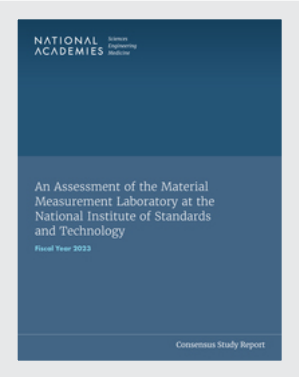

An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2023 (2023)

DETAILS

126 pages | 8.5 x 11 | PAPERBACK

ISBN 978-0-309-71068-8 | DOI 10.17226/27257

CONTRIBUTORS

Panel on the Assessment of the National Institute of Standards and Technology (NIST) Material Measurement Laboratory; Laboratory Assessments Board; Division on Engineering and Physical Sciences; National Academies of Sciences, Engineering, and Medicine

SUGGESTED CITATION

National Academies of Sciences, Engineering, and Medicine. 2023. *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2023*. Washington, DC: The National Academies Press. https://doi.org/10.17226/27257.

NATIONAL ACADEMIES Sciences Engineering Medicine

NATIONAL ACADEMIES PRESS
Washington, DC

An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology

Fiscal Year 2023

Panel on the Assessment of the National Institute of Standards and Technology (NIST) Material Measurement Laboratory

Laboratory Assessments Board

Division on Engineering and Physical Sciences

Consensus Study Report

NATIONAL ACADEMIES PRESS 500 Fifth Street, NW Washington, DC 20001

This activity was supported by Contract SB134117CQ0017, Task Order 1333ND23FNB100012 between the National Academy of Sciences and the National Institute of Standards and Technology. Any opinions, findings, conclusions, or recommendations expressed in this publication do not necessarily reflect the views of any organization or agency that provided support for the project.

International Standard Book Number-13: 978-0-309-71068-8
International Standard Book Number-10: 0-309-71068-4
Digital Object Identifier: https://doi.org/10.17226/27257

This publication is available from the National Academies Press, 500 Fifth Street, NW, Keck 360, Washington, DC 20001; (800) 624-6242 or (202) 334-3313; http://www.nap.edu.

Printed in the United States of America.

Suggested citation: National Academies of Sciences, Engineering, and Medicine. 2023. *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2023*. Washington, DC: The National Academies Press. https://doi.org/10.17226/27257.

The **National Academy of Sciences** was established in 1863 by an Act of Congress, signed by President Lincoln, as a private, nongovernmental institution to advise the nation on issues related to science and technology. Members are elected by their peers for outstanding contributions to research. Dr. Marcia McNutt is president.

The **National Academy of Engineering** was established in 1964 under the charter of the National Academy of Sciences to bring the practices of engineering to advising the nation. Members are elected by their peers for extraordinary contributions to engineering. Dr. John L. Anderson is president.

The **National Academy of Medicine** (formerly the Institute of Medicine) was established in 1970 under the charter of the National Academy of Sciences to advise the nation on medical and health issues. Members are elected by their peers for distinguished contributions to medicine and health. Dr. Victor J. Dzau is president.

The three Academies work together as the **National Academies of Sciences, Engineering, and Medicine** to provide independent, objective analysis and advice to the nation and conduct other activities to solve complex problems and inform public policy decisions. The National Academies also encourage education and research, recognize outstanding contributions to knowledge, and increase public understanding in matters of science, engineering, and medicine.

Learn more about the National Academies of Sciences, Engineering, and Medicine at **www.nationalacademies.org**.

Consensus Study Reports published by the National Academies of Sciences, Engineering, and Medicine document the evidence-based consensus on the study's statement of task by an authoring committee of experts. Reports typically include findings, conclusions, and recommendations based on information gathered by the committee and the committee's deliberations. Each report has been subjected to a rigorous and independent peer-review process and it represents the position of the National Academies on the statement of task.

Proceedings published by the National Academies of Sciences, Engineering, and Medicine chronicle the presentations and discussions at a workshop, symposium, or other event convened by the National Academies. The statements and opinions contained in proceedings are those of the participants and are not endorsed by other participants, the planning committee, or the National Academies.

Rapid Expert Consultations published by the National Academies of Sciences, Engineering, and Medicine are authored by subject-matter experts on narrowly focused topics that can be supported by a body of evidence. The discussions contained in rapid expert consultations are considered those of the authors and do not contain policy recommendations. Rapid expert consultations are reviewed by the institution before release.

For information about other products and activities of the National Academies, please visit www.nationalacademies.org/about/whatwedo.

PANEL ON THE ASSESSMENT OF THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY (NIST) MATERIAL MEASUREMENT LABORATORY

ELSA REICHMANIS (NAE), Lehigh University, *Chair*
ROBERT ARLEY BEVER, Bode Technology
AUGUST W. BOSSE, ExxonMobil Technology and Engineering Company
KENNETH M. CALDERONE, Confocal, Leica Microsystems
IULIANA CERNĂTESCU, Pratt and Whitney
STEVEN C. FREILICH, Andlinger Center for Energy and the Environment
GARY S. GROENEWOLD, Independent Consultant, Idaho National Laboratory (retired)
MINKI HONG, Kyulux North America, Inc.
MOHAMMAD A. KHALEEL, Oak Ridge National Laboratory
RICHARD A. LESAR, Iowa State University
FRANCES S. LIGLER (NAE), Texas A&M University
QUINGHUANG LIN, Linktech International, LLC
DAVID MELLOR, Center for Open Science
NICOLA POHL, Indiana University Bloomington
JAYAKANTH RAVICHANDRAN, University of Southern California
JAMES W. RINGER, Innovative Process Solutions, LLC
GEORGE RODRIGUEZ, ExxonMobil Technology and Engineering
JAMES E. SAAL, Citrine Informatics, Inc.
MARC SALIT, The MITRE Corporation
ISAAC C. SANCHEZ (NAE), The University of Texas at Austin
ALIX L. SCHMIDT, The Dow Chemical Company
JESSE C. SEEGMILLER, University of Minnesota
JOHNNA S. TEMENOFF, Georgia Institute of Technology and Emory University
CRISTINA U. THOMAS, 3M (retired)
OCKERT J. VAN DER SCHIJFF, Exponent, Inc.

Staff

KATIE BRATLIE, Director, Laboratory Assessments Board
JAMES MYSKA, Senior Program Officer, *Study Director*
AZEB GETACHEW, Administrative Assistant
JAYDA WADE, Research Associate (until August 4, 2023)

LABORATORY ASESSMENTS BOARD

[1] Resigned from the board on October 25, 2023.

Reviewers

This Consensus Study Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process.

We thank the following individuals for their review of this report:

ASAD ABIDI (NAE), University of California, Los Angeles
LYNDA CATHERINE BRINSON, Duke University
CHANTELLE FERLAND-BECKHAM, Cohen Veterans Bioscience
STEVEN MCKNIGHT, Department of Energy
NGA LEE NG, Georgia Institute of Technology
ANNE ELISABETH OSBOURN (NAS), John Innes Centre, United Kingdon
STYRON N. POWERS, Independent Safety Consultant
ANN SALAMONE (NAE), Rochal Industries, LLC
SHIJING SUN, University of Washington

Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations of this report nor did they see the final draft before its release. The review of this report was overseen by **DAVID W. JOHNSON,** University of Minnesota, Minneapolis, and **JENNIE S. HWANG (NAE),** H-Technologies Group, Inc. They were responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the authoring committee and the National Academies.

Contents

SUMMARY 1

1 INTRODUCTION 6

2 OVERVIEW OF THE MATERIAL MEASUREMENT LABORATORY 11

3 APPLIED CHEMICALS AND MATERIALS DIVISION 16

4 BIOSYSTEMS AND BIOMATERIALS DIVISION 23

5 BIOMOLECULAR MEASUREMENT DIVISION 30

6 CHEMICAL SCIENCES DIVISION 38

7 MATERIALS MEASUREMENT SCIENCE DIVISION 50

8 MATERIALS SCIENCE AND ENGINEERING DIVISION 58

9 OFFICE OF DATA AND INFORMATICS 65

10 OFFICE OF REFERENCE MATERIALS 72

11 MATERIAL MEASUREMENT LABORATORY'S RESPONSES TO THE FINDINGS AND RECOMMENDATIONS OF THE FISCAL YEAR 2020 ASSESSMENT REPORT 76

12 OVERARCHING THEMES, KEY RECOMMENDATIONS, AND CHAPTER-SPECIFIC RECOMMENDATIONS FROM THIS ASSESSMENT 95

APPENDIXES

A Acronyms and Abbreviations 105
B Panel Biographical Sketches 108

Summary

BACKGROUND AND TASK

Since 1959, the National Institute of Standards and Technology (NIST) has annually engaged the National Academies of Sciences, Engineering, and Medicine to assemble panels of experts—from academia, industry, medicine, and other scientific and engineering communities of practice—to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are six,[1] as well as the adequacy of the laboratories' resources. These reviews are conducted under contract at the request of NIST. In fiscal year 2023, NIST asked the National Academies to assess the Material Measurement Laboratory (MML). The assessment process included a site visit by the panel, including laboratory tours, individual engagement with MML researchers, and follow-on questions after the site visit. The panel then used its collective experience and expertise to assess MML according to the statement of task and make recommendations. MML is assessed in its entirety every 3 years.

The statement of task has four main components. First, the panel is asked to assess MML's technical programs, how the quality of research at MML compares to similar programs of research internationally, and whether the quality of the programs at MML are adequate for MML to achieve its objectives. Second, the panel is also asked to assess the portfolio of scientific and technical expertise at MML, whether it is world-class, and how well it supports MML's technical programs and MML's ability to meet its objectives. Third, the panel is asked to assess the adequacy of MML's budget, facilities, equipment, and human resources, and how well these support MML's technical work and achieving MML's goals. Finally, the panel is asked to assess the effectiveness of MML's efforts to disseminate products of its work including how well MML's work is driven by stakeholder needs, how effective and comprehensive the dissemination and technology transfer mechanisms are, and how well MML is monitoring the stakeholder use, and the impact of, MML's output.

MATERIAL MEASUREMENT LABORATORY

MML comprises six technical divisions and two offices. The two offices manage programs related to NIST standard reference materials and NIST data products. The technical divisions engage in research and development of the measurement science, standards, technology, and data required to support the nation's need to design, develop, manufacture, and use materials. These divisions interact extensively with both industry and public institutions to advance the economy and provide tools for the creation of knowledge.

The divisions and offices in MML are the Applied Chemicals and Materials Division, Biosystems and Biomaterials Division, Biomolecular Measurement Division, Chemical Sciences Division, Materials Measurement Science Division, Materials Science and Engineering Division, Office of Data and Informatics, and Office of Reference Materials. The Applied Chemicals and Materials Division is located

[1] The six NIST laboratories are the Communications Technology Laboratory, the Engineering Laboratory, the Information Technology Laboratory, the Material Measurement Laboratory, the NIST Center for Neutron Research, and the Physical Measurement Laboratory.

on the NIST campus in Boulder, Colorado. The remainder of the divisions and offices are located on NIST's campus in Gaithersburg, Maryland.

CONCLUSIONS AND RECOMMENDATIONS

Assessment and General Conclusions

Across the MML divisions and offices, research staff continue to demonstrate impressive productivity in scientific publications, standards interactions, intellectual property activity, and customer engagement.

The technical quality of the research at MML is excellent. The work being done at MML not only compares favorably with work being done at other national metrology institutes around the world, in some cases it is world leading. For example, there is cutting-edge work being done in standards for additive manufacturing, a new albumin standard reference material that will allow for far more accurate testing for kidney disease, and a new hair peptide analysis technique that is free from concerns about DNA contamination and might be sensitive enough to tell the difference between identical twins. The quality of the technical work is generally adequate for MML to meet its technical objectives. There is room for improvement, however, and this is addressed in each of the chapters where the panel saw the need.

The portfolio of scientific and technical expertise at MML is impressive and is highly recognized in the scientific community worldwide. The expertise resident at MML is world-class in the areas of MML's mission and objectives. MML staff are active in many standards bodies, often in leadership roles. They produce an impressive output of technical papers and work products. MML staff have won many awards, such as being named fellows of ASM International, ASTM International, and the American Physical Society. They have received the ASTM International Award the Chemical Society of Washington's Charles Gordon Award, of Merit, and many Department of Commerce and NIST named awards. As with the technical programs, there are places where there is room for improvement; these are addressed in the chapters where they occur.

In contrast with the quality of the technical work and expertise at MML, there are challenges in the areas of budget, facilities, equipment, and human resources. While these are addressed in more detail in the report, generally MML is experiencing budget stress including flat budgets that either barely hold or lose ground to inflation, some of its equipment that is dated and in need of refreshing, and serious challenges regarding MML's human resources support. The biggest challenge faced by MML's staff, and across NIST, is the condition of many of MML's facilities. There are serious deficiencies in places that actively impede MML's work. These are not issues that MML can address on its own; they require action by NIST headquarters and work is underway at the headquarters level to address MML's—and all of NIST's—facilities problems. All of these issues are discussed in the body of the report. Regarding facilities, this report notes MML-specific challenges and ties to the National Academies' 2023 report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023; hereafter the "*Capital Facility Needs* report").

Regarding the dissemination of program outputs, MML engages in extensive collaborative work, across MML, NIST, and an impressive number of external stakeholders. In essence, MML continues its essential role of supporting U.S. industry metrology, technology, and standards needs. The strong support of its industrial stakeholders is shown in part by the significant number of cooperative research and development agreements in this review along with an increase in nondisclosure agreements. MML researchers are highly published and influential, they are very active in international standards bodies, holding several leadership positions in those bodies, and they hold many patents. Generally, MML's work is responsive to stakeholder needs and its dissemination and technology transfer mechanisms are effective. While there is significant evidence of the impact of MML's work, the panels make some

recommendations about better tracking this impact and thus more effectively demonstrating MML's value.

The recommendations in report's chapters are grouped by division or office to provide actionable suggestions that address each division's unique needs. This Summary highlights overarching, cross-cutting themes that emerged over the course of the 2023 assessment.

KEY RECOMMENDATIONS

Adequacy of Facilities

As highlighted in the National Academies' 2020 MML assessment, *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020* (NASEM 2021), and more recently in *Capital Facility Needs* report (NASEM 2023), aging facilities and infrastructure present significant handicaps. Notably, the 2023 report found that NIST research staff spent from 10 to 40 percent of their time working around facility shortcomings, with the typical reported values being 20 percent (NASEM 2023). As direct consequence of these limitations, at NIST generally and specific to this report, MML researchers are left to mitigate these limitations through repeating their work or implementing workarounds with limited research budgets.

The MML laboratories in Boulder, Colorado, and Gaithersburg, Maryland, are negatively affected by poor temperature and humidity control in addition to inadequate air flow in their laboratories, which are not compatible with state-of-the-art measurements and instrumentation. On the Gaithersburg campus in 2022, aging infrastructure led to serious flooding of MML research laboratories, resulting in a loss of millions of dollars of equipment and time. The facilities are generally inadequate for the performance of modern materials chemistry related processes. Much of the infrastructure, both buildings and equipment, has exceeded its expected life, leading to time spent inefficiently compared to the capabilities of state-of-the-art facilities and equipment in academic and industry laboratories and at metrology institutes around the world. Researchers have had to repeat experiments multiple times. They have had their ability to work interrupted by utility failures. Postdocs have ended their postdoc without having been able to do the work needed to author a publication. The impacts are building, and MML broadly is becoming a less and less appealing place to work. MML is already at a compensation disadvantage compared to industry, now it cannot always offer world-class facilities, either. While MML research efforts are world-leading, *aging facilities and infrastructure are such that MML is at the cusp of losing its world-leading position and its ability to continue to attract new generations of world-leading researchers*. It needs to be noted that MML—or any of NIST's laboratories—have a very limited ability to address facilities inadequacies. Major facilities work—the construction, renovation, and modernization that is needed to resolve the worst of the problems—is managed and funded by NIST's Office of Facilities and Property Management (OFPM). As detailed in the report Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology, OFPM has a coordinated recovery plan to fix NIST's facilities. The most important thing for MML to do is to ensure that OFPM is fully aware of its facilities issues and that MML's priorities are reflected in the coordinated recovery plan.

> **Key Recommendation 1: The Material Measurement Laboratory (MML) and the National Institute of Standards and Technology Office of Facilities and Property Management should work together to identify and document critical laboratory infrastructure issues. They should collaborate to prioritize items that need to be addressed and create a plan with an associated timeline to address those needs. MML should actively encourage its researchers to document facilities issues and all associated time lost repeating experiments, and the portion of the research budget spent on working around facility issues.**

The identified infrastructure issues also represent *safety* issues: floods can easily lead to sparks that can in turn initiate fires; inadequate exhaust will lead to contaminated laboratory air that can negatively impact research product quality and in the long term can impact the health of research staff. As a whole, aged infrastructure and equipment can have an impact on the overall attitude of the staff toward safety. Safety requires intimate and active management involvement, creating and driving an overall safety culture. Participation in the Occupational Safety and Health Administration's Voluntary Protection Programs might be a useful way to approach safety at MML.[2]

Key Recommendation 2: Safety is as much a line management responsibility as an individual one. Leaders should recognize that every task can be done safely, and every task has inherent risks. That attitude needs to be transmitted down the line in order for each individual to take responsibility for not only maintaining but also improving the safety of their environment and the environments of those around them. The Material Measurement Laboratory (MML) should maintain statistics of leading indicators of safety risks and facilities dangers that represent the base of the safety pyramid. These statistics should be socialized within the organization in such a way that a safe and safety-conscious environment is created that results in a safety culture that supports continuous improvement. MML should consider engaging with experienced industrial partners who can bring a fresh perspective on the safety risks as a way of providing an unbiased and fresh pair of eyes to the situation.

Adequacy of Scientific and Technical Expertise

MML conducts research at a very high level. It has formal arrangements with renowned institutions such as Brookhaven National Laboratory and the Institute for Bioscience and Biotechnology Research, a joint institute with the University of Maryland, College Park, and the University of Maryland, Baltimore. MML has primary responsibility within NIST for producing and curating standard reference materials and standard reference data. In addition to maintaining critical standard reference materials and standard reference data, MML has developed newer standards products based on biology. The balance of maintaining legacy standard reference materials versus redirecting limited resources toward producing standard reference materials and standard reference data in new and emerging areas presents both a challenge and an opportunity. MML notes that areas of new opportunities include the bioeconomy and engineering biology, data science and engineering, artificial intelligence, and the circular economy.

The robustness of MML's program against retirements or unforeseen departures could be improved. In some places there needs to be more systematic succession planning to prevent gaps from occurring. Cross-training to provide backup coverage in case the primary cognizant scientist leaves is a further way to protect against disruption. In other instances, retraining staff to take on emerging issues requiring different disciplinary knowledge was lacking.

Pandemic restrictions limited onboarding and other processes that contribute to a cohesive work culture, which has been recognized by the MML leadership team. The lack of cohesion negatively impacts an organization or culture where career mentoring and professional development for the population of term-limited scientific appointees becomes uneven.

Key Recommendation 3: The Material Measurement Laboratory (MML) should work with National Institute of Standards and Technology human resources to develop effective processes and procedures for hiring and career development of staff. Processes to ensure timely support to MML in hiring and onboarding of postdocs, term, and permanent employees should be developed and implemented.

[2] More information about the Voluntary Protection Programs and how to participate can be found at Occupational Safety and Health Administration, "Voluntary Protection Programs," https://www.osha.gov/vpp.

Key Recommendation 4: The Material Measurement Laboratory (MML) should require mentorship training for all research staff within the laboratory to ensure quality vertical mentorship and sponsorship in order to increase the impact of the postdoc and early career population both within MML and later in industry, academia, or government positions. MML should increase the number of employees who have formal leadership training to standardize mentoring and onboarding of new personnel. The training should include a formalization of clear mentor and mentee expectations in terms of work, in-person meetings, and supervision. MML should consider a standard message about the processes of transitioning from a postdoc or term appointee to a permanent staff member, and the probability thereof so as to minimize the uncertainty around this process.

Data Management and Data Infrastructure

Data science represents an increasingly important part of MML's work to meet its mission. Within MML, the Office of Data and Informatics is a dedicated, service-oriented data resource with domain expertise in biological, chemical, and materials sciences, specializing in large and information-rich data sets.

Across MML, data collection, storage, analysis, and movement appear to be handled by multiple, fragmented platforms, and computational data does not appear to be managed in a centralized platform. In addition, not all of the experimental measurement systems have a consolidated and automated data infrastructure, which results in a fragmented data infrastructure that, unfortunately, leads to discrete, inefficient, and stovepiped experimental data infrastructure across MML. These observations lead to opportunities to unify all computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management.

Key Recommendation 5: To the extent possible, the Material Measurement Laboratory should launch an initiative to unify all computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management. This data science initiative could be applied to machine learning deployment and expand capabilities in laboratory automation, high-performance computing, and artificial intelligence. Computing infrastructure should, to the extent possible, be updated to meet current laboratory standards.

REFERENCES

NASEM (National Academies of Sciences, Engineering, and Medicine). 2021. *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020*. Washington, DC: The National Academies Press. https://doi.org/10.17226/26048.

NASEM. 2023. *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology*. Washington, DC: The National Academies Press. https://doi.org/10.17226/26684.

1
Introduction

The National Academies of Sciences, Engineering, and Medicine have, starting in 1959, annually assembled panels of experts—from academia, industry, medicine, and other scientific and engineering communities of practice—to assess the quality and effectiveness of the National Institute of Standards and Technology (NIST) measurements and standards laboratories, of which there are six,[1] as well as the adequacy of the laboratories' resources. These reviews are conducted under contract at the request of NIST.

STATEMENT OF TASK

The National Academies shall appoint a panel to assess independently the scientific and technical work performed by the NIST Material Measurement Laboratory. The panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the Material Measurement Laboratory. Visits will include technical presentations by NIST staff, demonstrations of NIST projects, tours of NIST facilities, and discussions with NIST staff. The panel will deliberate findings in closed sessions and will prepare a report summarizing its assessment findings and recommendations.

NIST has requested that the laboratories be assessed against the following broad criteria:

1. Assess the organization's technical programs.
    a. How does the quality of the research compare to similar world-class research in the technical program areas?
    b. Is the quality of the technical programs adequate for the organization to reach its stated technical objectives? How could it be improved?
2. Assess the portfolio of scientific expertise within the organization.
    a. Does the organization have world-class scientific expertise in the areas of the organization's mission and program objectives? If not, in what areas should it be improved?
    b. How well does the organization's scientific expertise support the organization's technical programs and the organization's ability to achieve its stated objectives?
3. Assess the adequacy of the organization's budget, facilities, equipment, and human resources.
    a. How well do the facilities, equipment, and human resources support the organization's technical programs and its ability to achieve its stated objectives? How could they be improved?
4. Assess the effectiveness by which the organization disseminates its program outputs.
    a. How well are the organization's research programs driven by stakeholder needs?

[1] The six NIST laboratories are the Communications Technology Laboratory, the Engineering Laboratory, the Information Technology Laboratory, the Material Measurement Laboratory, the NIST Center for Neutron Research, and the Physical Measurement Laboratory.

b. How effective are the dissemination methods and technology transfer mechanisms used by the organization? Are these mechanisms sufficiently comprehensive?
c. How well is this organization monitoring stakeholder use and impact of program outputs? How could this be improved?

CONDUCT OF THE ASSESSMENT

In 2023, at the request of the director of NIST, the National Academies formed the Panel on Assessment of the National Institute of Standards and Technology (NIST) Material Measurement Laboratory (the "panel"), having earlier established the statement of task described above.

The panel's review covered the six divisions and two offices that comprise MML. The panel conducted its review in person on May 16–18, 2023, with a split meeting between Boulder, Colorado, and Gaithersburg, Maryland. The panel was divided into 8 sub-panels. After an opening plenary session with general presentations and discussions, the panel broke out into its sub-panels to work independently, receiving briefings, engaging in discussions, and going on tours. By design, each sub-panel was focused on the division or office that it assessed. There was a final working plenary where the panel deliberated as a whole and then a session for it to confirm its understandings with MML leadership. NIST staff further provided written responses to the panel's queries.

To accomplish its mission, the panel reviewed the material provided by MML prior to and during the review meeting. The choice of projects to be reviewed was made by MML. The panel applied a largely qualitative approach to the assessment, using the members' professional experience, expertise, and judgment to conduct the assessment. Given the non-exhaustive nature of the review, the omission in this report of any particular MML project should not be interpreted as a negative reflection on the omitted project. Similarly, the natural variations between the chapters in terms of length, level of detail, and approach convey no message about the quality of work being performed by MML or the information provided to the panel. Each chapter was an independent sub-panel focused on a specific division or office and conveyed the information they believed to be important based on their interactions with the staff of the particular division or office that they assess. It must be noted that this panel's charge is not to opine on what work MML should be doing. That is guidance provided by another independent NIST advisory committee, the Visiting Committee on Advanced Technology. This panel's charge is confined to assessing how well MML is doing its work.

Special Considerations

There are two items that need to be addressed to fully understand this report.

Comparison to International Research Efforts

One of the questions in the statement of task (item 1.a) is "How does the quality of the research compare to similar world-class research in the technical program areas?" The panel was impressed with the quality of research conducted at MML and found it to be generally world-class or world-leading. As with all other assessment topics, this is based on the panelists' individual and cumulative expertise and experience. However, within the time constraints of this project, there was not time to engage in extensive additional research. Therefore, the report might have fewer concrete examples in regard to this item of the statement of task than the others. Any lack of examples should not be taken as a lack of quality.

Safety

Also, the panel makes observations and a recommendation on safety. It was very careful in doing so. Safety is not part of the formal charge to the panel, but MML leadership indicated that they would like to receive any feedback the panel had on this issue. Two panelists—Elsa Reichmanis and Steven Freilich—have laboratory and leadership safety experience, but the panel was not composed to conduct a rigorous safety review (as it was not tasked to do so). Accordingly, the report notes some things that the panel observed that are of concern to it and makes a high-level safety key recommendation to draw attention to the panel's concerns and suggest a path forward withing the limits of the scope, information available to the committee, and the panel's collective expertise. Due to these limitations, the panel took a relatively light touch on this matter.

SUMMARY OF THE 2023 TECHNICAL ASSESSMENT OF THE CAPITAL FACILITY NEEDS OF THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY REPORT

In February 2023, the National Academies released the report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023; hereafter the "*Capital Facility Needs* report"). The authoring committee was tasked to assess NIST's facilities and utility infrastructure, review and assess plans and projects to reinvigorate NIST's facilities and utility infrastructure, the cost estimates for doing so, and the factors that NIST should consider in developing a comprehensive capital strategy for the facilities and utility infrastructure at NIST's campuses in Boulder, Colorado, and Gaithersburg, Maryland. The committee that authored the 2023 Capital Facilities report engaged with the Department of the Interior, the National Institutes of Health, the U.S. Army Engineer Research and Development Center, and the Johns Hopkins University Applied Physics Laboratory to learn about their methods and metrics for assessing facility conditions and maintaining their facilities.

The condition of NIST's facilities and utility infrastructure has been a concern since 2002 when the Visiting Committee on Advanced Technology issued a report calling NIST's facilities condition and the related funding situation "alarming" and "critical." Over the following 20 years, the Visiting Committee on Advanced Technology returned consistently to this theme with increasingly dire language. Eventually, the conference report accompanying the Consolidated Appropriations Act of 2021 (P.L. 116-260) requested that NIST "contract with an independent entity to develop a report that assesses the comprehensive capital needs of NIST's campuses." In response, NIST's Office of Facilities and Property Management approached the National Academies to conduct a study based on a successful study and report completed for the National Institutes of Health in 2019 (NASEM 2019). The result was the 2023 *Capital Facility Needs* report (NASEM 2023).

The committee that authored the *Capital Facility Needs* report visited both the Boulder, Colorado, and Gaithersburg, Maryland, campuses. They discovered that many NIST facilities are inadequate to support the world-leading research that is NIST's mission. Both the quality and the reliability of power can be problematic, resulting in slowed work, lost work, and unnecessary time spent recalibrating sensitive instruments. Inadequacies in basic environmental controls can result in laboratories that are too hot or cold, too humid or not humid enough, and lack proper vibration insulation. In one 1950s-era Boulder laboratory the gaps between the windows and frames allow dust to blow straight into the laboratory. Roof leaks have destroyed multimillion-dollar pieces of equipment, such as tunneling electron microscopes in both Boulder and Gaithersburg. A water leak in Gaithersburg resulted in permanent damage to the world-leading Kibble balance that tied the standard kilogram to the speed of light. There are many more instances and stories. In all, the committee that authored the 2023 *Capital Facility Needs* report found that the NIST research staff loses between 10–40 percent of its working time fighting against facility inadequacies, also consuming research money to do so.

That committee concluded that the situation has reached the point where:

- NIST researchers will not be able to continue their world-class research no matter their efforts;
- This is already impacting the ability to recruit and retain staff and the willingness of foreign researchers to do work at NIST;
- At risk is also NIST's international credibility and influence and its ability to support national security, U.S. international competitiveness, medical therapeutics, and a wide range of other activities upon which users in the U.S. government, industry, and academia rely.

In the course of its work, the authoring committee found that NIST's internal facility and property management policies are not responsible for this situation. Rather, the cause is more than two decades of erratic, unpredictable, and inadequate funding for NIST's Construction of Research Facilities budget, which includes facility sustainment, restoration, modernization, and expansion. Exacerbating this problem is congressionally directed pass-through funding for things like building laboratories on university campuses that are not used by NIST. This pass-through funding is not revenue-neutral to NIST, costing staff time and money to administer, draining even more much-needed money from NIST's facilities coffers.

In short, the committee that authored the 2023 *Capital Facility Needs* report found that the situation requires serious and sustained attention, particularly from leadership levels above NIST. The authoring committee also endorsed the coordinated recovery plan drafted by NIST's Office of Facilities and Property Management and recommended its continued refinement and shortening it to complete it in 12 years. Critically, the authoring committee identified the need for significant and sustained funding to address NIST's facilities and utility shortcomings and bring them to the standard necessary for modern metrology. This funding is the critical piece of the recovery plan. The committee that authored the 2023 *Capital Facility Needs* report recommends $420 million to $550 million per year in funding for NIST's Construction of Research Facilities budget over at least 12 years. As shown in Table 1-1, this includes $120 million to $150 million per year for sustainment, capacity, maintenance, and major repairs funding to address the more than $800 million deferred maintenance backlog and bring existing facilities to an acceptable condition and keep them there. It also includes $300 million to $400 million per year over at least 12 years for the construction and major renovations budget to upgrade, renovate, and build the new laboratories with the new capabilities needed to conduct modern metrology research.

The picture is not unremittingly bleak. NIST has already begun to modernize laboratories as its current budget allows. These new laboratories are state of the art and enable the cutting-edge, world-leading research that is NIST's mission. As an example, one NIST research group—after waiting 18 months to be relocated into a new, modern laboratory—won the 2021 Physics World Breakthrough of the Year award for a previously unprecedented demonstration of the quantum entanglement of micro-resonators. NIST's staff is world-class and capable of producing amazing results, results that will serve the nation and inspire the next generations of researchers, provided they are given the facilities and tools needed to do their work.

TABLE 1-1 Overview of NIST Facility and Infrastructure Funding Needs

Funding Component	Amount Needed Annually
Construction and Major Renovations (CMR)	$300 million to $400 million
Safety, Capacity, Maintenance, and Major Repairs (SCMMR)	$120 million to $150 million
Total needed for Construction of Research Facilities (CRF)	$420 million to $550 million

NOTE: CRF funding is the sum of CMR and SCMMR funding.
SOURCE: NIST (2022).

STRUCTURE OF THIS REPORT

This report opens with this introductory chapter, followed by an overview of MML. Each division and office of MML is then assessed in its own chapter. The structure within each of these chapters is aligned with the statement of task presented above to aid the reader in understanding the panel's assessment. Within the common structure of each chapter, each sub-panel had the flexibility to implement a substructure that it believed made the most sense for the information that it wanted to convey. This results in different substructures among the chapters. After the assessment chapters is a chapter that presents the recommendations from the fiscal year (FY) 2020 MML assessment report (NASEM 2021) and MML's responses to those recommendations. The final chapter presents the recommendations from this report in one place for ease of reference. Any issue that the panel believed applies to MML as a whole is addressed with a key recommendation. These are presented in the Summary, in the chapters in which they appear, and in the final recommendation summary chapter. The structure of the report chapters lays out thus:

- Chapter 1: Introduction
- Chapter 2: Overview of the Material Measurement Laboratory
- Chapter 3: Applied Chemicals and Materials Division
- Chapter 4: Biosystems and Biomaterials Division
- Chapter 5: Biomolecular Measurement Division
- Chapter 6: Chemical Sciences Division
- Chapter 7: Materials Measurement Science Division
- Chapter 8: Materials Science and Engineering Division
- Chapter 9: Office of Data and Informatics
- Chapter 10: Office of Reference Materials
- Chapter 11: Material Measurement Laboratory's Responses to the Findings and Recommendations of the Fiscal Year 2020 Assessment Report
- Chapter 12: Overarching Themes, Key Recommendations, and Chapter-Specific Recommendations from This Assessment

REFERENCES

NASEM (National Academies of Sciences, Engineering, and Medicine). 2019. *Managing the NIH Bethesda Campus Capital Assets for Success in a Highly Competitive Global Biomedical Research Environment*. Washington, DC: The National Academies Press. https://doi.org/10.17226/25483.

NASEM. 2021. *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020*. Washington, DC: The National Academies Press. https://doi.org/10.17226/26048.

NASEM. 2023. *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology*. Washington, DC: The National Academies Press. https://doi.org/10.17226/26684.

NIST (National Institute of Standards and Technology). 2022. "NIST Facilities Summary for Representative Trone," Point Paper. Office of Facilities and Property Management. June.

2
Overview of the Material Measurement Laboratory

The Material Measurement Laboratory (MML) is one of the National Institute of Standards and Technology's (NIST's) six major laboratories and one of NIST's fundamental metrology laboratories. The preponderance of MML activity occurs at the Gaithersburg, Maryland, campus, where more than 80 percent of the staff and associates are located. One MML division, Applied Chemicals and Materials, is located on the NIST Boulder, Colorado, campus. Smaller deployments are scattered across a further four sites, including the Institute for Bioscience and Biotechnology Research in Rockville, Maryland; the Hollings Marine Laboratory in Charleston, South Carolina; NIST Beamlines at the Brookhaven National Laboratory; and the NIST Pacific Islands Program in Oahu, Hawaii.

MML describes itself as serving as "the Nation's primary resource for advancing measurements essential to the chemical, biological, and materials sciences and related engineering disciplines" to "bring focus to the development of exceptional measurement science expertise and capabilities, reference products and standards, and data science and data dissemination capabilities." The work of MML is overall subsumed under three scientific and technical goals: (1) measurement science excellence, (2) measurement service excellence, and (3) data science and data management capabilities. There are a further two goals: (4) strategic partnering and customer engagement and (5) organizational excellence.

MML is organized into six divisions and two offices. Five of the divisions—Materials Science and Engineering, Materials Measurement Science, Biosystems and Biomaterials, Biomolecular Measurement, and Chemical Sciences—and the two offices—Office of Data and Informatics and Office of Reference Materials and are primarily located on the NIST campus in Gaithersburg, Maryland. The sixth division, Applied Chemicals and Materials, is located at the NIST campus in Boulder, Colorado. The divisions are focused on research and the offices are focused on measurement services. MML identified challenges include aging and outdated building infrastructure and "large" equipment needs and uses.

The Applied Chemicals and Materials Division focuses on creating and maintaining tools to measure the properties and structures of fluids and materials of importance to industry, with the goal of providing measurement tools and models, as well as critically evaluated data, to a diverse set of stakeholders. Their work is designed to support the creation of better products, and, importantly, new and improved standards.

The Biosystems and Biomaterials Division aims to advance measurement science, standards, and technology to promote U.S. biosciences and biotechnology, enhance economic security, and improve competitiveness of the U.S. bioeconomy, inclusive of increasing the resilience and flexibility of the bio-supply chain. The division is also tasked with developing cybersecurity technologies for the unique needs of genomic and biomedical-based systems.

The Biomolecular Measurement Division provides measurement science, technologies, and standards for the evaluation of biomolecules, including proteins, oligonucleotides, carbohydrates, lipids, metabolites, and complexes including such molecules. Key stakeholders include the pharmaceutical community, makers of analytical instruments, and clinical and forensics laboratories.

The Chemical Sciences Division manufactures and curates standard reference materials; develops chemical measurement science and technology, including development and fabrication of standard reference instruments; generates and curates standard reference data, including chemical informatics that

are tied to stakeholder needs; and organizes and performs quality assurance tasks. The division is motivated by the need for regulatory rigor that is stipulated by legislation, and by industry, which needs accurate measurement science in order to be competitive.

The Materials Measurement Science Division conducts mission-based fundamental research and engages in standards production and applied science and engineering. This work enables innovation in U.S. industry and addresses measurement science needs of a range of other agency stakeholders. The division's technical work is focused in 6 areas: safety and security, forensics and public health, micro- and nano-plastics, semiconductors, climate mitigation, and ceramic additive manufacturing. These focus areas are centered around core capabilities in multiscale materials characterization, atomic and nanoscale metrology, as well as leveraging growing computational science, artificial intelligence, and data science expertise.

The Materials Science and Engineering Division is engaged in the research and development of materials measurement science, standards, technology, and data. It supports the NIST MML mission in advanced manufacturing, including the Materials Genome Initiative 2.0, additive manufacturing, and biomanufacturing. This division also has programs in advanced electronics, circular economy, climate, and the environment.

The Office of Data and Informatics provides leadership and expertise to meet the data needs of MML and NIST research data infrastructure. It also provides services to MML and to NIST through its expertise, guidance about data science, and the resources it offers in order to enhance the discoverability, usability, and interoperability of data.

The Office of Reference Materials serves a significant and prominent role in translation of NIST measurement science to stakeholders. The office's administrative activities include managing business operations, administrative oversight, product sales, and technical support for the NIST standard reference material program. Through its responsibility for managing working capital and standards development funding, the office has a strong influence in selecting and resourcing the technical work that is developed and disseminated.

OVERARCHING THEMES AND KEY RECOMMENDATIONS

Facilities and Safety

As highlighted in prior review reports and more recently in the 2023 National Academies' report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023; hereafter the "*Capital Facility Needs* report"), aging facilities and infrastructure present significant handicaps. Notably, the report found that NIST research staff spent from 10 to 40 percent of their time working around facility shortcomings, with the typical reported values being 20 percent (NASEM 2023). Furthermore, NIST researchers are left to mitigate these limitations through repeating their work or implementing workarounds with limited research budgets.

Similar issues became apparent across MML research laboratories at both the Gaithersburg and Boulder campuses during this assessment. For instance, current research in Buildings 2 and 24 at Boulder is negatively affected by the poor control of temperature and air flow in their laboratories. On the Gaithersburg campus, in 2022, aging infrastructure led to serious flooding of MML research laboratories, with resultant loss of equipment and lost time. In addition, neither the Gaithersburg nor the Boulder facilities have the humidity and temperature control needed for many state-of-the-art measurements, which seriously limits output; and laboratory exhaust systems are inadequate for the performance of modern materials chemistry related processes. Aging computer systems limit data-sharing and data analysis that are critical for MML to achieve its technical goals. Much of the infrastructure, both buildings and equipment, has exceeded its expected life, leading to time being spent inefficiently compared to the capabilities of state-of-the-art facilities and equipment. While MML research efforts are world-leading,

aging facilities and infrastructure are such that MML is at the cusp of losing its world-leading position and its ability to continue to attract new generations of world-leading researchers.

> **Key Recommendation 1: The Material Measurement Laboratory (MML) and the National Institute of Standards and Technology Office of Facilities and Property Management should work together to identify and document critical laboratory infrastructure issues. They should collaborate to prioritize items that need to be addressed and create a plan with an associated timeline to address those needs. MML should actively encourage its researchers to document facilities issues and all associated time lost repeating experiments, and the portion of the research budget spent on working around facility issues.**

The facilities issues observed in the course of this assessment are not only infrastructure issues. Critically, they also represent *safety* issues. With an abundance of electronic equipment, floods can easily lead to sparks that can in turn initiate fires; inadequate exhaust will lead to contaminated laboratory air that can negatively impact research product quality and in the long term can impact the health of research staff. As a whole, aged infrastructure and equipment can have an impact on the overall attitude of the staff toward safety. In addition, MML laboratory tours suggested a risk of safety incidents as a result of a perception that the risks, in many cases, are minimal. Safety and excellence go together. The Safety Pyramid provides a basis for a safe working environment (Prpich and Unnerstall 2022).

Safety involves an entire organization, including and particularly line management. Managers set the tone and monitor the progress against metrics. They participate in safety inspections. They lead investigations of incidents and near misses. In so doing they create the environment that ultimately grows into a safety culture. Safety is not a grassroots effort, and management needs to do more than establish the objectives; managers at all levels needs to recognize their responsibility and accountability for what happens at the same organizational intensity level as revenue and productivity targets. Participation in the Occupational Safety and Health Administration's Voluntary Protection Programs might be a useful way to approach safety at MML.[1]

> **Key Recommendation 2: Safety is as much a line management responsibility as an individual one. Leaders should recognize that every task can be done safely, and every task has inherent risks. That attitude needs to be transmitted down the line in order for each individual to take responsibility for not only maintaining but also improving the safety of their environment and the environments of those around them. The Material Measurement Laboratory (MML) should maintain statistics of leading indicators of safety risks and facilities dangers that represent the base of the safety pyramid. These statistics should be socialized within the organization in such a way that a safe and safety-conscious environment is created that results in a safety culture that supports continuous improvement. MML should consider engaging with experienced industrial partners who can bring a fresh perspective on the safety risks as a way of providing an unbiased and fresh pair of eyes to the situation.**

Portfolio of Scientific Expertise

As enumerated in Chapters 3 through 10, the MML research staff continue to demonstrate impressive productivity in scientific publications, standards interactions, intellectual property activity, and customer engagement. Over the past 3 years MML personnel have participated in more than 180 standards committees with leadership positions in more than 45 of those committees. The strong

[1] More information about the Voluntary Protection Programs and how to participate can be found at Occupational Safety and Health Administration, "Voluntary Protection Programs," https://www.osha.gov/vpp.

participation of MML personnel on these committees is of critical importance to the NIST mission, making it possible for MML to continue its essential role of supporting U.S. industry technology and standards needs. The strong support of its industrial stakeholders is shown in part by a significant number of cooperative research and development agreements in this review period (259 since the 2020 assessment) along with an increase in nondisclosure agreements. MML research staff are engaged and highly recognized in the scientific community. The record of peer-reviewed publications is impressive. Since 2020, MML has produced 1,292 archival journal papers, 74 conference proceedings, 184 inter-agency reports, 33 workshop reports, and 29 books or book chapters.

MML appears to have a limited number of mid-career staff, with large numbers of established late-career staff. There does not appear to be a clear succession path to bring in newer staff and fold them into the work of MML. While MML has no control over, and limited information about, when staff might leave, the lack of a succession plan is troublesome. More systematic succession planning may prevent gaps from occurring in mission critical areas. Cross-training to provide backup coverage in case the primary cognizant scientist leaves is a further way to protect against disruption. Alternatively, retraining staff to take on emerging issues requiring different disciplinary knowledge could be considered.

Also, regarding staffing, support from the centralized human resources office operation could be significantly improved. Hiring new administrative and research staff appears inordinately slow, taking up to 6 months just to release standard advertisements. Even when the jobs are posted and interviews conducted, there are reported instances where a new hire was agreed upon, but the notification letter never went out from human resources to the prospective employee. The procedure for hiring federal scientists and engineers was not clear to either the postdoctoral and temporary staff or the panel. The availability of positions related to MML programs and mission-focused areas appears de-prioritized compared to time-limited, emergent activities like staffing to support the work that NIST will be getting under the CHIPS and Science Act of 2022. More timely support from human resources would ease the frustrations of existing staff whose progress is hampered by vacancies in administrative support, hiring of postdoctoral fellows, or staffing of existing mission areas.

Over the course of the discussions with postdocs and limited term employees, it became clear that pandemic restrictions limited onboarding and other processes that contribute to a cohesive work culture. The MML leadership team is actively working to rebuild these processes, although this work is especially challenging given the spread of people across buildings and the limited availability of shared public spaces. Career mentoring and professional development for the population of term-limited scientific appointees appears uneven. The panel also noted an uneven level of formal leadership training among the MML staff.

Key Recommendation 3: The Material Measurement Laboratory (MML) should work with National Institute of Standards and Technology human resources to develop effective processes and procedures for hiring and career development of staff. Processes to ensure timely support to MML in hiring and onboarding of postdocs, term, and permanent employees should be developed and implemented.

Key Recommendation 4: The Material Measurement Laboratory (MML) should require mentorship training for all research staff within the laboratory to ensure quality vertical mentorship and sponsorship in order to increase the impact of the postdoc and early career population both within MML and later in industry, academia, or government positions. MML should increase the number of employees who have formal leadership training to standardize mentoring and onboarding of new personnel. The training should include a formalization of clear mentor and mentee expectations in terms of work, in-person meetings, and supervision. MML should consider a standard message about the processes of transitioning from a postdoc or term appointee to a permanent staff member, and the probability thereof so as to minimize the uncertainty around this process.

Data Management and Data Infrastructure

Integral to its mission, MML collects, stores, analyzes, and transmits data in all of its research, measurement, standards-making, and dissemination activities. Accordingly, data science represents an increasingly important part of the laboratory's work to meet its mission. Within MML, the Office of Data and Informatics is a dedicated, service-oriented data resource for physical sciences with domain expertise in biological, chemical, and materials sciences, specializing in large and information-rich data sets.

MML projects often result in the development of many different computational and theoretical methods, which while impressive are performed as part of individual projects. Across MML, data collection, storage, analysis, and movement appear to be handled by multiple, fragmented platforms, and computational data does not appear to be managed in a centralized platform. In addition, not all of the experimental measurement systems have a consolidated and automated data infrastructure, which results in a fragmented data infrastructure that unfortunately leads to discrete, inefficient, and stovepiped experimental data infrastructure across MML. Often, aging computer systems limit data-sharing and data analysis which are critical for MML to achieve its technical goals. There are many instances where old computers—year 2000 or older—using outdated operating systems such as Windows XP and Windows 2000 are in use. Reliance on outdated computing infrastructure could compromise data integrity. However, some of the use of older computers is driven by legacy instruments that cannot work with newer operating systems.

To overcome these deficiencies, the Office of Data and Informatics was effective in consolidating many vastly different operating systems of discrete sets of measurement equipment into a virtual machine. This virtual machine approach unified the measurement equipment operating systems and afforded a unified infrastructure for data management infrastructure, use, and security. The virtual machine approach may be a practice that could be useful throughout MML as it balances computational infrastructure needs with budgetary constraints.

> **Key Recommendation 5: To the extent possible, the Material Measurement Laboratory should launch an initiative to unify all computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management. This data science initiative could be applied to machine learning deployment and expand capabilities in laboratory automation, high-performance computing, and artificial intelligence. Computing infrastructure should, to the extent possible, be updated to meet current laboratory standards.**

REFERENCES

NASEM (National Academies of Sciences, Engineering, and Medicine). 2019. *Managing the NIH Bethesda Campus Capital Assets for Success in a Highly Competitive Global Biomedical Research Environment.* Washington, DC: The National Academies Press. https://doi.org/10.17226/25483.

NASEM. 2023. *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology.* Washington, DC: The National Academies Press. https://doi.org/10.17226/26684.

Prpich, G., and R. Unnerstall. 2022. "Translating Industrial Lab Safety Practices to Academia." *Chemical Engineering Progress* 118(5):29–34.

3
Applied Chemicals and Materials Division

The Material Measurement Laboratory's (MML's) Applied Chemicals and Materials Division, located in Boulder, Colorado, focuses on creating and maintaining tools to measure the properties and structures of fluids and materials important to industry, with the goal of providing measurement tools and models, as well as critically evaluated data, to a diverse set of stakeholders. Their work is designed to support the creation of better products and importantly, new and improved standards.

The division is organized into the following five groups, which have the same structure and same leadership team as in the fiscal year (FY) 2020 MML review (NASEM 2021):

- Thermodynamics Research Center
- Fatigue and Fracture Group
- Nanoscale Reliability Group
- Fluid Characterization Group
- Thermophysical Properties of Fluids Group

In addition, a briefing on "3D Materials Research", an effort led by Edward Garboczi, a NIST Fellow in the Applied Chemicals and Materials Division headquarters, was presented.

The work in the Applied Chemicals and Materials Division is extremely broad, focusing on measurements and modeling of materials in their gas, liquid, and solid states. The division has two somewhat competing demands for its resources. On one hand, they have a responsibility to continue to fund and maintain their traditional role as a developer of standards for both the United States and international partners. These standards serve very important roles in developing and using materials by industry, government, and academic partners. The division, however, has to balance those responsibilities with new challenges that arise from the changing needs for measurement science in response to new materials systems and new funding sources.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

The technical work in the Applied Chemicals and Materials Division was all very good to excellent, with several new and promising technical advances in metrology science. The mix of technical activities is quite broad in topics and consists of a strong mix of ongoing work in NIST's traditional role of providing standard reference materials and standard reference data to industry and other external customers combined with new areas of high-impact research and development of new metrology science. Here are a few highlighted examples, starting with the work on standard reference materials and data.

All of the work in standard reference materials and data is very good and has a high impact on industries and other users of their work. The Charpy Machine Verification Program each year sells standard reference materials to more than 1,900 customers in 73 countries that are used to certify Charpy impact test machines for ensuring the quality of steel used in industry and construction. It has a huge impact worldwide, bringing in $2.3 million of support for the sample manufacturing and for activities at

the Applied Chemicals and Materials Division. The Reference Fluid Thermodynamic and Transport Properties Standard Reference Data provides thermophysical property data for 140 industrially important fluids and their mixtures and is used by tens of thousands of engineers across hundreds of organizations. The ThermoData Engine standard reference data set contains tens of thousands of materials, including pure compounds, mixtures, and chemical reactions, and underlies process simulation tools used by industry. This data set is built by compiling data reported in scientific journals; MML is not generating the data, it is finding it and compiling it for community use. One of their challenges, however, is that there is significant loss of experimental data owing to incomplete or inaccurate reporting in the journals. To address this issue, they have developed a set of principles for *Good Reporting Practice for Thermophysical and Thermochemical Property Measurements* (Bazyleva et al. 2021), which was published as an International Union of Pure and Applied Chemistry Technical Report. NIST collects fees from its users of its thermophysical properties data, which only accounts for about 50 percent of the total cost of the program to division.

Several key advances were made by the Applied Chemicals and Materials Division over the past 3 years. In metrology science, they developed key instrumentation and applications. The development of extreme ultraviolet atom probe tomography, the only one of its kind in the world, will revolutionize the chemical characterization of nanoscale structures and interfaces by overcoming the limitations of commercially available atom probe tomography instruments. (Most such instruments use high temperatures or high electrostatic fields to drive atoms off the surface, which can lead to changes in the local atomic structure via diffusion and other mechanisms. Extreme ultraviolet atom probe tomography uses a wavelength that drives atoms off the surface with little change in the local structure.) The Fluid Characterization Group has pioneered novel uses of nuclear magnetic resonance that enable the concurrent determination of composition, pressure, and temperature for vapor, liquid, or combined vapor and liquid samples. This nuclear magnetic resonance method is being used, in addition to other applications such as sequestering CO_2 in cement, to do ground-breaking, in situ vapor-liquid equilibrium measurement in which they can measure temperature, pressure, vapor-phase composition and liquid-phase composition, which will lead to better thermodynamic models. Making use of a novel method that the Fluids Characterization Group previously developed for vapor pressure measurements over six orders of magnitude, members of the group have participated in a pilot study measuring tetrahydrocannabinol (i.e., THC) in breath aerosols before and after legal-market product inhalation as part of a project to create a cannabis breathalyzer in a project funded in part by the Department of Justice.

Work in the Applied Chemicals and Materials Division has also led to advances in materials for use in additive manufacturing. First, standardization of photopolymer additive manufacturing technologies will significantly accelerate the adoption of the additive manufacturing of plastics, soft materials, and biological materials. Second, division staff discovered a novel fatigue-resistant additive manufacturing titanium microstructure and developed an inexpensive process control technique to significantly improve fatigue performance, which will enable that alloy to be used in medical device applications, such as hip replacements.

Opportunities and Challenges

The Fluid Characterization Group has undergone a rather large change in personnel since the FY 2020 review, losing 7 staff and adding 2 new permanent staff and 3 term staff. To give a sense of the significance of this change, the group has 6 permanent staff and 2 associates. It did at the time of the prior assessment, too. As part of this change, there was a dramatic change in the makeup of their staff, with all of their new staff being chemists, while losing 2 of the four chemical engineers and both of the mechanical engineers. Despite these changes, the group remains a small but engaged, highly collaborative, productive group conducting and disseminating impactful research. Although small, they have made significant advances. However, longer-term program building requires a more stable

workforce. The Fluids Characterization Group will be moving their research to renovated labs in Building 1, Wing 4.

The nanoscale reliability team has several legacy projects that are ideally suited to impact the upcoming investments through the CHIPS and Science Act of 2022. The team has received advanced characterization instrumentation shared with other groups across NIST Boulder (through the precision imaging facility), which puts them in an ideal position to lead characterization efforts for projects related to the CHIPS Act. The CHIPS Act has the promise of a major source of funds over the next few years. Applied Chemicals and Materials Division has hopes of spending $20 million in funds from this act in the 2024–2025 time frame for purchasing major pieces of equipment, such as scanning electron microscopes and transmission electron microscopes.

Hydrogen-assisted fracture and cracking remains a vexing and poorly understood phenomenon in high strength materials such as precipitation-hardened and age-hardening steels, which are essential in the oil and fracking industry because of the increased depth of oil and gas wells. The work of the Fatigue and Fracture Group at MML contributes greatly to the metals industry as a whole to better understand the mechanisms associated with these phenomena with high value for industry. It is not clear how much cooperation and support there is from manufacturers of alloy steels that are susceptible to hydrogen cracking and if such partnership can be exploited better to grow and expand the program.

How the Applied Chemicals and Materials Division moves forward and maintains their competitiveness, however, is not as clear given that one of their buildings (Building 24) is rated so poorly that it would be less expensive to tear it down than renovate. For example, while the Fatigue and Fracture Group has unique instrument capabilities (e.g., a million-pound load frame and the hydrogen research facility), it is housed in old buildings (including Building 2) without modern support systems and features. Reportedly, there have been long standing issues with stable electrical power and chilled water. While the chilled water provision is now reportedly working well after major campus level upgrades in 2022, the electrical power stability remains very problematic and is a site wide issue at NIST-Boulder. The temperature control in all three buildings (2, 8, and 12) is also not good and has to be accounted for in equipment and experiment design and execution. Even if new buildings are constructed, we were told that relocating much of the current equipment will be cost prohibitive and there is a need to couple the buildings with investment on new equipment.

Perhaps the biggest challenge that the Applied Chemicals and Materials Division faces is how to continue support for their legacy work in light of the new opportunities arising from the CHIPS Act and the recent development of new materials for meeting the challenges of global climate change. As noted elsewhere, salary costs at NIST are growing about twice as fast as their base funding, requiring them to find new funding just to keep even. How they respond to new initiatives thus becomes of grave concern. The Applied Chemicals and Materials Division may have to retire old programs to free up funds for new, and highly impactful, work. How the division makes those decisions will be a challenge and when asked, they admitted that it is very difficult for them. However, they have relatively recent experience in doing this, ending a 20-year program in measuring vapors to find explosives and moving toward the cannabis breathalyzer and potentially, breath-based diagnoses of illnesses. What we would have liked to see is a plan for how they will make those decisions.

Recommendation 3-1: The Applied Chemicals and Materials Division should develop a process to evaluate the maturity and current and future importance of ongoing projects relative to new opportunities to help decide which programs could be cut in effort or retired completely.

ASSESSMENT OF SCIENTIFIC EXPERTISE

Accomplishments

The Applied Chemicals and Materials Division possesses a breadth of scientific expertise to further the organization's mission and project objectives as noted below. This expertise adequately supports the organization's technical programs and the organization's ability to achieve the objectives to further the mission of both the division and NIST.

The division, with 55 scientists—a decrease of 5 percent from the 2020 reporting period—continues to demonstrate impressive productivity in scientific publications, standards interactions, intellectual property activity, and customer engagement. The frequency of publication in archival journals continues to average more than 1.3 articles per year per scientist.

Over the past 3 years Applied Chemicals and Materials Division personnel have participated in 69 standards committees (an increase of 25 over the 2020 review) with leadership positions in 17 of those committees. The strong participation of division personnel on these committees is of critical importance to the NIST mission, making it possible for the division to continue its essential role of supporting U.S. industry by initiating, evaluating, and maintaining industry standards. The strong support of its industrial stakeholders is shown in part by a significant increase in the number of cooperative research and development agreements in this review period (46) over that in the 2020 review (13), along with an increase in non-disclosure agreements (17 in this review versus 11 in 2020). The staff of the Applied Chemicals and Materials Division have also developed a new Research Grade Test Material Reference Resin for Photopolymer Additive Manufacturing, which already has 20 material transfer agreements completed or in progress.

A clear measure of the scientific expertise of Applied Chemicals and Materials Division researchers is seen with the major advancements in metrology over this review period. A short list of those advances includes the development of a pulsed extreme ultraviolet radiation source that greatly extends the applicability of atom-probe tomography (patented and licensed); development of a novel additive manufacturing microstructure for critical fatigue applications than enables additive-manufactured titanium alloys to be used in hip-replacement implants; and an invented measurement approach for in situ mechanical measurement for voxel-scale bioprinting and additive manufacturing.

Finally, members of the Applied Chemicals and Materials Division have received important awards from NIST for their work on creating a digital verification program for Charpy standards and from the Department of Commerce for increasing cardiac device reliability through improved measurements and standards.

Opportunities and Challenges

Looking at the demographics of the research staff in the Applied Chemicals and Materials Division, there seems to be a gap in the mid-career staff, with large numbers of established late-career staff, but with no clear succession path to bring in newer staff and fold them into the division's work. While division has no control on when staff might step down, the lack of a succession plan is troublesome.

The panel met with a group of postdoctoral fellows, associates, and young staff. While some were content with the current situation, there were others who raised several concerns, including uncertainty about conversions to permanent staff in spite of clear needs, the pay differential between federal government scientists and engineers compared to industry, and remote work by mid and senior staff members significantly inhibiting postdoc and early career scientist productivity and career advancement. In a later question and answer session with the Applied Chemicals and Materials Division director and the MML deputy director, these issues were probed. Management described a system of mentoring and evaluation of mentors that is part of their yearly assessment. The resulting impression is that neither the

expectations of management nor the expectations of young staff and postdoctoral fellows were being consistently met.

Recommendation 3-2: The Applied Chemicals and Materials Division, and the Material Measurement Laboratory broadly, should have a streamlined and standardized mentoring plan with suitable evaluation of the mentors.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

The budget of the Applied Chemicals and Materials Division in FY 2023 was $23.371 million, comprising $13.993 million from appropriations, $4.899 million from reimbursable work, and $4.478 million from providing services and a working capital fund. It has a total of 91 staff, comprising 55 scientists, 2 technicians, 4 support staff, 1 fellow, and 29 associates.

Accomplishments

To carry out its mission, the Applied Chemicals and Materials Division needs onsite access to new, state-of-the-art, advanced characterization tools. The division has been successful in finding creative solutions (e.g., partnering with other divisions and purchasing equipment from U.S. government surplus listings) to not only upgrade their current equipment but to also obtain funding for developing new and unique instruments that are not widely available elsewhere (e.g., MML's extreme ultraviolet atom probe tomography instrument and nuclear magnetic resonance to probe the vapor-liquid phase equilibria).

A glaring issue, which is adequately highlighted in prior review reports, are aging facilities and infrastructure, which handicaps the research efforts in the Applied Chemicals and Materials Division. The division has been successful, however, in finding funds to renovate laboratory space in the newest building, Building 81. They have also found funding and have plans in place to do further renovation in Wing 4 of Building 1, with a planned construction start of 2024 or 2025.

Opportunities and Challenges

While the appropriated funds from NIST to the Applied Chemicals and Materials Division increased by about 9.4 percent since the 2017 review (FY 2016), the Scientist-4 (ZP-IV) midpoint salary increased over twice as fast (by more than 20 percent) over the same time period. There is a variety of reasons for this. A major driver in salary growth was a market salary survey and resulting upward adjustments to MML staff salaries to be more competitive. The disparity between funding growth and salary growth means that increased funding from outside projects is required to just maintain the division's budget situation, which has the potential to adversely affect both program development and maintaining standards and the ability of the division to move into new areas of research to better meet future industrial needs. The panel noted that experienced, and more expensive, PhD-level scientists are involved in many routine-seeming tasks related to ongoing activities such as the production of standard reference materials and data sets. It might be possible to increase the use of technicians, who are typically less expensive, to conduct routine tasks and thereby stretch limited funding further while supporting ongoing work and developing new work.

Given the funding issues just described, it would be good if the Applied Chemicals and Materials Division could recover more funds from users who use their products and services. The Charpy program, for example, generates about $2 million from external payments, which covers most or all of its costs. The division's standard data products, however, seem to recover only about 50 percent of their costs. However, MML contends that the division is charging as much as users would be willing to pay and that charging more would result in fewer users for the division's standard data products. It would seem that a

detailed market assessment might be a way to assess and maximize the return on the long-term investment in generating and maintaining MML's data-based products.

Current research in Buildings 2 and 24 is significantly affected by the poor control of temperature and air flow in their laboratories. Indeed, Building 24 has been assessed with a facilities condition index of –13, indicating that it would be more cost effective to tear down that building and replace it than to attempt to renovate it to address the needs of the research conducted in this building. It is worth noting that according to the 2023 National Academies report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023), there is a plan in preparation to address facility conditions for MML and all of NIST. This plan and associated funding are discussed in more detail in Chapter 1 of this report and in the 2023 report.

Making use of CHIPS Act funding, the Applied Chemicals and Materials Division has an aggressive plan to work with the Physical Measurement Laboratory to spend $20 million to substantially improve the NIST-Boulder Precision Imaging Facility in the 2024–2025 time frame. The plan includes the purchase of new tools, including electron microscopes and focused-ion beams.

As noted in the FY 2020 MML assessment (NASEM 2021), the Applied Chemicals and Materials Division's dependence on associate staff may lead to potential program continuity issues as the tenure for short-term employees ends. The division may not succeed in sustaining additional program growth through reliance on increases in future associates.

Recommendation 3-3: To maximize outcomes from the use of external funds, the Applied Chemicals and Materials Division should make greater use of technicians for maintaining legacy projects and provide adequate staff time for new initiatives.

Recommendation 3-4: The Applied Chemicals and Materials Division should carry out a detailed market assessment to assess and maximize the return on the long-term investment in generating and maintaining Material Measurement Laboratory's' data-based products.

EFFECTIVENESS OF DISSEMINATION EFFORTS

Accomplishments

The programs at the Applied Chemicals and Materials Division that span emerging topics such as photopolymer additive manufacturing and legacy historical needs such as Charpy testing and are largely driven by the stakeholder needs. There is significant interaction between the stakeholders and division to continuously improve the program outputs to serve the stakeholder needs.

The Applied Chemicals and Materials Division has been very effective in disseminating its outputs in several different ways. Division personnel publish substantially in the open literature, with 229 papers in archival journals, 18 in conference proceedings, 9 book chapters, and 24 reports during the period between the 2020 assessment and this assessment. This amounts to a journal publication rate of approximately 1.3 papers per researcher per year. The staff members actively participate in seminars, workshops, and conference presentations with 160 invited presentations in the past 3 years. The division has worked closely with a variety of organizations, such as the American Society for Testing and Materials, the International Organization for Standardization, and the American National Standards Institute in developing standards. As noted above, the staff participates in as many as 69 standards committees with numerous staff members assuming leadership positions on these committees.

The Applied Chemicals and Materials Division has also been very successful at disseminating their work on standards. Currently there were 21 standard reference material and reference material activities and 6 standard reference data activities in the division. There are several notable examples of programs driven by stakeholder needs, most notably the Charpy Impact Machine Verification Program and the Thermophysical Properties of Fluids Group. The Charpy Impact Machine Verification Program

sells 17 distinct standard reference materials and provides associated services to more than 1,900 customers in 73 countries to enable certification of the Charpy Impact Test Machines used to ensure that the steel produced is in compliance with American Society for Testing and Materials and International Organization for Standardization standards. It has remained the leading NIST standard reference material year after year. The division's Reference Fluid Thermodynamic and Transport Properties standard reference data database has 1,423 annual licenses and is a go-to source of thermophysical property data for the refrigeration, natural gas, aerospace, and other industries. This program calculates the thermodynamic and transport properties of 140 industrially important fluids and their mixtures and is used by tens of thousands of engineers across hundreds of organizations for product and process design. The NIST Standard Reference Database 103b (the ThermoData Engine) contains original thermodynamic experimental data collected from archival scientific journals for ~29,000 pure compounds, ~75,000 binary mixtures, ~24,000 ternary mixtures, and ~8,200 chemical reactions with a total of more than 8,000,000 individual data points.

The Applied Chemicals and Materials Division has focused on engaging with their customers through a variety of activities, including hosting 18 focused workshops, developing 46 cooperative research and development agreements, 18 material transfer agreements, 17 nondisclosure agreement, 11 interagency agreements, 2 memoranda of understanding, and 4 consortia over the past 3 years. These mechanisms allow the division to monitor the use and impact of the program outputs.

The Applied Chemicals and Materials Division has been awarded 1 patent with 7 additional invention disclosures and patent applications over the past 3 years.

Overall, the Applied Chemicals and Materials Division does an excellent job of disseminating its output to all stakeholders.

Opportunities and Challenges

While the Applied Chemicals and Materials Division has created significant impact with key standard reference data and standard reference materials, it needs to, as much as feasible, increase revenues from those products so it can better fund these activities, which would enable the division to explore both new solutions to its ongoing work and new programs focused on the changing needs for alternative materials.

REFERENCE

Bazyleva, A., J. Abildskov, A. Anderko, et al. 2021. *Good Reporting Practice for Thermophysical and Thermochemical Property Measurements (IUPAC Technical Report)*. https://www.degruyter.com/document/doi/10.1515/pac-2020-0403/html.

4
Biosystems and Biomaterials Division

The Biosystems and Biomaterials division is tasked with advancing measurement science, standards, and technology to promote U.S. biosciences and biotechnology, enhance economic security, and improve competitiveness of the U.S. bioeconomy. This includes increasing the resilience and flexibility of the bio-supply chain. They have also been tasked with developing cybersecurity technologies for the unique needs of genomic and biomedical-based systems. There are four main research areas: regenerative medicine and advanced therapies, precision medicine, engineering biology, and microbial metrology. Research groups collaborate extensively with each other to accomplish the goals of the division. They also collaborate with and disseminate results to outside groups including industry, academia, federal agencies, and standards developing organizations.

In April 2023, based on the data that were presented to this panel, the division had 106 staff, including 55 scientists, 36 associates, and 8 technicians. This group is diverse in its scientific backgrounds—including chemistry, biology, engineering, and statistics—as well as in its gender makeup and age range. Postdoctoral fellows, term-limited appointees, and visiting students also regularly bring in new ideas and contribute significantly to the division's mission. Over this review period, individuals in the division have earned 12 Department of Commerce and National Institute of Standards and Technology (NIST) awards, and 2 external awards (Outstanding Young Scientist Award from Maryland Science Center, and the Dirks Prize in Molecular Programming from the California Institute of Technology [Caltech]) in recognition of individual contributions to science.

The division is supported by a $24.6 million budget, comprising appropriations ($20.9 million), funds from interagency agreements ($3.4 million) and additional funds ($306,000) for service work. The division also receives episodic and term-limited funding for specific work, such as that related to the COVID-19 pandemic.

The division's products include measurement science data and protocols, which are disseminated in publications, reference materials and reference data. Overall, during the review period the Biosystems and Biomaterials Division has published more than 95 peer-reviewed articles, organized 26 conference proceedings, and presented their research in 118 invited presentations. In regard to stakeholder engagement, the division has more than 150 partnership agreements including 4 large consortia and has participated in 22 workshops to develop and disseminate information. They have developed 22 standards and reference materials and received 4 patents, with 3 additional applications filed.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

The division is currently divided into four main research areas: regenerative medicine and advanced therapies, precision medicine, engineering biology, and microbial metrology. There is strong collaboration and sharing of resources and expertise between personnel associated with each of these areas. Overall, it was clear that the division was highly accomplished during this review period despite the restrictions owing to the COVID-19 pandemic. The research overall, as demonstrated in numerous high-quality publications and invited talks (see the section "Effectiveness of Dissemination Efforts" below), is

extremely rigorous and forward-thinking. The technical program organization and the cross-cutting nature of the groups, and the high quality of the research products are well aligned to support the division in reaching its overall goals in the quickly changing field of biometrology.

The Regenerative Medicine and Advanced Therapies Program is integral to developing standards for the growing bioeconomy. They have developed numerous standards published by the International Organization for Standardization (ISO), including the development of a common biotechnology genome editing vocabulary to improve communication between stakeholders. They oversee the Genome Editing, Flow Cytometry Standards, and Rapid Microbial Testing Methods consortia. They have developed methods to evaluate the quality of gene delivery systems, infectious virus titer measurements, and are working on extracellular vesicle characterization and reference materials. The standards developed for gene delivery systems are integral to increasing confidence in the CRISPR (Clustered Regularly Interspaced Short Palindromic Repeats) era of genetic modifications for use in clinical and experimental research.

The Flow Cytometry Standards consortium is a particularly successful public-private partnership to increase the confidence and comparability in flow cytometry data to support the bioeconomy. This consortium has developed calibration standards, standard operating procedures to ensure comparability between different cytometer platforms and is developing a global filename convention for data dissemination. The Rapid Microbial Testing Methods consortium has enabled new characterization of existing materials, including flow-based methods to quantify genomes and feasibility studies of *E. coli* reference materials. They have also worked to develop and encourage the adoption of reference standards across more than nine parameters of cell function. The Regenerative Medicine and Advanced Therapies Group has also created an open access tool (the Counting Method Evaluation Tool, known widely as COMET[1]) to analyze the performance of cell counting methods based on an ISO standard. The group also significantly contributed to the development of this ISO standard. This research team has also developed new microscopy and spectroscopy techniques to improve stem cell throughput and capabilities through liquid media.

The Precision Medicine Program is tasked with identifying and developing the infrastructure to ensure that measurement methods and materials give reproducible results for personalized healthcare. In the period covered by this assessment report, this research area has published 10 papers to develop benchmarks and best practices and collaborated to evaluate and improve methods with 14 papers. They have developed intensity scales for microscopy and a strong evaluation tool of flow cytometers for industrial and academic use. This group also runs the Genome In A Bottle consortium, which has characterized variants in 7 human genomes, developed open consent cell lines to meet clinical needs, and is developing an artificial intelligence model to improve confidence. This consortium improves confidence in genome sequencing and variant calling. More than 50 commercial products are available based on Genome In A Bottle Personal Genome Project cell lines. Precision Medicine researchers also support the Pangenome Reference consortium to further understand the normal and abnormal diversity of the human genome. They are collaborating to develop somatic variant reference samples in order to support the validation of next-generation sequencing of cancer biomarkers for diagnostics. Cancer biomarker reference materials are being developed to improve clinical measurements through interlaboratory studies. The liquid biopsy cancer biomarker project operates under an interagency agreement with the National Institutes of Health (specifically the National Cancer Institute) to improve standards of extracellular vesicle measurements, circulating tumor DNA measurements, and DNA methylation measurements.

The Engineering Biology Program is focused on developing measurement tools and standards to support the control and design of biological functions. This includes living measurement systems, which are focused on growth, manipulation, sample preparation, and measurement of engineered microbes, and systems designed to improve the consistency of biological research and development. They are currently

[1] For more information, see Standards Coordinating Body, "NIST Develops Cell Counting Method Evaluation Tool (COMET)," https://www.standardscoordinatingbody.org/release-comet.

focused on three main goals: biological sensors, biological computation, and development of a chassis. The chassis refers to a cell-free biological system to use as a testbed of protein synthesis. They have developed a living measurement systems foundry to increase the consistency and throughput of biological systems development. This is designed to be an automated system to improve throughput and consistency.

The Microbial Metrology Program is focused on the human microbiome as a target for diagnostics and therapeutics. Biosurveillance has particular importance in the post-COVID era. This group has hosted workshops on standards for microbiome research and biosurveillance. The biosurveillance group within the microbial metrology research area has partnered with the Defense Advanced Research Projects Agency to develop pathogen detection within samples containing large numbers of microbes. Wastewater surveillance allows diagnostics throughout larger regions of communities. They developed an Mpox[2] virus assay and positive controls. Considering that the first and second Food and Drug Administration–approved microbiome therapeutics have been approved within the past 2 years, the need for standards has increased. This group has created the human fecal reference material to develop diagnostic standards.

Challenges and Opportunities

Building on the current success of all research areas within the division, but especially the engineering biology and microbiome areas, there is an opportunity to further develop standards and reference materials in the area of biotechnology for agricultural use (clean energy and food sustainability). This would further the division's broad goals to support the growing bioeconomy and promote customer outreach to an even broader set of academic and industry stakeholders (see the section "Effectiveness of Dissemination Efforts" below).

ASSESSMENT OF SCIENTIFIC EXPERTISE

Accomplishments

The Biosystems and Biomaterials Division is a recognized leader in biometrology within the United States and internationally. This is demonstrated by the division's leadership in standards development, particularly in the area of advanced therapeutics which has led to more than 40 ISO standards; leading in a number of NIST consortia (Genome In A Bottle, Flow Cytometry Standards, Genome Editing, and Rapid Microbial Testing Methods); and publications in high-quality journals.

The four programmatic research areas have continued from the past review period: engineering biology, regenerative medicine and advanced therapies, precision medicine, and microbial metrology. Expertise in each of these areas is deep, and well aligned to promote the division's objectives. In engineering biology, expertise has centered around supporting the transition of engineering biological systems from a costly, laborious, trial-and-error approach to a routine, automated, design-build-test-learn workflow. Expertise in the Regenerative Medicine and Advanced Therapies Group allows the researchers to provide measurement infrastructure and platform technologies, as well as standards to promote manufacturing innovation, improve supply chain resilience, and support characterization and testing to facilitate regulatory approval of advanced therapeutics. In precision medicine, expertise has focused on supporting the identification, validation, and accurate measurement of biomarkers, especially for cancer diagnosis and treatment. Expertise in the Microbial Metrology Group allows the researchers to provide complex reference materials and measurement capabilities to support a wide range of industrial activities, including microbial therapeutics to treat disease, soil probiotics that enable more robust agricultural processes, novel approaches to biofuel production, and bioremediation and carbon capture for the

[2] Mpox is the new name for monkeypox.

environment and climate. Moreover, the focus of the researchers in each area on a subset of use cases or "test-beds" (e.g., Chinese Hamster Ovaries cells and specific viral vectors for genetic modification) helps to unify the division's research teams and encourage knowledge sharing among research teams.

Through these consortia, the division team has developed reference standards, innovative and reliable reference methods, benchmark sets, data, publications, and harmonized lexicons. The division's work has been recognized by numerous awards by the Department of Commerce and NIST awards, including 4 Department of Commerce Gold Medals. In addition, the division's impact has been recognized by several external awards, including the Outstanding Young Scientist Award from Maryland Science Center, and the Dirks Prize in Molecular Programming from Caltech.

Since 2020, the groups in Biosystems and Biomaterials Division continue to grow in national prominence in the areas of both mammalian and microbial biologics. During this review period, the division's programs have supported the development of the Executive Order on Advancing Biotechnology and Biomanufacturing Innovation for a Sustainable, Safe, and Secure American Bioeconomy (Executive Order 14081), the National Biodefense Strategy, and associated research and development strategy documents. The division has built cutting-edge expertise in robotic platforms for bioassays and biomanufacturing to accelerate productivity. The division's success in enhanced group activities stems from efficient integration of staff among the groups and the use of modular and flexible capabilities (such as a new modular laboratory currently used for cell expansion). This integrated structure allows the division to remain flexible to meet unexpected demands on their expertise, such as the COVID-19 pandemic, where they helped produce a SARS-CoV-2 polymerase chain reaction reference-grade testing material (led by the Biomolecular Measurement Division) and ISO standards on SARS-CoV-2 testing. Another laudable example is that the division's staff was able to use their collective expertise and creative redeployment of resources to produce a Mpox DNA standard within 30 days in response to this emerging health threat.

Opportunities

Notably, during this review period, the Biosystems and Biomaterials Division has paired extensively with the National Aeronautics and Space Administration's Jet Propulsion Laboratory (JPL) to build on JPL's capabilities to provide a well-architected data management environment (LabCAS/LIMS) to support the capture, curation, management, distribution, and analysis of data science activities within the division. This work is currently using the JPL cyberinfrastructure for several test cases within the Biosystems and Biomaterials Division. Data curation and analysis is of utmost importance for further analysis of results from biosystems, biomanufacturing, and bioassays to direct the future of these fields over the next 5–10 years. Given the importance of this capacity across the division, there is an opportunity to further build (1) expertise in the division and (2) data management capacity within the division by both continuing existing programs such as the JPL partnership, as well as continue to partner with data scientists at NIST and externally to develop a cohesive data management plan for all data gathered within the division.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

Accomplishments

The division's leadership works with the six group leaders who oversee the five groups of the division (Complex Microbial Systems, Biomarkers and Genomics Sciences, Biomaterials, Cell Systems Science, and Cellular Engineering). Personnel in these five subgroups in turn are deployed as needed within the division's four programmatic research areas (or research groups) listed in previous sections. Although most groups have a single leader, the Biomarkers and Genomics Sciences Subgroup is co-led by a team of two leaders. The division leader has been very strategic in deployment of resources to have

maximal impact. The chief and deputy chief have fostered a climate of open discussion necessary for the highest level of work and cultivated a very enthusiastic staff. A pathway to promotion from lab technician to team leader and flexible work options within the division has enabled the retention of talent.

The Biosystems and Biomaterials Division has been very proactive in the incorporation of automated liquid handling and other robotics platforms into work routines. The division has an AI-enabled Living Measurements Systems Foundry and Prototype Cell Assay Measurement Platform. These automated systems aid in reproducible, higher throughput quantitative sample preparation and measurements of complex living systems and processes.

Challenges and Opportunities

The division is supported by a $24.6 million budget. This support comes from appropriations ($20.9 million), funds from interagency agreements ($3.4 million), and additional funds for service work ($306,000). The division also receives episodic and time-limited funding for specific programs such as those related to the COVID-19 pandemic. During this review period, the Biosystems and Biomaterials Division's programs have supported the development of standards related to COVID-19 and Mpox outbreaks, the development of the Executive Order on Advancing Biotechnology and Biomanufacturing Innovation for a Sustainable, Safe, and Secure American Bioeconomy (Executive Order 14081), the National Biodefense Strategy, and associated research and development strategy documents. However, despite this growing demand for the division's expertise, the overall budget has decreased in inflation-adjusted support since the past review in 2020.

> **Recommendation 4-1: Owing to increasing demands on the unit resulting from new bioeconomy initiatives, the Material Measurement Laboratory should prioritize allocations to the Biosystems and Biomaterials Division within budgetary constraints to ensure adequate support and the Biosystems and Biomaterials Division should continue to prioritize its efforts mindful of its limited budget.**

The division works in laboratories spread across two buildings on the NIST campus in Gaithersburg, Maryland. The groups work closely together yet are physically located in separate locations. This separation slows down the work physically (requiring moving of samples a 15-minute or more walk each way), as well as slowing idea transfer. Moreover, the state of these buildings has been well described in the 2023 report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023). Room temperatures vary from too hot to too cold such that the reliability of modern scientific equipment and measurements is imperiled. Humidity and power control are also too variable for consistent operation of sensitive equipment, such as lasers.

> **Recommendation 4-2: The Material Measurement Laboratory leadership should evaluate space allocations to co-locate the Biosystems and Biomaterials Division in a single building with adequate temperature, humidity, and power control for continuous instrument function.**

The pandemic restrictions did limit onboarding processes and other processes that contribute to a cohesive work culture. The division's leadership team is actively working to rebuild these processes, although this work is especially challenging given the spread of people across buildings and the lack of shared public spaces like the cafeteria. Career mentoring and professional development for the population of postdoctoral fellows and other term-limited scientific appointees is uneven. The path to employment within NIST or within its corporate and academic partners or elsewhere is not clear to many of these appointees. Increased mentor training within this population (for horizontal mentorship) and within the division overall (for vertical mentorship and sponsorship) would increase the impact of this population

both within NIST and later in industry, academia, or government positions. A larger strategy consistent with the mission of NIST would be to partially fund NIST postdoctoral fellows in laboratories of stakeholders such as industry, academic, and agency partners in areas of needed expertise development for the division, with the expectation that they would spend time within both NIST laboratories and the partner institution. This practice would enhance collaborations, the cross-fertilization of knowledge, and broader awareness of the work of the Biosystems and Biomaterials Division.

Recommendation 4-3: The Biosystems and Biomaterials Division leadership should require mentorship training for all laboratory employees and increase the number of employees who have formal leadership training to standardize mentoring and onboarding of new personnel and to make career development opportunities more uniform.

EFFECTIVENESS OF DISSEMINATION EFFORTS

Accomplishments

The Biosystems and Biomaterials Division has been very active in disseminating its protocols, materials, and expertise. It has maintained robust participation in national and international consortia and national and international working groups through the pandemic years. It is clearly recognized around the world. Since the past review in 2020, the division has published almost 100 peer-reviewed articles in high-impact journals, published 5 books or book chapters, given 118 invited presentations at conferences, and contributed to a dozen workshop reports. The division has actively engaged the industrial community and others through 22 workshops, 91 cooperative research and development agreements, and almost 60 material and data transfer agreements. They also participate actively in four consortia, including the Flow Cytometry Standards Consortium and the NIST Rapid Microbial Testing Methods Consortium that was launched in June 2020. Four patents have been issued (two in 2020 and two in 2022) and 3 patent applications were filed in 2022.

The division is proactive in maintaining an international presence through participation on 22 standards committees (including 8 leadership positions) and the development of 1 standard reference data product, 1 research grade test material, and 22 standard reference materials. This work is critical for the development and the success of the biotechnology industry. The U.S. Technical Advisory Group to the ISO Technical Committee 276 (which works on Biotechnology), along with the NIST-administered U.S. Mirror Committee, has published more than 50 documentary standards to support biomanufacturing and biotechnology. A living reference material for certain yeast cells was developed to support the Department of Homeland Security's efforts to benchmark the detection and quantification of microbes. The Biosystems and Biomaterials Division was also instrumental in developing a SRM (standard reference material) (SRM 2917) in collaboration with the Environmental Protection Agency to estimate total fecal pollution and the sources of this type of pollution in water. The Mpox outbreak led to the production of a positive control material (RGTM 10223) to assess Mpox diagnostic kits. This division is very responsive to the development of standards and protocols needed to drive assay development within government and for-profit organizations.

Challenges and Opportunities

The Biosystems and Biomaterials Division maintains exceptionally strong networks of stakeholders and collaborators including other NIST units, other government entities, industry, and academic institutions. These networks contribute to the very strong technical programs and scientific capabilities of the division. The challenge will be to continue to expand these assets sustainably to contribute to the bioeconomy across industries from health to energy, and from chemicals to agriculture. The division has the opportunity to actively reach out to an even broader set of academic institutions

across broader geographic areas of the United States to further promote the dissemination of the division's products and capabilities. Such broader geographic outreach is particularly important to reach more stakeholders involved in the growing number of bioeconomy initiatives. In addition, NIST also offers very good incentives for the filing of patents, but many staff are not aware of them. There is therefore an opportunity to increase awareness for all staff, including new arrivals, about the process and outcomes of filing patents through NIST.

5
Biomolecular Measurement Division

The Biomolecular Measurement Division provides measurement science, technologies, and standards for the evaluation of biomolecules, including proteins, oligonucleotides, carbohydrates, lipids, metabolites, and complexes including such molecules. Key stakeholders include the pharmaceutical community, makers of analytical instruments, and clinical and forensics laboratories. The core competencies are built around methods for biomolecular measurements including mass spectrometry, mass spectrometry data analysis and library development, separations, biophysical methods, capillary electrophoresis, polymerase chain reaction techniques, genome sequencing, and production and validation of standard research materials and research-grade material standards.

The key focus areas of programmatic activity in the Biomolecular Measurement Division include mass spectrometry to support other projects and Reference Library expansion, forensics (genetics and drugs of abuse), clinical analyses (protein and nucleic acid markers), and biotherapeutics (biomanufacturing and engineering biology). The 77 federal employees and 25 associates in the Biomolecular Measurement Division are divided into five groups: the Mass Spectrometry Data Center, the Biomolecular Structure and Function Group, the Bioanalytical Science Group, the Applied Genetics Group, and the Bioprocess Monitoring Group. These groups seem to interact seamlessly within and externally to division to achieve the goals of each program area. For this reason, the following discussion is organized by program area and not research group.

Between April 2020 and March 2023, the Biomolecular Measurement Division published 135 papers, 4 workshop reports, 22 data sets, and 3 databases of standardized analytical measurements. Four patent applications have been issued, and most of these are licensed. They produced 20 standard reference materials and reference materials, 3 standard reference data sets, and 2 research-grade test materials. The division staff serve on 25 standard committees and 19 working groups—12 of these in leadership positions. The balance of activities includes basic science related to technology development (e.g., dyes for protein sequencing, sub-zero chromatography for hydrogen/deuterium exchange-mass spectrometry, and artificial intelligence for tandem mass spectrometry peptide identification), customer-driven projects, and mission-oriented product development.

The breadth and depth of the projects is impressive. The following analyses are not exhaustive, but endeavor to distill the observations from 2 days of tours, the read-ahead materials provided to the panel, and the members' expertise and experience to recognize excellence, offer suggestions for possibilities to increase staff productivity, and provide pertinent examples.

ASSESSMENT OF TECHNICAL PROGRAMS

The technical programs are focused on developing processes and information relevant to the National Institute of Standards and Technology (NIST) mission. There are only a few examples of research that could be considered as basic, and that work seemed to be very targeted toward solving specific problems in the program areas through technology improvements. While this type of work is useful, seed projects involving research potentially relevant for meeting more long-term mission needs would be important for the Material Measurement Laboratory (MML) to pursue, if not already in progress. None were presented to us.

The work under way in response to stakeholder needs and in support of the NIST mission focus areas was quite impressive. The research addressed both the fundamental challenges in measurements relevant for major areas important to our society—with impact both nationally and globally, building consortia with customers, and providing high quality measurement processes and standards. Below are short comments about each of these areas.

Mass Spectrometry

The technical approach that the Biomolecular Measurement Division is taking to develop mass spectrometry libraries is world class. They are selecting molecules to be added to the libraries through a process based on the potential of the data to help address important societal problems. The selection of compounds to be analyzed is based on an algorithm the group developed, taking into account commercial availability, cost of the compound, and the national need for the information (e.g., chemicals in plastics, designer drugs, or food allergens). The compounds they purchase must be more than 90 percent pure prior to initiating the careful mass spectrometry required for addition of a new molecule to the library. The compounds and fragmentation profiles are then vetted, and peaks are assigned by scientists. The objectives of the group are clear, and productivity is exemplary in this program area, as illustrated by the addition of more than 40,000 compounds to the existing mass spectrometry spectral libraries, even through the COVID-19 pandemic. The staff engaged in this program area are efficient and highly productive.

The new Biomolecular Measurement Division hair peptide analysis technique was developed as part of MML's forensics initiative and is designed to identify specific individuals; it is also scientifically impressive. The group exploited the mutations of specific hair proteins, one being keratin, and demonstrated the discrimination between individuals in terms of subtle variations in proteins. This capability is unique in that a hair strand is one sample and cannot be contaminated by DNA from other individuals (unlike many samples used for DNA analysis). This technique is quite robust and may even differentiate between hairs from identical twins. The results are outstanding, and the staff is encouraged to further validate and bolster their findings for this potential paradigm shift in forensic analysis using mass spectrometry.

The mass spectrometry project to support the circular economy mission through plastic recycling made impressive use of liquid chromatography mass spectrometry. The staff in the mass spectrometry program area are building a library of spectra of plastic components by extracting polymeric subunits and additives out of the plastic for careful analysis. This program area may benefit from the integration of other analytical techniques (e.g., Raman spectroscopy), simultaneously building a library with spectra from both methods. This would allow for simple spectroscopy methods, such as Raman spectroscopy, to be employed in the field while coupling the field methods to the more precise liquid chromatography-mass spectrometry data acquired in a center of excellence.

The development of the NIST Urine Albumin Standard Reference Material 2925 now provides for global standardization of this critical marker in the urine. Presently, clinical laboratories—with Food and Drug Administration–approved diagnostic methods—can differ from one another by more than 40 percent in concentration measurements. This variability is significant as there are clinical guidelines that supply urine albumin cutoff values for the diagnosis of chronic kidney disease. MML will partner with external laboratories to develop reference measurement procedures using the albumin standard reference material for calibration. This global standardization of urine albumin measurements will enable consistent chronic kidney disease diagnosis across the world. Once the standardization system is in place, the staff in this program area are prepared to disseminate the information through publications and promotions to the health care community. This program area is partnered with the International Federation of Clinical Chemistry, the National Institute of Diabetes and Digestive and Kidney Diseases, and the Joint Committee for Traceability in Laboratory Medicine to achieve this mission. The Biomolecular

Measurement Division is addressing an important problem with this albumin standard and its continued collaborations with external partners.

Forensics

The Applied Genetics Group is a recognized leader in the forensic community. Their research on the statistical interpretation of DNA mixtures, use and validation of DNA sequence-based genetic loci, and introduction of novel peptide variant markers (discussed in the previous section) is high-quality and will be used to support forensic stakeholders such as law enforcement laboratories and the U.S. legal system. The applied genetics technical programs focus on meeting national goals by supporting current legacy technologies as well as providing standard reference materials and validating processes to be used with newly emerging technologies such as the next generation sequencing of forensically relevant genetic loci. They currently use next generation sequencing to analyze specific areas of the genome associated with ancestry, kinship, visible phenotypes, and personal identification. Additionally, forensic scientists have used whole-genome technologies to lay the foundation for forensic investigative genetic genealogy, which generates leads for unsolved violent crimes or the identification of missing persons. The laboratories are well equipped with the requisite instrumentation typically used in conventional forensic laboratories; Access to whole-genome sequencing equipment, which is finding significant utility in state-of-the-art laboratories, is only available through an external source. This is adequate for now, but plans for obtaining newer generation, lower cost equipment need to be considered as such equipment becomes more commercially available and used more broadly.

The standard reference materials produced by the Applied Genetics Group are used routinely by forensic laboratories for the quantitative and qualitative measurement of genetic markers. This group is revising their standard reference materials based on stakeholder needs as more genetic markers are being developed for forensics. This is demonstrated by the 2023 revision and implementation of Standard Reference Material 2391d, a polymerase chain reaction-based DNA Profiling Standard, by adding more than 11,000 additional genetic markers to it. Furthermore, they are in the process of developing a research reference material that will be used for interlaboratory studies relevant to the analysis of samples including mixtures of DNA from multiple individuals.

Clinical Analyses Using Protein and Nucleic Acid Markers

The research and development efforts in this area have focused on exhaustive development of methods for analyzing IgG and RNA. The RNA efforts produced usable standard materials for SARS-CoV-2 and Mpox in amazingly short time frames, demonstrating the skill and responsiveness of the staff to meet critical national and international needs. The methods used to analyze these molecules are widely applicable to other important proteins and nucleic acids. There is also some excellent underlying research that is important for analyzing particulates used in plastics recycling and therapeutics that will be relevant for both the circular economy project and biotherapeutic product manufacturing.

Biotherapeutics, Biomanufacturing, and Engineering Biology

The focus in this program area leveraged the availability of the NIST monoclonal antibody (NIST mAb) and the NIST Chinese Hamster Ovaries cell line that produces the monoclonal antibody to validate protein manufacturing processes and products. These are great tools, and both are and will continue to be important standards. Furthermore, the group developing these standards appreciates their value for education. For example, the NIST Chinese Hamster Ovaries cells can be put through bench-scale fermentation procedures to produce antibodies in teaching laboratories with minimal facilities development—a very powerful tool for workforce development, especially when coupled with metrics for the processes and their products. The research staff is interested in developing new tools for

biomanufacturing and bioprocess monitoring but does not possess much expertise outside of their current analytical methods, most of which are too expensive or impractical for implementation in a large-scale biomanufacturing operation. Thus, the staff's focus on providing information from high-resolution systems that can validate lower resolution data in processing operations makes sense.

The staff in this program area has developed simulations for overall biotherapeutic product stability and manufacturing quality control. This cutting-edge approach was achieved by combining nuclear magnetic resonance, electron paramagnetic resonance spectroscopy, small-angle X-ray scattering, small-angle neutron scattering, and hydrogen/deuterium exchange mass spectrometry techniques to validate the simulations. These approaches are on the forefront of biomanufacturing technologies and definitely position the team to lead these efforts in the field.

ASSESSMENT OF SCIENTIFIC EXPERTISE

The Biomolecular Measurement Division has a deep pool of knowledgeable scientific staff. This pool includes chemists, physicists, data and computer scientists, life and biological scientists, and forensic scientists. This matrixed expertise has produced world-class results and assisted the United States in staying at the forefront of biomolecular measurements. The expertise at NIST supports the technical programs well, meeting deadlines and achieving the overall goals for the organization and its stakeholders.

Mass Spectrometry

In terms of mass spectrometry, based on the presentations the panel received, tours, and interactions with the staff, MML definitely has a group that is world-class. The mixture of mass spectrometrists and data and computer scientists is particularly strong. The mass spectroscopy reference library is supplied, along with periodic updates that include expanded analyses, with spectrometers sold by most major suppliers and are critical to analytical laboratories worldwide. Thus, this product makes a major contribution to NIST's international reputation. In addition, the mass spectrometry group develops new methods for analytics that pushes the capabilities for molecular analysis at the cutting edge.

Forensics

The Biomolecular Measurement Division has a portfolio of scientists that are considered leaders in the global forensic genetics community and are well recognized in the field through their publications, presentations, and workshops. The applied genetics scientists support the organization's mission by providing best methods to interpret data through focused research on rapid DNA analysis, mixture interpretation, development of novel genetic markers, validation studies of new instrumentation and forensic genetic test kits, and coordination of interlaboratory studies associated with measurement of genetic data. The scientists support the division's mission by improving the legacy standard reference materials to include new genetic loci and systems. An area that could potentially use more expertise is the application of genomic techniques, particularly in the area of forensic investigative genetic genealogy, as this technology becomes increasingly accessible and moves into forensics laboratories. This expertise could be gained through collaboration with other NIST divisions supporting human genome science, especially the Biosystems and Biomaterials Division.

Clinical Analyses Using Protein and Nucleic Acid Markers

The research staff have the expertise to use a wide variety of analytical methods to evaluate protein and nucleic acid biomarkers. The choice of problems on which the staff focus is largely driven by

their responsiveness to big companies or industry-government consortia, demonstrating that the staff are very responsive to national needs in biomanufacturing. The two standard methods for assessing albumin in urine (mentioned above) were developed in response to stakeholder requests. The same is true for the standards under development for diagnosing food allergens (a growing area). The development of standards for RNA identification from viruses of immediate concern (e.g., SARS-CoV-2 and Mpox) showed how fast and how well the staff can produce vital results, giving high credibility to their expertise. The exploration of methods for analyzing extracellular vesicles and nanoparticles is a developing area that will be extremely important in the future as these types of therapeutics are expanding rapidly. MML will be at the forefront of defining acceptable product metrics for use in vaccines, drug delivery, and regenerative medicine. The staff have the expertise and drive to conduct important applied research and early-stage development in this area, especially in separations as well as analytics.

Biotherapeutics, Biomanufacturing, and Engineering Biology

This team seems to be relatively new. They are just building their expertise base and could use more staff (as well as redeveloping the facilities in space available to the Biomolecular Measurement Division in the Institute for Bioscience and Biotechnology Research [IBBR]). Biotherapeutics is an important area for the U.S. economy, and the need for standard analytical methods during processing as well as for product validation is critical, especially analytics for use in-line during biomanufacturing processes. NIST is relying on its customers and the National Institute for Innovation in Manufacturing Biopharmaceuticals collaborators for technical expertise, which is good, but NIST needs to strengthen its in-house expertise to make a long-term impact in biomanufacturing.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

In fiscal year 2023 the budget of the Biomolecular Measurement Division was $36 million—61 percent of this comes from appropriations; 32 percent from providing standard reference materials and data and a working capital fund; and 7 percent from reimbursable work for other federal agencies.

All of the groups in the Biomolecular Measurement Division are generating tremendous amounts of data. They need more expert staff support in laboratory information management systems development and data management. While the mass spectrometry group includes these experts, as well as bioinformatics experts, the level of computational support was highly variable across the mission areas. The groups that rely on centralized support from information technology and data management experts received inconsistent support. More personnel to support the other groups would leverage their existing expertise and increase productivity.

The staff is very dedicated to their missions and invested in disseminating the products of their labors. The young federal staff members are especially enthusiastic about the opportunities they have for expanding their research endeavors and developing leadership skills. The postdocs enjoy what they are doing, and in many cases really appreciate the independence they have to focus on projects of their choosing, but some of them feel very isolated and uncertain about what future directions they could pursue after time at NIST. Mentoring of postdocs seems to be uneven, and postdocs in particular could benefit from a mentoring program that includes information about what constitutes short-term success in MML and long-term career development opportunities.

The support from the human resources office, especially in terms of replacing lost staff, could be significantly improved. Hiring new administrative staff is inordinately slow, taking up to 6 months just to release standard advertisements. Even when the jobs are posted and interviews conducted, instances were reported when the group has agreed to hire someone and the notification letter never went out from human resources to the prospective employee. Bringing postdocs on board can take months after they accept the offer and complete their PhD, during which time some of the new postdocs have no income. The procedure for hiring federal scientists and engineers was not clear. The availability of positions

related to MML programs and mission-focused areas seems to have been put on the back burner as human resources work priorities focus on hiring to support new work deriving from the CHIPS and Science Act of 2022. These problems will impact group productivity and need to be fixed.

Conclusion 5-1: The current staff is scientifically outstanding, but maintaining a critical mass of scientists and engineers with critical expertise is challenging. More timely support from the human resources department would make the projects more competitive and ease the frustrations of existing staff whose research progress is hampered by vacancies in administrative support, hiring of postdoctoral fellows, or staffing of existing mission areas. Postdocs could benefit from increased mentorship in terms of networking and career development.

Recommendation 5-1: The Biomolecular Measurement Division should work with the Material Measurement Laboratory (MML) leadership and the National Institute of Standards and Technology's headquarters human resources personnel to develop effective procedures for the hiring and career development of staff. Internally, MML should improve their mentorship of postdoctoral fellows to address career development planning.

In terms of facilities, Building 227 is old and outdated, but still functional. The air handling and plumbing systems are a particular problem. Building 221 appears to be an ongoing disaster and a calamity waiting to happen. Too much high-tech equipment is crowded into a space that is under-resourced in terms of air handling, electrical supply, and safety infrastructure. Facility upkeep by NIST maintenance workers appears to be an issue, especially with inadequate heating, ventilation, and air conditioning systems. The mass spectrometry equipment is considered state of the art and adequate for the projects being undertaken and to complete all of the tasks for stakeholders. However, temperature fluctuations already threaten the quality of the mass spectrometry data, which is critical for a key NIST product, the Mass Spectrometry Data Library. These mass spectrometry instruments are very sensitive to temperature changes; if the room temperature varies too much—e.g., between 68 to 85 degrees Fahrenheit—the mass spectrometers may produce erroneous results as the spectral peaks will be shifted. This can limit productivity for the group and will be an ever-present issue until remedied. The infrastructure problems in Building 221 have reached a critical stage; building 227 also needs upgraded heating, ventilation, and air conditioning systems. Funding for these types of major renovations needs to come from appropriated funds as the level of funding from overhead income is far from sufficient.

In contrast, space at IBBR is high quality. Moving the entire division to IBBR would solve its space problem, provide space in Building 227 for other NIST researchers (as well as present an opportunity for renovation), and encourage increased interactions with researchers from universities across Maryland who also work in IBBR. The space is currently available at IBBR and some funding to begin appropriate renovation in preparation for them to move in has already been identified.

Conclusion 5-2: Existing facilities do not support continued work at the world-class level. Facilities staff are fighting a losing battle trying to keep existing systems—especially the heating, ventilation, air conditioning, plumbing, and building integrity—operational. The research staff lose valuable time making ad hoc workarounds to facility shortcomings and are, at times, unable to operate and maintain high-tech equipment owing to maintenance issues. Facilities renovation is too expensive to be covered by internal Material Measurement Laboratory funding.

Recommendation 5-2: The Biomolecular Measurement Division (BMD) should work with Material Measurement Laboratory leadership and the National Institute of Standards and Technology to identify, as soon as possible, laboratory facilities with the level of temperature and humidity control, and space required by BMD to perform its work safely and at a world-class level. A move of BMD to the Institute for Bioscience and Biotechnology Research could be part of this solution.

While much of the equipment is aging, most of it is working well. There is some need for new instruments to integrate new capabilities into the analytical capabilities, for example, next-generation gene and protein sequencing systems. A definite need exists for more automation of contiguous separations and analytics to increase sample throughput. Dedicated funds for both equipment and expertise in laboratory robotics would benefit multiple operations and improve the efficiency of long-term data output.

Conclusion 5-3: Much of the work in the Biomolecular Measurement Division is repetitive and highly amenable to automation. With the introduction of appropriate robotic systems and expertise, the existing staff could be even more productive. Automation is used throughout the stakeholders' labs. Increased automation within the division would also enable the Material Measurement Laboratory to provide guidance on automated processes to its stakeholders.

Recommendation 5-3: The Biomolecular Measurement Division should increase laboratory automation to support critical steps in production of standard products and processes.

EFFECTIVENESS OF DISSEMINATION EFFORTS

The Biomolecular Measurement Division disseminates its results in multiple ways: research publications, conference presentations, round-robin trials with customers, workshops, staff participation in standards groups, and the production of standard products—both the well-characterized standard reference materials for which NIST is well known and now research-grade standards. The inclusion of the mass spectrometry libraries with commercial mass spectrometers, as well as triannual updates, is very broadly valued across academia and industry. The active participation of the Applied Genetics Group staff in the forensic standards-setting organizations—Scientific Working Group on DNA Analysis Methods and the Organization of Scientific Area Committees for Forensic Science—as well as the dissemination of peer-reviewed publications is vital to forensic stakeholders as they present scientific evidence to the courts. The extent to which NIST documentation is viewed as a source of unbiased validation of current and emerging instrumentation, protocols, and data interpretation algorithms by the U.S. legal process is noteworthy.

Across all four of its focus areas, the Biomolecular Measurement Division has strong interactions with users and manufacturers. This two-way interchange disseminates the value and results of NIST's work and has produced a good understanding of the value chain for potential standards products. Even junior staff are encouraged to take on leadership responsibilities in working with consortia of stakeholders and do so very effectively. There is a limit to how extensive such operations can be, since there are limits on staff and funding, but the choices of where to focus the division's energies and resources are thoughtful and effective in terms of the opportunities for the Biomolecular Measurement Division to have a real impact for its customers. As the United States puts more resources into biomanufacturing, this would be a logical area for expansion.

The involvement of the Biomolecular Measurement Division with commercial partners is consistent with MML's mission to support the national economy with measurement science and technologies. The delivery of standards is one good metric of the division's impact on the commercial sector and clinical practice (as described above for proteins, genes, and viruses), but the division is doing much more. There are two areas of additional Biomolecular Measurement Division activity that merit increased support: the dissemination of products to the educational sector involved in workforce development (activities in this area have begun largely through participation in the National Institute for Innovation in Manufacturing Biopharmaceuticals and educational partnerships at IBBR) and providing information to researchers on the potential advantages of using NIST standards across research endeavors

(e.g., the use of the albumin standard reference materials as calibration material for proteomic researchers using mass spectrometry).

Conclusion 5-4: The current dissemination of research and development and standards to traditional stakeholders is very effective. Products recently developed for biomanufacturing and forensics can be extremely impactful in multiple communities, including some that are less aware of these standards and processes. The dissemination of standard reference materials made by the Biomolecular Measurement Division and the documentation of processes for dissemination to both the education community that is critical for workforce development and the forensics legal community could be highly impactful.

Recommendation 5-4: The Biomolecular Measurement Division (BMD) should increase engagement with communities focused on workforce development and forensics analysis, and compile data on how often their resource materials are used. For biomanufacturing workforce development activities, instructional information related to using BMD standards and standard processes could be provided to educational and professional groups providing training for biomanufacturing. Dissemination of information about how often BMD's published validation studies, research findings, and standard reference materials are used by the stakeholders in forensic activities could increase the appreciation of the value they provide to the legal community.

6
Chemical Sciences Division

The general objective of the Chemical Sciences Division is to provide measurement services, which encompasses standard reference data and computational tools, reference measurement procedures, quality assurance programs, and a wide range of reference materials (e.g., standard reference materials). This includes several databases and codes that are maintained and curated by the division. Over the past 8 years, the division has accommodated more than 4,500 technical inquiries related to standard reference materials, which originated from all fifty states, and 96 countries. Two additional areas with more restricted scope but a high level of significance include a standard reference photometer for ozone calibration, and the calibration of ozone and mercury vapor generators. Of the more than 1,000 standard reference materials generated and maintained by the National Institute of Standards and Technology (NIST), the Chemical Sciences Division is responsible for 76 percent of them, and handles 56 percent of the 29,000 standard reference material units sold annually. The large numbers of standard reference materials that are handled by the division are indicative of the importance of the NIST reference materials program, particularly within Chemical Sciences Division, whose leadership accurately describes the reference materials as indispensable core services to industry.

The motivation behind these activities is the need for regulatory rigor that is stipulated by legislation and by industry, which needs accurate measurement in order to be competitive. The work of the Chemical Sciences Division can be broadly divided into two categories: the production of standard reference materials and data, and research and development of new measurement methods and technologies. The production and research and development activities occurring within the Chemical Sciences Division is also motivated by the need to ensure the safety of food and pharmaceutical products.

The Chemical Sciences Division organization consists of 135 scientists and technicians, parsed into eight research groups. The organization has not appreciably changed compared to the past assessment, which was conducted in 2020. The panel believes that the fact that the organizational structure of the division has not changed is indicative that it is well organized to address its numerous functions and missions. The research groups are: Inorganic Chemical Metrology, Organic Chemical Metrology, Gas Sensing Metrology, Chemical Informatics, Chemical Process and Nuclear Measurements, Biospecimen Science, Optical Measurements, and Biochemical and Exposure Science.

The majority of the Chemical Sciences Division is situated at the Gaithersburg, Maryland, campus of NIST. There are, however, significant facilities at the Hollings Marine Laboratory (in partnership with the National Oceanic and Atmospheric Administration [NOAA]), the Center for Marine Debris Research (together with Hawaii Pacific University), and the NIST Synchrotron Science Group (at Brookhaven National Laboratory).

ASSESSMENT OF TECHNICAL PROGRAMS

The research conducted by the staff of the Chemical Sciences Division is of consistently high quality, at least as good as that done by other institutions in the United States and worldwide, and, in some cases, better. The uniqueness of the division's missions and research, and the diverse range of the measurement science conducted, make a direct comparison with other institutions difficult. The division's work is driven by stakeholder needs and industrial and academic stakeholders make extensive use of the

reference data, standard reference materials, measurement protocols, and instrumentation produced or curated by the division. The division actively benchmarks its work against other leading international metrology institutes to ensure the quality of its work. The breadth of the division's work is challenging, but it has been able to achieve accuracy and precision in metrology that enable industry and other research institutions to conduct their functions.

Accomplishments

Inorganic Chemical Metrology Group

The Inorganic Chemical Metrology Group provides a wide range of measurement services that encompass reference measurement procedures, quality assurance programs, and reference materials. A particularly noteworthy example of the group's activities is the work of the ozone measurement group, which is an excellent example of a unique, long-term research program that enables accurate ozone measurement by domestic and international extramural research groups. The group fabricates ozone generators coupled with spectrophotometers that enable calibration of secondary instruments. A network of 12 standard reference photometers is maintained, and 64 of these instruments have been deployed worldwide. It is worthwhile noting that this level of demand is insufficient for an instrument manufacturer to enter the market, however, the environmental community is dependent on these devices for ozone calibration (note that the Central Calibration Laboratory for ozone resides in the Gas Sensing Group). The research enables specification of National Ambient Air Quality Standards for ozone. Ozone measurement performance is benchmarked versus the Bureau International des Poids et Mesures, which is an international standards organization. The production of standard reference materials for air toxics, notably mercury, is also notable.

Organic Chemical Metrology

The Organic Chemical Metrology Group is focused on providing primary standard reference materials, quality assurance programs, and reference methods and tools that are critical for maintaining quality for food and nutrition products, clinical diagnostics, natural products, dietary supplements, environmental contaminants, and forensics. The group leverages its research via collaborations with other federal agencies like the Environmental Protection Agency, Federal Bureau of Investigation, U.S. Department of Agriculture, Food and Drug Administration, Centers for Disease Control and Prevention, National Institutes of Health, and a large number of non-governmental organizations that participate in the group's quality assurance programs. A key objective is to enable stakeholders to make accurate chemical measurements that are needed for label requirements, regulatory limits, and product quality.

The production of creatinine standards in frozen human serum affords an impactful example, owing to the critical need for these standards by clinical and academic laboratories and manufacturers of in vitro diagnostic devices. This is important because creatinine concentration is an indicator of kidney function. Another noteworthy example is the generation of standard reference materials for perfluoro and polyfluoroalkyl substances (PFAS) which are critical for accurate measurement in environmental and biological samples. PFAS are important because they have been linked to adverse health effects involving metabolism, fertility, fetal growth, cancers, and immune system function and are a huge emerging pollutant problem for the United States (Fenton et al. 2021). The division also operates a cannabis laboratory, which is becoming increasingly important as more states legalize the drug.

Chemical Informatics Group

The Chemical Informatics Group's objective is to use computational tools to study complex systems such as fluid behavior and CO_2 adsorption. The group also maintains stable isotope and trace

element databases, and a library of materials, both of which are accessible to stakeholders with interests in food safety and environmental chemistry.

This group has demonstrated computational methods that could enable future collaboration with bench scientists, directly supporting experimental work. For example, the group has compiled libraries of X-ray absorption near-edge spectroscopy data for arsenic analysis, which directly support food safety. Research in organizing and comparing two-dimensional nuclear magnetic resonance data generated from monoclonal antibody characterization enables differentiation of oxidized samples, a significant contribution because of the importance of monoclonal antibody standards. Libraries of prompt gamma activation analysis spectra facilitate identification of a wide range of materials including coal and coke, oils, concrete, and forensic glass samples.

Molecular simulation and computation research including the Free Energy and Advanced Sampling Simulation Toolkit is an example of deploying a simulation capability to the extramural user community, which has resulted in impact that extends beyond NIST researchers. Simulations of monoclonal antibody solutions for the purpose of predicting physical properties are noteworthy, given that monoclonal antibody-based products account for 5 of the 10 top pharmaceuticals worldwide. The NIST Adsorption Database is also curated by the Chemical Informatics Group, which is applicable to CO_2 capture and adsorption modeling that supports the climate strategic focus.

Gas Sensing Metrology Group

The objectives of the Gas Sensing Metrology Group are to (1) certify and disseminate gaseous standard reference materials, and (2) provide high quality SI-traceable gas measurements. The research conducted by this group provides benchmarks important for compliance with U.S. and state regulations related to environmental regulation, climate change issues, and fair trade issues. They are responsible for 68 standard reference materials, and the NIST Traceable Reference Material Program for Gas Standards.

The group provides ozone, mercury, and monoterpene gas reference materials. These activities are motivated by a number of domestic stakeholders that include the Environmental Protection Agency, the California Air Resource Board, NOAA, the National Aeronautics and Space Administration, and the U.S. specialty gas industry. A notable research emphasis is the development of a breath biomarker reference material, which has the potential to benefit both forensic and medical applications. Research to quantify CO_2 adsorption to cylinder walls holds the potential to further improve accuracy.

Chemical Process and Nuclear Methods Group

The objective of the Chemical Process and Nuclear Methods Group is to provide metrology of chemical and physical transformations, with specific emphasis in heterogeneous catalysis, particle metrology, CO_2 removal and conversion, and elemental analysis using neutron activation conducted by the NIST Synchrotron Science Group, located at Brookhaven National Laboratory and part of MML's Materials Science and Engineering Division. The Chemical Process and Nuclear Methods Group's research emphasizes measurement of rate constants for atmospherically relevant reactions, CO_2 conversion reactions on surfaces, and the advancement of the measurement science of nanoplastics in water. The neutron activation research focuses on characterizing standard reference materials, specifically glass standard reference materials needed by the forensic science community. However, the reactor was shut down in 2021 following an incident and was back up to full operation at the time this report was drafted.

Optical Measurements Group

The Optical Measurements Group is focused on developing optical measurement methods with the intent to maintain the SI traceability of field instruments used by practitioners. The group's research

emphasizes remote sensing of natural and anthropogenic species, emission monitoring, carbon cycle research, and atmospheric radiative transfer. Experimentally, the group pursues development of an ensemble of advanced laser-based spectroscopic measurement techniques. An overarching goal is to improve greenhouse gas sensing by removing physical artifacts and complex calibration chains.

Applications include SI-traceable isotopic ratios, specifically $^{13}C/^{12}C$ ratios of standard reference materials, and development of calibration-free $^{14}CO_2$ concentration using bench-top cavity ringdown spectroscopy instrumentation. These techniques may be relevant to future regulations and are currently being used by industry stakeholders to verify claims of sustainable or "green" carbon sourcing. Methane emissions monitoring is also an area of significant research.

Biospecimen Science Group

Another important research capability is the NIST Biorepository and Cryogenic Reference Material Production Facility, which is situated in the Hollings Marine Laboratory and staffed by the Biospecimen Science Group. The group develops methods for generating cryogenic standard reference materials, and approaches for preserving those standards using advanced cryogenic storage technology to ensure stability and reproducibility. The standard reference materials support food quality and safety, and also environmental protection activities. The group is unique in its expertise, and standard curation capability and has unique laboratory capabilities.

Biochemical and Exposure Sciences Group

The Biochemical and Exposure Sciences Group maintains a capability both at the Hollings Marine Laboratory in Charleston, South Carolina, and at the Center for Marine Debris Research in Oahu, Hawaii. The Biological Responses subgroup, at the Hollings Marine Laboratory, is focused on understanding proteomic and metabolomic responses, a subject of interest to both governmental and industrial stakeholders. Challenges in the "omics" areas are the lack of standard reference materials for many proteins and metabolites that are important for identifying environmentally induced alterations in proteins and metabolites. This group is developing standard reference materials that are related to human health, including blood, urine, liver, and stool materials. Along with the standard reference materials, the omics groups are developing best practices for reporting proteomic and metabolomic responses.

The Plastic Pollution Measurements group is situated at the Hawaii Pacific University Center for Marine Debris Research. This group is involved with characterizing the growing volume of waste plastics in the oceans, emphasizing characterization of plastic micro- and nanoparticles. The group works to standardize measurement methods, and to produce plastics reference materials. These efforts enable identification of derelict fishing gear and monitoring plastics ingestion in seabirds, turtles, and fish. The group has cultivated a large number of academic, other government, and industrial partners with its research of polymer weathering, along with microplastics fate and transport.

Challenges and Opportunities

The following items represent opportunities to improve the quality of the technical programs and the ability of the organization to reach its stated technical objectives.

Safety

Several safety-related challenges were noted that are rooted in communication, facilities, and funding issues. Issues derived from facility problems are noted below in the "Budget, Facilities, Equipment, and Human Resources" section. There are several actions that would positively bear on the

Chemical Sciences Division's safety posture. Placing placards outside of each laboratory specifying the laboratory's hazards and the required safety behaviors and personal protective equipment requirements would increase safety visibility. Facility issues such as roof leaks, and equipment shortcomings, are increasing safety hazards. While some of these issues are intractable to MML because they are addressed by other parts of NIST, any efforts that MML can make, such as with gas sensors and alarms, would improve the situation. Another step that could improve the safety environment would be to collaborate with MML's industrial partners to help strengthen MML's safety program with things like root cause investigations and a near miss database.

Static Resources and the Increasing Demand for Standard Reference Materials

The development of new standard reference materials relies on the same staff, instrumentation, and facility resources that are needed for maintaining existing standard reference materials, resulting in difficulty in meeting the needs of both activities. The consequence is that staff members are oversubscribed. There may be opportunities to clarify prioritization of activities in order to balance incoming requests for new standard reference materials with maintenance of existing standard reference materials.

The pricing of the standard reference materials in some cases may not be commensurate with the cost of starting materials, instrumentation, and PhD staff time that are needed for production and technical support. Funding challenges result in a need to emphasize standard reference material production, which generates a revenue stream. However, production of existing standard reference materials impedes development of new standard reference materials that will be needed in the future. Working with the Office of Reference Materials to appropriately price materials may alleviate some prioritization conflicts.

Workflow Modernization

Workflow modernization could have a huge impact on the organizational resources and technical delivery on program objectives. More efficient, digitally enabled work processes could free significant time for staff to address new research. This is especially true considering that production of standard reference materials follows standard and repeatable workflows, making them a straightforward choice for data automation.

The committee noted success in the Biochemical and Exposure Sciences Group with a staff member whose research interests migrated into the data science and engineering space to build the "data plumbing" for the high-volume omics labs. It was indicated that this staff member is doing a rotation in the Office of Data and Informatics as a part of a rotational effort to transfer data engineering skills and culture throughout MML as well as showcasing the value of data engineering to the organization. Replicating the success of the Biochemical and Exposure Sciences Group "data plumbing" effort may well improve staff productivity and increase data stewardship skills across the Chemical Sciences Division.

NIST Center for Neutron Research Shut Down

An ongoing challenge is that the nuclear reactor that provides the neutron beamlines for the NIST Center for Neutron Research has not been available for research since February 2021. It was shut down following an incident in the reactor. It was restarted in March 2023, and is operating at low power for testing and training. However, the center plans to shut it down again in 2024 to upgrade the reactor.

Data and Chemical Informatics Group Alignment

The alignment of the Data and Chemical Informatics Group with the other Chemical Sciences Division groups having more direct program objectives (e.g., those delivering metrology expertise or standard reference materials, and standard reference data) is somewhat obscure. A closer alignment of the group with the bench chemists, who have clear alignment to program objectives, may be beneficial. A clearer understanding of whether the Data and Chemical Informatics Group is meant to support NIST metrology research or outside research is needed to appropriately manage the group's portfolio.

Another potentially valuable function of the Data and Chemical Informatics Group would be to act as a focal point for Chemical Sciences Division-generated data, that could enable strategic development of data infrastructure in support of the on-going program areas. Prior MML assessment reports recommended increasing staff training to build a culture of "data as an asset," but it does not appear that much progress has been made. In alignment with the leadership directive that the Data and Chemical Informatics group is to prioritize the support of MML researchers, implementing improved data extraction, transform, and load practices could be a very impactful activity. Note many researchers do not understand the value that the modeling team could bring to a program.

Conclusion 6-1: Enhanced benefits from the Data and Chemical Informatics Group may be realized by reviewing its alignment with the missions and objectives found in other areas of the Chemical Sciences Division. Clear delineation of intramural collaborative research versus independent research efforts may help clarify management of the group's research portfolio. Further benefit could emerge from a more intentional communication of the capabilities and functions of the Data and Chemical Informatics Group to the broader Chemical Sciences Division and Material Measurement Laboratory community.

ASSESSMENT OF SCIENTIFIC EXPERTISE

Accomplishments

In many of the research areas being pursued within the Chemical Sciences Division, the scientific expertise of the staff is on a par or better than other laboratories, either domestic or internationally. Frequently, the division's staff constitute a nearly singular repository of expertise in several technical areas, that is, other research institutions rely on expertise within the Chemical Sciences Division, and accordingly have not replicated it. Generally, the division's scientific expertise is finely tuned to its technical programs.

An example of staff expertise is found in the group conducting primary ozone measurement and instrumentation fabrication for national metrology institutes across the globe. Additionally, Chemical Sciences Division expertise was recognized and called on by NOAA to generate marine samples and called on by ASTM International[1] to develop methods for measuring CO_2 in concrete. The division's scientific expertise is strengthened by ongoing interactions with Bureau International des Poids et Mesures and other national metrology institutes. This ensures and builds the credibility of the Chemical Sciences Division staff among peer organizations worldwide. The panel endorses these interactions and continuing opportunities to maintain engagement with these organizations (i.e., support interactions, provide time for leadership roles, and travel support).

The publication rate of the Chemical Sciences Division staff is appropriate for the size of the organization, as noted in the "Effective of Dissemination Efforts" section.

The extremely broad scope of the Chemical Sciences Division's technical programs require expertise and capability across many subdisciplines, which presents a staffing challenge for the division.

[1] Formerly known as the American Society for Testing and Materials.

This challenge can be addressed by intramural collaboration (i.e., with other MML groups), and by identifying extramural collaborators to fill gaps in expertise critical to an application area. The committee observed that the Chemical Sciences Division is adept at implementing this collaborative approach. An example of such an extramural collaboration partnership involved the need to develop methods for the improved microanalysis of glass, which emerged from the forensics community. The Chemical Sciences Division combined its in-house expertise in neutron activation analysis with fabrication expertise at Corning Glass to produce unique glass standards that have been used to calibrate instrumentation at local forensics laboratories, of sufficient quality to be admissible to courts of law.

Challenges and Opportunities

In multiple areas, the demand for standard reference materials and standard reference data is so great that staff lack the time to pursue improvements in production efficiency, measurement capabilities, or research. The Chemical Sciences Division leadership noted that the maintenance of hundreds of standard reference materials and measurement services results in "far too many tasks for too few staff," an assertion backed by observations. The situation would normally motivate addition of new scientist- and technician-level staff; however, this solution is not easily implemented on account of budget constraints noted below. Without such changes, the ability of Chemical Sciences Division staff to remain ahead of the metrology needs of industry and provide timely research and materials may be compromised. The division has responded by cross training staff, which helps address staff redundancy vulnerability, but this is unlikely to overcome growing research capacity limitations.

> Finding 6-1: The broad range of standard reference materials and standard reference data products, and the high volume of demand for those products, is close to exceeding the capacity of the staff to meet those demands. This leads to an over-extended span of research and lack of functional redundancy for many of the activities the staff undertake.

> **Recommendation 6-1: The Chemical Sciences Division should look for ways to add new scientist- and technician-level staff to continue to service the existing array of standard reference materials and free up staff resources to pursue development of new standard reference materials. In addition, the division should continue to emphasize staff cross training to ensure functional redundancy. The Chemical Sciences Division should continue to prioritize internal and external collaboration as a solution to maintaining the significant breadth and depth of expertise.**

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

In fiscal year 2023 the Chemical Sciences Division's budget was $35.561 million, comprising $23, 402 million from appropriations, $3.645 million from reimbursable work for other federal agencies, and $8.514 million from services such as providing standard reference materials and a working capital fund. It has 134 staff, comprising 94 scientists, 4 technicians, 6 support staff, and 30 associates.

Accomplishments

Chemical Sciences Division staff are enthusiastic, well informed in their metrology subdisciplines, and passionate about NIST's purpose. These observations were manifest in a high level of motivation toward further the metrology research and a remarkable customer service attitude. Work was always clearly aligned to a valued motivation that they could clearly articulate.

Staff displayed the ability to quickly pivot to respond to emergent urgent needs aligned with their expertise (e.g., Mpox [see below] and PFAS). This was reported to be exciting and motivating to the

researchers, although these activities did put pressure on standard reference material production which often fell behind schedule as a result of responding to emergent needs.

The Chemical Sciences Division's support of NIST's diversity and inclusion principles is evidenced by things such as when the Biospecimen Science Group worked with local indigenous groups in Alaska and the Pacific Islands to gather samples in accordance with cultural guidelines.

Challenges and Opportunities

Budget

The essentially flat MML budget has challenged the organization in program execution. Increasing labor costs resulting from merit and cost of living adjustments increase the fraction of the budget allocated for labor, and decrease the fraction of the budget available for instrument refreshment and repair, and facility maintenance and modification. In addition, budgetary constraints limit the ability of Chemical Sciences Division leadership to hire staff and, in the longer term, to conduct significant succession planning.

Insufficient funding has impacted the capabilities needed to advance many of the different required technologies for existing MML missions and newer research areas like omics, chip manufacturing, biomaterials, PFAS, and microplastics. This problem was particularly apparent in the Inorganic Chemical Metrology Group, which relies on funding from sales of reference materials, requiring the group to prioritize standard reference material production and thus limiting the ability of the group to address new challenges.

It was noted that efforts on Mpox characterization were not explicitly funded, but nevertheless were required as part of the Chemical Sciences Division's research scope. The division addressed the problem by moving resources and funding from other programs to the Mpox effort, which is unlikely to be a sustainable long-term approach.

> Finding 6-2: Static funding levels have adversely impacted the ability of the Chemical Sciences Division to execute its mission owing to three factors: staff, whose costs have increased as a result of cost-of-living increases; instrument maintenance and refresh; and facility upkeep. Mission sustainability at current funding levels is likely to be problematic.

Staff—Span of Control and Adjustment to New Work Norms

The Chemical Sciences Division's PhD staff are heavily involved with and sometimes entirely responsible for operational production of standard reference materials and other samples. These operations activities, both sample production and continued technical service to customers, preclude their ability to conduct research, outreach, and global leadership activities.

These challenges are consistent with the decrease in numbers of staff; as of the writing of this report in 2023, the Chemical Sciences Division had 135 staff members, which is a 20 percent decrease compared to 2020, when there were 170. The staff includes 35 associates, which consist of guest researchers from industry and academia, postdoctoral fellows, and students. Within the division, the fraction of associates appeared to be less than that for MML overall. A specific example is provided by the Organic Chemical Metrology Group, which is challenged by the need for additional staff; in several important program functions, the group relies on a single staff member. Two examples of research that was deprioritized because of the demands of standard reference material production include the development of a standard reference material for CO_2 in seawater, and a breath standard of volatile organic compounds for medical diagnostics.

The limited staffing does not just affect the ability of the Chemical Sciences Division to conduct new research. In some cases, even production of mission-critical standard reference materials and other

samples is conducted by a single individual or using a single instrument. This presents a significant risk to the ability of the division to fulfill its current mission. The real-world commercial implications of this risk cannot be underestimated.

In a second illustrative example of razor thin staffing, a single staff researcher oversees the standards that enable quality assurance testing of infant formula for essentially all of the western world. Without these standards, industry suppliers cannot safely release infant formula to the public. Those efforts are in direct competition with responsiveness needed for the development of methods and standards for PFAS in food. Both of these high-profile high-importance endeavors rely on a single expert on staff with the skills to work on both areas. Additionally, the Gas Sensing Metrology Group previously had 4–5 people who were trained and skilled in making gas standards; now there is a single expert to complete this production. The commerce that depends on NIST would be adversely impacted by a supply shock caused by certification requirements, which are in turn dependent on NIST standards and methods that are reliant on a very small number of NIST staff.

Staff—Rebalancing

There may be opportunities for rebalancing staff so that technician-level personnel are conducting the bulk of the operational standard reference material production, which has the potential to improve cost efficiency, and would provide opportunities for the PhD staff to expand research and development activities. Cross-training of personnel and replication of unique facilities together with instrument investments could result in a more resilient and sustainable supply of standard reference materials, standard reference data, and other critical products.

Demands on the staff are exacerbated by the fact that National Research Council postdoctoral classes are shrinking, although this may be a transient phenomenon related to the COVID-19 pandemic that will rectify once MML staff are able to resume attendance at scientific meetings.

Another challenge is posed by the fact that some skill sets cannot be recruited. For example, metrology, standard reference materials, and standard reference data research are relatively unique to NIST and need to be taught to new NIST staff once onboard. This requires duplicating staff for some functions and teaching new staff unique skills; however, the budgetary constraints are not compatible with this approach.

Negotiating the new work environment may be challenging as a result of the need to achieve balance between the need to bring staff back to campus for certain types of work, reconditioning workspaces, and establishing a hybrid environment that encompasses both in-person work and telework.

Lastly, in the culture of the laboratory, standard reference material and standard reference data production operations have not historically been esteemed as highly as have the more basic measurement research and development activities, in part because the latter present more opportunity for publications and patents. However, there has been a noteworthy evolution in culture regarding the perceived hierarchy between standard reference material production and research within Chemical Sciences Division. The two objectives are now viewed as having more equal importance, as indicated by discussions with early career staff. Chemical Sciences Division leadership noted that promotion criteria were adjusted to reflect the equal importance of the two objectives. In addition to recognition, both production and research staff indicated a comparable sense of purpose and value. Maintaining this progress will be even more important if Recommendation 6-1 is pursued.

Instrumentation—Maintaining and Augmenting State of the Art

The ability of the staff to execute Chemical Sciences Division missions is increasingly impacted by dated instrumentation, which results from advances in the state of the art of instrumentation leaving current generations behind, and difficulties stemming from instrument upkeep. The committee observed several instances where instrument control and data acquisition were performed by computers using

operating systems that are no longer supported. This poses a risk to research functions that are relying on the outdated equipment, and likely poses barriers to the data availability across the Chemical Sciences Division. A specific example was the rebuild of an instrument that provides the certified measurements for the pH standards. The rebuild took 1.5 years, in part because the instrument was being operated using a year 2000-vintage computer, and exacerbated by the lack of staffing in the laboratory. The consequence was significant inefficiency owing to an instrument that needs to be replaced rather than repaired.

A second notable example of dated instruments is the nuclear magnetic resonance, mass, and optical spectrometers that are heavily relied on by the Organic Chemical Metrology group. Several instruments are no longer cutting edge, which will eventually erode the ability of the group in making state-of-the-art measurements. State-of-the-art analytical instrumentation is also an ongoing need for the Biochemical and Exposure Science Group focused on Chemical Metrology for Omics.

The problems are exacerbated by difficulty refreshing instrumentation, which is related to the high cost of investment in cutting-edge scientific equipment and maintenance. The staff noted that these problems are also aggravated by the business processes at NIST, particularly a slow and cumbersome procurement process.

Like most laboratory institutions that house state-of-the-art instrumentation, there is a historical culture of individual ownership of high-end equipment. This is understandable since it is desirable to have a single point of contact for cutting-edge spectrometers and microscopes. However, productivity can be impeded by an "ownership" culture that is uncomfortable with sharing facilities. The division is working on instilling a philosophy of broad access to instrumentation and facilities while ensuring their proper operation and maintenance.

All of the challenges discussed above will be exacerbated as competition between the needs of the existing program portfolio and scope of anticipated new work emerging from the CHIPS and Science Act of 2022.

Facilities

Chemical Sciences Division leadership noted an ongoing need for more laboratory space, an observation consistent with the division's increasing scope of research. Lack of space availability constrains efforts to expand the division's scope of work in research and standards. This is true both in Gaithersburg and in the Hollings Laboratory. The Biospecimen Science Group in particular is challenged by constraints on availability of storage space for its biorepository. All of the laboratory areas that were toured were fully used and did not have the capacity to readily take on more work. Creative approaches for increasing laboratory space may be needed.

The division's leadership noted that problems with the physical laboratory facility continue to adversely affect the ability of the staff to successfully execute their diverse missions. Specifically mentioned were environmental controls, and areas where the roof is leaking. Facility repairs and renovations are slow and expensive. Aging laboratory facilities are continuing to display points of failure, which in some instances is impacting production and research activities.

In several instances the degradation and disrepair of laboratory facilities have led to the potential for compromised safety. For example, the oxygen depletion sensor in the gas sensing laboratory has not functioned for multiple years; the staff creatively installed a work-around system which does alarm locally in the event of an uncontrolled gas release. However, the work-around system doesn't notify site security. A second example is in the cylinder storage room, which has a ceiling leak that has persisted for several years, causing valves to corrode and covers to stick on the gas cylinders. Potential safety hazards include gas leaks and upset cylinders resulting from the need for augmented force to overcome cap and valve seizure resulting from corrosion. The problem also has the potential to destroy inventory and invalidate calibrations.

The information gathering for this assessment concluded that NIST's buildings and infrastructure are outdated, to the extent that a normal level of maintenance is inadequate to keep facilities functional.

Problems with facilities are exerting a negative impact on the ability of staff to meet mission objectives. In addition, the inventory of critical standard reference materials is put at risk by facilities conditions that compromise their quality. When analytical measurements require controlled temperature and humidity, generation of valid measurement data can be compromised, resulting in significant delays in projects.

Laboratory procurement processes were cited by staff as an administrative impediment. A specific example involved the procurement of creatinine, a required ingredient in at least two standard reference materials (creatinine, and creatinine in frozen human serum) that are prepared up to 3 years in advance of anticipated inventory depletion. Lack of administrative support staff for purchasing necessitated involvement of scientific staff. The combination of a slow procurement process and a bad lot of creatinine from a supplier resulted in the inventory of the standard reference material being exhausted, with subsequent complaints from industry customers. The problem impacted both industry stakeholders and the research agenda of the scientific staff.

EFFECTIVENESS OF DISSEMINATION EFFORTS

Accomplishments

The Chemical Sciences Division uses a variety of approaches for disseminating information and technology transfer. The committee believes that with regards to the stakeholders, the dissemination approaches are effective. The Chemical Sciences Division leadership is keenly attuned to the use of the division's products and employs a number of measurement and modeling tools that enable evaluation of the accuracy and precision of standard reference data, and the fidelity of standard reference materials. The division aggressively monitors analytical performance in the measurement of component concentrations in gas mixtures, organic, and inorganic species in many matrices. Accuracy and precision are compared with results from a number of other national metrology institutes. These comparisons provide invaluable benchmarking, a basis for confidence in the standard reference material and standard reference data products NIST generates.

Publications

As noted above, the publication rate of the Chemical Sciences Division staff is appropriate for the size of the organization. From the beginning of 2022 through approximately the midpoint of 2023, the Division generated 97 publications and 242 conference or seminar publications. This level of productivity is noteworthy given that research and the resulting publications must be balanced together with the production of data, standards, materials, and quality control programs that the division also produces.

The Chemical Sciences Division provides excellent support for publication opportunities to maintain and enhance reputation of the staff and the Division, to disseminate information products, and to build staff expertise, particularly among more junior staff members and postdocs. It is very important that this support be continued.

Outreach

The Chemical Sciences Division exhibits good support for staff outreach activities to the technical community, which is impactful for communicating data and standards products to the stakeholder communities, and to anticipate future needs. Examples include conference attendance—which had been on hold during the pandemic but is now becoming a routine activity for the scientific staff—and organizing workshops, specifically for planning and coordination. Other activities might be described as workforce building efforts, which involves training of regulatory employees. Another commendable observation is the Biospecimen Science Group report on best practices for biobanking. These actions increase the impact of each research project.

A noteworthy example is seen in the gas sensing group, which is pursuing transfer of some standards productions out of NIST to the specialty gas industry. This action would diversify the supply of these standard reference materials and would reduce the need for their production within the Chemical Sciences Division. If successful, the transfer process will be a model for moving the production of other standard reference materials from the Chemical Sciences Division to outside stakeholders, which would free up staff and facilities needed for generating new data and standard reference materials. Similarly, the Biochemical and Exposure Science Group on Oahu has a strong partnership with Hawaii Pacific University, which serves as a vetted recipient for Chemical Sciences Division technology once development is complete.

Chemical Sciences Division support for industry workshops serves as an effective dissemination strategy. For example, staff from the neutron activation group led several workshops per year and initiated a strong collaboration with NAATBatt, an international battery manufacturer organization. These and other forms of industry engagement are critical to support NIST's mission by listening well enough to anticipate the measurement needs of the future.

Challenges and Opportunities

Universities and other government agencies accounted for well over half of the Chemical Sciences Division collaborations featured by leadership during the assessment, suggesting that research originating from industry is funneled through academic and government entities. This could mean that in many cases, MML may be one layer removed from direct industry partners, which could impede its understanding of and alignment with stakeholder needs, limit Chemical Sciences Division's ability to transfer standard reference material production out to industry and obscure the size of Chemical Sciences Division's impact on industrial commercialization organizations. If possible, more direct partnerships with industry could provide better visibility into the needs of industry stakeholders and increase Chemical Sciences Division's impact.

Research in the application of machine learning to Chemical Sciences Division's work is highlighted in its publications. However, it is unclear how this research is generalized to platform-level tools, and how it is more broadly promoted. An example is the Free Energy and Advanced Sampling Simulation Toolkit for Monte Carlo simulations, which is recognized by industry. The socialization of this toolkit could serve as a template for how to make software products more broadly available.

There is an opportunity for expanding the use of impact metrics, to both advocate for MML as well as recognize achievements of their staff. Several leaders noted that depending on where a standard reference material falls in the supply chain, it may have few sales but high significance (e.g., a standard reference material that has low demand, but is critical for maintaining accurate measurement for pharmaceutical or food products).

REFERENCE

Fenton, S.E., A. Ducatman, A. Boobis, et al. 2021. "Per- and Polyfluoroalkyl Substance Toxicity and Human Health Review: Current State of Knowledge and Strategies for Informing Future Research." *Environmental Toxicology and Chemistry* 40(3):606–630.

7
Materials Measurement Science Division

The mission of the Materials Measurement Science Division is to strengthen the personal safety of American consumers and the economic security of the nation. The division develops purposeful solutions to critical, uniquely challenging materials science problems. It leverages an inspired and diverse workforce to conduct rigorous metrology-focused research.

The division is organized into nine groups: the division office and eight technical groups, which are structured around scientific, engineering, and programmatic expertise. The nine groups are the Materials Measurement Science Division headquarters, the Microscopy and Microanalysis Research Group, the Nano Materials Research Group, the Data and Artificial Intelligence-Driven Materials Science Group, the Surface and Trace Chemical Analysis Group, the Synchrotron Science Group, the Materials Structure and Data Group, the Nanomechanical Properties Group, and the Security Technologies Group.

Collaboration between groups is common and often required to fulfill the division's mission, reach program milestones, and address stakeholder needs. Furthermore, based on the panel's observations, at least two of the groups function as central capabilities, leveraged by a wide range of programs: the Data and Artificial Intelligence-Driven Materials Science Group and the Synchrotron Science Group.

In addition to the formal group structure, the Materials Measurement Science Division has identified a range of core competencies and capabilities. While an explicit mapping of the core competencies and capabilities to the groups was not discussed, it appears that some of the core competencies and capabilities have a center of mass in a particular group, while others span a wide range of groups.

The division's research portfolio is organized into six focus areas, each with distinct goals:

1. *Safety and Security*—to deliver test methods, measurements, and standards to various stakeholder communities for problems ranging from trace detection to impact mitigation.
2. *Forensics and Public Health*—to develop and facilitate the implementation of scientifically valid, robust measurement tools for the chemical characterization of synthetic drugs.
3. *Micro- and Nano-plastics*—to provide the U.S. regulatory agencies a standardized platform for the quantification of micro- and nano-size plastic particles for assessing potential risk and exposure of these emerging contaminants.
4. *Semiconductors*—to develop standardized, quantitative tools for the assessment of the three-dimensional distribution, morphology, and size features in real, complex semiconductor devices.
5. *Climate Mitigation*—to develop an autonomous sorbent materials foundry for the rapid evaluation of materials for direct air capture of carbon dioxide.
6. *Ceramic Additive Manufacturing*—to facilitate the advancement of standards through industry-partnered engagements.

The division's research activities were presented in terms of these focus areas, along with three special topics: Super-Resolution Microscopy, Artificial Intelligence and Data Science, and the Material Measurement Laboratory's (MML's) partnership facility at Brookhaven National Laboratory.

Accordingly, the assessment of technical work below is organized along the lines of these focus areas and special topics.

The Materials Measurement Science Division has 92 federal employees and 49 associates (i.e., contractors and guest scientists). Most of the personnel are located at the National Institute of Standards and Technology (NIST) campus in Gaithersburg, Maryland. Seven of the federal employees and four of the associates in the division are stationed at the National Synchrotron Light Source II facility at Brookhaven National Laboratory in Upton, New York. The division receives approximately 25 percent of its funding from other federal agencies or external sources. These external funding sources are non-permanent and usually tied to specific deliverables.

ASSESSMENT OF TECHNICAL PROGRAMS

Accomplishments

Safety and Security

The division's work in the Safety and Security Focus Area provides the necessary measurement science to address technical problems related to the nation's safety and security. Work in this focus area generally falls into three categories: improving national security, enhancing public safety, and advancing personal protection for law enforcement and first responders. The work in this focus area leverages a range of Materials Measurement Science Division core competencies and capabilities including multiscale measurements of physical, mechanical, and transport properties for engineered materials and atomic and nanoscale metrology for structure, chemistry, and composition. Research is focused on a range of challenges including trace contraband detection, through-barrier imaging, threat detection, riot gear evaluation and standards, ballistic and stab-resistant body armor, blunt trauma and concussion prevention, nanomedicine, micro- and nano-plastics and microfibers, mask efficiency measurements, and the Rapid Drug Analysis and Research program.

Forensics and Public Health

The Forensics and Public Health Focus Area supports local, state, and federal partners to address the critical measurement challenges surrounding forensic chemistry by developing implementable solutions through collaborative research. Work in this focus area generally falls into four categories: sample handling and preparation, sample analysis, data analysis and interpretation, and topics that are beyond traditional forensics, such as novel types of evidence. The work in this focus area relies heavily on a range of advanced individual and combined characterization platforms, including gas and liquid chromatography, mass spectrometry, infrared and Raman spectroscopy, and electron microscopy and spectroscopy. Research is focused on a range of challenges including identifying and quantifying background material and chemical compositions (e.g., the baseline or natural concentration of a material or chemical in the environment), modeling the handling of evidence, expanding screening capabilities for illicit materials, analysis of novel materials, rethinking forensic workflows, developing new forensic algorithms and software, spectral databases, physical standards, the Rapid Drug Analysis and Research program, the Rapid Emerging Drug Deployment project, and evaluating and establishing new types of evidence.

Micro- and Nano-Plastics

Work in this focus area generally falls into three categories: test material production; detection, identification, and abundance of micro- and nano-plastics; and sampling, separation, and characterization of micro- and nano-plastics. Advanced separation and spectroscopic characterization methodologies are

used, along with machine learning tools to facilitate the rapid analysis of complex data. The staff in this focus area are working to develop methods for size-based separations of micro- and nano-plastics from complex matrices, chemical characterization protocols for micro- and nano-plastic, and test materials for the quantification of micro- and nano-plastics.

Semiconductors

Work in this focus area generally falls into three categories: three-dimensional structural and chemical imaging, nanomechanical property measurements, and thermal property measurements. The work in this focus area uses a wide range of advanced measurement capabilities including electron microscopy and spectroscopy; X-ray spectroscopy, scattering, and diffraction; and scanning probe microscopy. The staff in this focus area are working with the U.S. semiconductor industry to identify and solve metrology needs and challenges based on techniques such as scanning transmission electron microscopy, atom probes, nanocalorimetry, nanoscale strain measurements, thermal property measurements, intermittent-contact resonance atomic force microscopy, beamline-based measurements (e.g., with Brookhaven National Laboratory), and modeling techniques to complement the above. With the passage of the CHIPS and Science Act of 2022, the strategic importance of this focus area is likely to grow substantially.

Climate Mitigation

Work in this focus area falls into three categories: advanced material for carbon capture, catalysis for CO_2 conversion, and chemical aspects of carbon sequestration (e.g., carbonation of cement). The purpose of the work in this focus area is to provide benchmark data, measurement science, and standards to address the global climate crisis. This work relies heavily on X-ray and neutron metrology, nanoscale metrology and fabrication, accelerated material science and data analysis tools, and measurement standards and services. Current efforts include development of an X-ray testbed for breakthrough catalyst measurements (for CO_2 conversion, but this appears to be, in fact, a very general framework), development methods and data to facilitate material discovery (for materials that would directly capture CO_2 from the air), and measurements of carbonation reactions in sequestration materials (e.g., cement).

Ceramic Additive Manufacturing

The Materials Measurement Science Division found a lack of standards and metrology focused on ceramic additive manufacturing and established this focus area to address that lack. Work falls into a range of categories: computational tools to simulate the entire manufacturing process, feedstock characterization, feedstock data, standards for part characterization, and measurements to enable post-processing (e.g., binder burnout and sintering). This work relies on a range of capabilities, including scanning probe microscopy, rheometry, X-ray and neutron scattering and diffraction, computation and modeling, and additive manufacturing platforms such as photopolymerization and direct-ink writing. Current efforts are focused on feedstock metrology, product property characterization and standards, in-situ synchrotron-based characterization, and microstructure and rheology measurement and correlations.

Data and Artificial Intelligence–Driven Materials Science Group

This group develops methods, algorithms, data, and tools to accelerate the discovery, development, commercialization, and circularity (i.e., the reuse, recycling, or sustainability) of industrially relevant materials. The group works across a range of focus areas, including climate mitigation and semiconductors, and it partners with the Synchrotron Group (discussed below) to enable

high-throughput measurement and advanced modeling. Core competencies and capabilities include autonomous and artificial intelligence–driven systems and data and protocols. The group is involved in more than a dozen projects both inside of the Materials Measurement Science Division and MML, and beyond.

Brookhaven National Laboratory MML Partnership Facility (Synchrotron Science Group)

In this special topic, the Synchrotron Science Group per se was not the primary focus; rather, the presentation highlighted the vast MML capabilities at Brookhaven National Laboratory, such as X-ray absorption spectroscopy, X-Ray diffraction, hard X-ray photoelectron spectroscopy, resonant soft X-ray scattering, microcalorimetry, near edge X-ray absorption fine structure spectroscopy, vector potential photoelectron microscopy, and the Large Area Rapid Imaging Analytical Tool. It was clear that this facility provides foundational support across the Materials Measurement Science Division focus areas and NIST more broadly.

Opportunities and Challenges

The quality of the technical work going on in the Materials Measurement Science Division is second to none. The panel approved of the general strategy of combining multiple measurement platforms, sometimes with a machine learning platform, to facilitate complex material measurements and allow for rapid and high-throughput measurements. In all focus areas, there was a very clear focus on metrology, measurement needs and challenges, stakeholder and customer needs, and standards. The focus area, core competency, and capabilities matrix structure were helpful when trying to understand the breadth of work and how the division articulates its impact.

MML largely has a flat base budget. At various times throughout the review it was noted that it can be challenging for division leaders to manage or balance its sustained base business research, as funded by Congress, with new, invariably temporary, federal initiatives that require an all hands on deck approach (e.g., the CHIPS and Science Act of 2022), and with efforts funded by external sources. This challenge creates a tension between the desire to maintain, develop, and grow core competencies and capabilities, and the need to deliver results on transient, albeit important, emergent research efforts.

> *Conclusion 7-1: With a largely flat base budget, growing into new areas while maintaining, developing, and growing the Materials Measurement Science Division's core competencies and capabilities is a challenge. Managers and focus area leads are compelled to choose to either secure temporary external funding to enable transient growth or focus on research connected to the base funding. Major federal initiatives (e.g., the CHIPS and Science Act of 2022) further complicate this dynamic, as such initiatives often result in substantial funding increases, but usually in a limited focus area and over a limited period of time.*

While the budget dynamics discussed above are in the context of MML, the general challenge of balancing capability development and growth, delivering results on base business efforts, and responding to critical emergent initiatives is typical of large research organizations. The type of matrix framework used by the Materials Measurement Science Division has been used successfully to manage research portfolios across a range of industries. In short, the focus area structure of the division can be used as a framework to prioritize research funding (e.g., one focus area might see an increase in funding at the expense of other focus areas), and in response to these changes, the core competency and capability resources (i.e., federal employees, associates, and capital) can be adjusted and shifted in response to the shift in focus area priorities. For example, with the CHIPS and Science Act of 2022, one could imagine the semiconductors focus area growing (i.e., in funding), perhaps at the expense of other division focus areas, followed by a redeployment of researchers and capital to work on programs in the semiconductors

focus area. The simplest implementation of this model often rests on the structure of the organization being roughly aligned with its core competencies and capabilities. It was not apparent in the course of this review that the division is using its matrix model to balance the demands of its base, ongoing research, and critical emergent initiatives.

Recommendation 7-1: The Materials Measurement Science Division should consider leveraging its focus area and core competency and capabilities matrix structure to manage the challenge of balancing ongoing base work with the needs of critical emergent initiatives, such as the CHIPS and Science Act of 2022.

ASSESSMENT OF SCIENTIFIC EXPERTISE

Accomplishments

The scientific expertise of the Materials Measurement Science Division is extensive, and an exhaustive accounting of such expertise here is unnecessary. A general accounting of scientific expertise was provided above, in the "Accomplishments" subsection of the "Assessment of Technical Programs" section.

In short, the overwhelming majority of the necessary expertise needed to advance the work reviewed was available in the Materials Measurement Science Division. In cases where specific expertise was needed that resided outside of the division, concerted, targeted collaborations were established to advance the research. For example, the effort to develop an X-ray testbed for breakthrough catalyst measurements requires a novel sensor; the Materials Measurement Science Division is partnering with the Physical Measurement Laboratory to design and build this sensor.

Opportunities and Challenges

While the overwhelming majority of the necessary expertise needed to progress the work reviewed was available and being leveraged, there were a few examples where important expertise appears to be minimal or absent. While a required expertise might not be part of the Materials Measurement Science Division's core competencies and capabilities, at a minimum, leveraging it, perhaps from other parts of NIST or with partners outside of NIST, could ensure the technical success of the associated programs.

For example, in the Climate Mitigation Focus Area, significant weight is given to motivating factors such as energy intensity and CO_2 accounting, yet it appears as if a life-cycle assessment or a techno-economic analysis has not been completed, likely owing to a lack of expertise on the research team. Life-cycle assessment or techno-economic analysis can provide clear motivation for specific research areas and elucidate otherwise unappreciated technical challenges. Furthermore, each of the three programs that were presented as part of the Climate Mitigation Focus Area appeared to lack expertise in the associated chemistry (e.g., catalysis, active materials and separations, and sustainable cement). The long-term impact of the work in this focus area could be limited by these apparent omissions.

Recommendation 7-2: The Materials Measurement Science Division should develop or leverage outside expertise in life-cycle assessment and techno-economic analysis in order to guide and focus its research in the climate mitigation focus area. Likewise, where complex measurement complements complex chemistry (e.g., catalysis, active materials and separations, and sustainable cement), the division should support a more substantial effort in the corresponding chemistries or leverage outside expertise to do so. This could include having a world-class catalyst chemist and metal-organic framework expert working side by side with the division's materials measurement scientists.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

In fiscal year 2023, the Materials Measurement Science Division's budget was $37.165 million, comprising $27.434 million from appropriations, $8.879 million from reimbursable work for other federal agencies, and $852,000 from providing services such as standard reference materials and a working capital fund. It receives approximately 25 percent of its funding from other federal agencies or external sources, and 75 percent of its funding from Congress as core or base funding. It has 136 total staff, comprising 81 scientists, 3 technicians, 6 support staff, 1 fellow, and 45 associates.

Accomplishments

Overall, the Materials Measurement Science Division staff exhibited an extraordinary ability to execute technically excellent work in less-than-optimal conditions. The sentiment communicated by the management, focus area leads, and staff was that everyone works hard to deliver results, despite the constraints that will be discussed below. While this division continues to produce impressive and cutting-edge work, its continued ability to do so is threatened by issues noted below in the "Opportunities and Challenges" section.

The division has a great deal of precision measurement and material science equipment, and this equipment is leveraged for much of the research portfolio. Nearly all programs presented rely on the internal discovery and development of measurement methods to deliver value to stakeholders. The division's facilities and equipment at Brookhaven National Laboratory were nothing short of extraordinary. The breadth and depth of capabilities at the Brookhaven National Laboratory MML Partnership Facility are second to none.

The Materials Measurement Science Division has 92 federal employees and 49 associates (i.e., contractors and guest scientists). Most of the division's personnel are located at the NIST campus in Gaithersburg, Maryland. Seven of the federal employees and four of the associates in the division are stationed at Brookhaven National Laboratory in Upton, New York. The National Research Council Research Associateship Program continues to be one of the premiere postdoc programs in materials science, and the program continues to attract world-class talent. The staff at all levels appeared to be excited about their work and dedicated to NIST's mission.

Opportunities and Challenges

While the work in the Materials Measurement Science Division is currently state of the art, there is a risk that the quality and output of work could be diminished unless care is taken to manage aspects of funding, facilities, equipment, and human resources.

Materials Measurement Science Division staff mentioned that some equipment, while functional and locally modified in order to maintain relevance, is dated and in need of replacement. Notable examples are associated with the Safety and Security Focus Area (e.g., large geometry secondary ion mass spectrometer) and the Semiconductor Focus Area (e.g., electron microscopes).

Materials Measurement Science Division staff noted, and this was strongly supported by discussions with postdoc and early career employees, that the time frame to complete facilities work (e.g., repairs and upgrades) can be very long, often disrupting the flow and delivery of—and even the ability to conduct—critical research. A notable example is the process to update facilities in the Advanced Measurement Laboratory—to address known flooding and water issues to enable the delivery and installation of new equipment required for work funded by the CHIPS and Science Act of 2022. Given the relatively short time frame associated with the funding in this act, this is concerning, to say the least.

Division staff also noted, and this was strongly supported by discussions with postdoc and early career employees, that a general lack of technician support means that principal investigators often spend

considerable time in the laboratory performing routine operations, often at the expense of advancing nonroutine and complex aspects of research.

Postdoc and early career staff noted that the NIST Human Resources office has been exceptionally slow and at times unresponsive. There are accounts of Human Resources not sending offer letters to new hires and not processing paperwork in a timely manner so that new employees are left in a period of limbo, without pay or benefits or even certainty of employment. This dynamic can clearly affect productivity directly, and it also produces considerable anxiety and distraction amongst the staff, thus affecting productivity indirectly. This is exacerbated by the reported de facto process of requiring approximately two term appointments before permanent employment is considered.

As mentioned above in the "Opportunities and Challenges" subsection of the "Assessment of Technical Programs" section, owing to a largely flat base budget, there is a persistent tension between the desire to maintain, develop, and grow core competencies and capabilities, and the need to deliver results on transient, albeit important, emergent research efforts. Conclusion 7-1 and Recommendation 7-1 presented there are relevant here as well.

Recommendation 7-3: The Materials Measurement Science Division should consider reallocating budget and staff support to facilitate refurbishment of the division facilities; purchasing of new equipment; increasing the number of technicians, especially in strategic areas or in areas where considerable routine laboratory work is required; and improving the response time and bandwidth of formal Human Resources activities.

Finding 7-1: Postdoc and early career staff noted that the uncertainty associated with the transition from postdoc to permanent employment at the National Institute of Standards and Technology can be a source of anxiety and distraction.

Recommendation 7-4: Materials Measurement Science Division management and postdoc advisors should consider a standard message about the chances and processes of transitioning from a postdoc to a permanent staff member to minimize the uncertainty around this process.

While the Materials Measurement Science Division has a central artificial intelligence and data group (Data and Artificial Intelligence-Driven Materials Science Group), it does not appear to have a central data infrastructure, such as curated or managed data repositories. Rather, it appears that data are managed by individual programs or projects. A central Materials Measurement Science Division or MML-curated or managed data repository could improve collaboration between teams and groups, increase productivity (e.g., speed up the time between data acquisition and analysis), and provide broader access to data for ad hoc use across program teams, NIST divisions, and external users.

Recommendation 7-5: The Materials Measurement Science Division should consider, perhaps in collaboration with other divisions in the Material Measurement Laboratory, establishing a managed data repository, or at least a common data management plan, to aggregate the division's data; facilitate sharing across program teams, National Institute of Standards and Technology divisions, and external users; and facilitate data analysis.

EFFECTIVENESS OF DISSEMINATION EFFORTS

Accomplishments

The read-ahead materials, along with the presentations from the Materials Measurement Science Division staff, illustrated numerous examples of recognized and effective dissemination efforts since the

previous assessment, such as 445 publications, 157 standards activities, 67 customer engagements, and a range of external recognition (e.g., the International Excellence Fellowship, granted by the Karlsruhe Institute of Technology) and Department of Commerce and NIST named awards (e.g., Bronze, Silver, and Gold medals, among many other internal awards).

As mentioned above, the Materials Measurement Science Division has a very clear customer focus, and about 25 percent of its budget is from external funding sources such as customers. These interactions are an acknowledged mechanism for dissemination of results. The division's dissemination efforts appear to be robust and fit for purpose.

Opportunities and Challenges

Generally speaking, the processes and avenues used to disseminate results were impressive. The programs appear to have strong connections to stakeholders, and publishing of results in various formats (e.g., research publications, standards, tutorials) is widely practiced. The only additional aspect worth considering is building stronger connections with instrument manufacturers. For example, the semiconductors focus area struggled to quantify program impacts owing to the confidentiality of the work of their stakeholders, customers, and partners, such as chip manufacturers. In short, the intellectual property concerns of organizations such as chip manufacturers mean that the division has received limited feedback on the utility of its work. Other efforts appeared to have a strong connection to the measurement practitioners of a given sector, but limited connections to instrument manufacturers. In both cases, there was a lack of direct interaction with measurement equipment manufacturers and vendors. Working to develop measurements and standards that are successfully implemented by measurement equipment manufacturers and vendors could increase the impact of the Materials Measurement Science Division's work in a clear and quantitative way.

Finding 7-2: There is a lack of direct interaction with measurement equipment manufacturers and vendors.

Recommendation 7-6: Where appropriate, the Materials Measurement Science Division's program staff should partner with measurement equipment manufacturers and vendors to facilitate the development and implementation of National Institute of Standards and Technology measurements and standards; this could improve the impact of a range of programs and help identify the quantitative impact of the division's work.

8
Materials Science and Engineering Division

The Materials Science and Engineering Division is dedicated to the research and development of materials measurement science, standards, technology, and data. It supports the National Institute of Standards and Technology (NIST) Material Measurement Laboratory's (MML's) mission in advanced manufacturing, including the Materials Genome Initiative 2.0, additive manufacturing, and biomanufacturing. The division also has programs in advanced electronics, the circular economy, climate, and the environment. Many of the topics are cross-cutting programs, and some programs are shared with other laboratories of NIST.

The division is made up of six groups. During this assessment, each group presented an overview of selected programs to the panelists. The six groups are the Polymers and Complex Fluids Group, Functional Polymers Group, Polymer Processing Group, Functional Nanostructured Materials Group, Mechanical Performance Group, and Thermodynamics and Kinetics Group.

The division also hosted two laboratory tours and a forum with postdoctoral fellows and early career researchers.

The division leads or collaborates with internal and external stakeholders on diverse programs important to the innovation and competitiveness of the nation's manufacturing. A few notable programs include the Center for Hierarchical Materials Design, Center for Theoretical and Computational Materials Science, NIST Center for Automotive Lightweighting, and Additive Manufacturing Benchmarks.

The division has 161 staff members at the time of this assessment; these include 60 permanent staff, 21 term employees, 20 postdoctoral fellows, and 60 associates. In 2020, there were 151 staff, indicating the total staff count has increased by 10 over the past 3 years. The division's staff represents about 19 percent of the total MML staff. The division's budget for 2023 was about $30 million, which is flat compared to 2020 when MML was last assessed. The average annual funding per full-time employee was about $186,000 in 2023.

The division's impact is closely connected to its collaboration with industry, government agencies, academic partners, standard organizations, and the dissemination of its research. The division holds an outstanding publication record, which includes 375 archival journals, 34 database publications, 16 NIST reports, 14 conference papers, and 6 book chapters since the past assessment. The division also has strong engagement with customers. It had 16 cooperative research and development agreements, hosted 2 consortia, and led or participated in 24 workshops in the past 3 years. The division's dissemination includes data, open-source software, and active participation in 96 standard committees with more than 21 leadership positions.

The scientific accomplishments and services of the division's researchers have been recognized by NIST and the Department of Commerce as well as by peers in professional societies. These awards include the Arthur S. Flemming Award, the NIST William P. Slichter Award, National Academy of Sciences Kavli Fellow, Microscopy Today Innovation Award, and fellowship of the American Physical Society, ASM International, and the Society of Rheology.

ASSESSMENT OF TECHNICAL PROGRAMS

The division determines the scope and the priorities of its research programs annually, with guidance from the Visiting Committee on Advanced Technology. One overarching division theme is leveraging its strength and core competences to advance science and technology in materials science, measurement technology, standards, and data to enhance U.S. manufacturing competitiveness in industries such as automobile, aviation, chemical, biotechnology, defense, pharmaceutical, and semiconductor. The division recruits and retains top-notch researchers and the quality of research is outstanding.

The Materials Science and Engineering Division supports the nation's need to design, develop, manufacture, and use materials. As such, the division interacts extensively with some of the leading players (with an aggregate 2022 annual revenue of more than $2 trillion) in industry. The division has had outstanding engagements with stakeholders in the semiconductor, and additive and automotive manufacturing industries, as well as the chemical and pharmaceutical industries. However, stakeholder engagement was not as clear in some other areas. The long-term impact of the division's programs on the nation's economy and innovations was not adequately documented and reported.

Researchers in the division developed unique multimodal capabilities to probe material composition, structures, and properties or functionalities simultaneously with wide ranges of spatial and temporal scales, coupled with modeling and simulation, to gain knowledge and provide insights for industrial applications. Some of the examples are highlighted below. The programs discussed below cut across the divisions research groups and involve collaboration with other parts of NIST and stakeholders outside of NIST.

Accomplishments and Challenges in Selected Programs

Advanced Manufacturing

The Materials Science and Engineering Division has a strong advanced manufacturing program, aimed at revitalizing the nation's manufacturing capabilities and the associated infrastructure. Advanced manufacturing is a cross-cutting theme within the division. It includes additive manufacturing with metals and polymers, advanced composites, the NIST Center for Automotive Lightweighting, biomanufacturing, and the nSoft consortium. The division leads a NIST-wide effort on additive manufacturing benchmarking to create a comprehensive benchmark database to validate numerical models over the full range of additive manufacturing processes.

As with other NIST programs, the division has engaged key external and internal stakeholders in advanced manufacturing to maximize its impact. External industrial partners are major players in manufacturing sectors such as automobile, aviation, biotechnology, chemical, defense, and pharmaceutical. Examples of these companies include 3M, Amgen, Boeing, Dow, Ford, General Motors, PPG, and Raytheon.

The division capitalizes on its strength in developing multimodal measurement techniques—many proprietary—to elucidate relationships between material composition, processing, structure, and properties or performance. These unique capabilities allow simultaneous spatial and temporal measurements of structure and performance over large swaths of time and space.

When division researchers encountered unavoidable challenges over the past 3 years, they rose to the occasion. For example, when some NIST facilities were closed during the COVID-19 pandemic, researchers in the division developed a mobile multimodal measurement module and shipped it around the world to maintain research momentum.

Advanced Electronic Materials

NIST has a long history of research on semiconductor technology and electronic materials. It is a recognized national center of excellence and is entrusted to administer the $50 billion CHIPS and Science Act of 2022. The Materials Science and Engineering Division will be a key part of this NIST effort. The division has a track record of fruitful collaborations with major players and key consortia in the semiconductor industry to develop technology roadmaps, spur innovations, and advance semiconductor measurements and manufacturing technologies. The external stakeholders include companies such as IBM, Intel, Honeywell, KLA, and the Taiwan Semiconductor Manufacturing Company; and consortia like the Semiconductor Research Corporation.

The division has a strong program in semiconductor lithography in X-ray-based dimensional metrology and photoresist materials. The metrology technology, called CDSAXS, employs X-rays to nondestructively measure high aspect-ratio, nano-scale critical features on 300-mm wafers, a feat that had been elusive to traditional semiconductor metrology methods. This exemplary technology has been adopted for manufacturing leading-edge three-dimensional memory products worldwide. The current focus is on providing the industry with standard reference materials for this measurement technology. This program's collaborators encompass semiconductor industry giants, including those who produce electronics products and those who create materials, equipment, process lines, and characterization tools for manufacturing electronics products.

Another focus area in semiconductor lithography is materials measurements technology for advanced photoresist materials. This work dates to foundational work at NIST in the early 2000s and has become increasingly important as the industry moves to extreme ultraviolet lithography for manufacturing the 5 nm node of electronic products and beyond. The division has been working on chemically specific direct measurements of nanoscale lateral interfaces that have greater relevance for new photoresist materials in extreme ultraviolet lithography.

Additionally, the division has an active program in electrochemical deposition of electrical conductors for the semiconductor industry. Researchers in the division demonstrated copper conformation super filling, which is important for wafer fabrications and advanced packaging.

Finally, the division pioneered research on biological ways to sort and place semiconducting carbon nanotubes as a potential future transistor technology to extend Moore's Law. Recent work on DNA templated dense carbon nanotube arrays is an important step toward future high-density, high-performance, and energy-efficient electronics.

The CHIPS and Science Act of 2022 investment is expected to significantly boost the division's advanced electronic materials research in the coming years.

Sustainability

The division's sustainability work is focused on three areas: (1) the circular economy of plastics, (2) polymer membranes for clean water, and (3) carbon dioxide (CO_2) capture.

The division partnered with major polyolefins manufacturers to advance measurement science through the synthesis of plastics with systematic variations of polymer sequence, chemistry, and chain architectures. This work led to a curated data and analysis framework of correlated measurements for post-consumer plastic identification and sorting facilities.

In a project focused on clean water, the division partnered with industry stakeholders to develop and advance integrated measurement platforms to characterize the key structural, thermodynamic, and kinetic properties of polymer membranes and sorbents that govern water and small molecule transport. This work led to design cues for water membranes with controlled chemistry, structure, and thickness; and standard testing protocols for the industry.

In the CO_2 capture project, the division endeavors to achieve CO_2 capture and the energy efficient, selective, and high-throughput conversion of CO_2 into chemical feedstocks and other specialty products.

While the plastics and CO_2 research quality is outstanding, the programs' long-term impacts are not adequately documented and reported.

Recommendation 8-1: The Materials Science and Engineering Division should develop more coordinated technical and stakeholder engagement plans for its effort in carbon dioxide capture and the circular economy of plastics and track the long-term impacts of the division's programs on the nation's economy and related innovations.

Data Science and Data Infrastructure

The Materials Science and Engineering Division collects, stores, analyzes, and transmits data in the course of all of its research, measurement, standards-making, and dissemination activities. Data science is an integral and increasingly important part of the division's work to meet its mission. Within MML, the Office of Data and Informatics is a dedicated, service-oriented data resource for physical sciences with domain expertise in biological, chemical, and materials sciences, specializing in large and information-rich data sets.

The division's efforts in data science are highlighted in three areas: (1) the Materials Genome Initiative 2.0; (2) Additive Manufacturing Benchmarking—a NIST-wide effort to create a comprehensive benchmark database for additive manufacturing; and (3) the NIST Center for Automotive Lightweighting data management system. In addition, the Center for Theoretical and Computational Materials Science provides a scientist-run, flexible production environment and testing ground for the development of new scientific software tools, computational workflows, and data management. This high-performance computing center hosts computers for both a shared public cluster (comprising approximately 70 compute nodes and 100 TB of data storage) and several private high-performance computing systems and clusters.

The Materials Genome Initiative 2.0 is an evolution from the Materials Genome Initiative 1.0. It focuses on data and informatics, laboratory automation, high-throughput computing, and artificial intelligence and machine learning methods. The goal is to accelerate materials discoveries and innovations by harnessing the power of artificial intelligence and machine learning.

The Center for Hierarchical Materials Design (ChiMad) is an extension and integral part of the Materials Genome Initiative. It developed broad research and outreach programs that involve participants from universities and NIST, and from automotive, aerospace, semiconductor, and polymer industries. It has made tremendous progress by integrating traditional computational materials tools with artificial intelligence and machine learning to accelerate material discovery and the technology deployment cycles. Since its inception, the center has published more than 600 papers and supported 14 dedicated NIST postdocs.

The center's active collaboration with industry has led to tangible results. For example, its researchers designed a new printable die-cast steel to enable Tesla Gigacasting and has transferred computational tools and data management approaches to major companies such as Intel and 3M. The center's researchers have also pioneered tools for the inverse design of sustainable plastics and nontoxic additives—tools that are highly sought after by industrial partners such as 3M, PPG, Solvay, and Apple in their efforts to transition into sustainable, fully recoverable materials cycles of use and reuse.

The Center for Hierarchical Materials Design has produced many fruitful outcomes and is coming to a natural end. The division's programs associated with the center will be redirected to other NIST priorities.

The Additive Manufacturing Benchmarking program aims to create a comprehensive benchmark data set to validate numerical models in additive manufacturing. This NIST-wide program, running since 2015, has 51 NIST staff and associates from 10 NIST divisions. This program adopted a challenge

approach to validate additive manufacturing models for specific additive manufacturing scenarios. It collects all of the relevant measurement data and metadata for a given scenario and makes it available to challenge participants—modelers—on a predetermined schedule. The challenge participants present the modeling results to the community at regularly scheduled conferences. In 2022, 34 challenge problems were posed. The Additive Manufacturing Benchmarking program received 138 submissions from the additive manufacturing modeling community and gave out 41 awards based on a set of predetermined model quality metrics. One data-related challenge in this program is that data collection, storage, analysis, and movement are handled by multiple platforms and are fragmented.

The NIST Center for Automotive Lightweighting aims to improve fuel economy and electric vehicle range while maintaining safety in the U.S. automotive industry by incorporating advanced lightweight materials into automobile designs. It develops foundational measurements, test methods, and standards for characterizing the material properties and behavior of automotive sheet materials under complex and real-life use conditions. This center is the largest and second-longest-tenured project in the division with strong partnership in the automotive industry. External partners include Ford, General Motors, and their suppliers. The center collects data from many test platforms with operating systems spanning several decades. It also has substantial modeling efforts. The NIST Center for Automotive Lightweighting faces similar data management challenges to the Additive Manufacturing Bench program, but on a larger scale. Not all of the experimental measurement systems have a consolidated and automated data infrastructure. This fragmented data infrastructure, unfortunately, leads to discrete ineffective experimental data infrastructure throughout this program (and the division).

One encouraging effort by the NIST Center for Automotive Lightweighting was to consolidate the vastly different operating systems of all of its measurement equipment into a virtual machine. This virtual machine approach not only unified the measurement equipment operating systems but also afforded a unified infrastructure for data management infrastructure, use, and security. The virtual machine approach as a best practice would be useful throughout the Materials Science and Engineering Division.

A large number of the Materials Science and Engineering Division's projects involve computational work and they often result in the development of many and different computational methods, varying from conventional finite element, thermodynamic methods to a density function theory-based comprehensive materials information system such as JARVIS. Although the computational works in the division are impressive, most of them are done as a part of individual projects. As a result, the computational data does not seem to be managed in a centralized platform.

Recommendation 8-2: The Materials Science and Engineering Division should launch an initiative to unify its computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management. This data science initiative could be applied to machine learning deployment and expand capabilities in laboratory automation, high-throughput computation, and artificial intelligence and machine learning methods.

ASSESSMENT OF SCIENTIFIC EXPERTISE

The Materials Science and Engineering Division's staff members are leading technical experts in their respective fields. These experts are passionate about addressing some of the nation's pressing challenges including manufacturing resurgence, sustainability, climate, and infrastructure. However, the skill set in machine learning or artificial intelligence is not adequate to support the division's needs to capitalize on the growing, diverse data sets and the division's overall goals in artificial intelligence, machine learning, and future initiatives in lab automation.

Recommendation 8-3: The Materials Science and Engineering Division should hire more scientists skilled in artificial intelligence, machine learning, and data science to build internal capabilities and capitalize on the growing, diverse sets of data the division has handled.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

In fiscal year 2023 the budget for the Materials Science and Engineering Division was $28.410 million, comprising $27.035 million from appropriations, $1.242 million from reimbursable work for other federal agencies, and $132,000 from providing services such as standard reference materials and a working capital fund. The division has maintained a steady funding and staffing level to meet its key mission and deliverables as outlined in the Introduction, provided that the division is able to complement its current staff with scientists with expertise in artificial intelligence, machine learning, and data science. The division has established a few new facilities such as the state-of-the-art materials measurement laboratory where the in situ fluorescence lifetime imaging microscopy equipment is housed. It also acquired new tools and capabilities such as the 300 MHz solid-state nuclear magnetic resonance spectrometer, the environmental transmission electron microscope, and the broad beam ion mill in recent years. It has strived to upgrade equipment or build its own tools. However, many of the buildings, facilities, and tools are several decades old. The maintenance, restoration, and modernization of facilities and capabilities have not kept up with the increasingly important role the division needs to play. Moreover, it took an unusually long time (more than 6 months) to receive approval for tools and capabilities. A more detailed assessment of NIST's facilities can be found in the 2023 National Academies report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023).

The division in general ascribes to proper safety procedures and practices. However, observations made during the laboratory tours and meetings suggest areas for improvement. For instance, it appeared that a researcher who typically wears prescription glasses does not universally use laboratory safety glasses that meet today's laboratory safety standards. Generally, it did not appear to the panel for it to be customary for researchers entering into a laboratory area to immediately don safety glasses upon entering a laboratory setting. On one occasion, an organic chemical odor was detected upon entering into a laboratory setting, which suggests the need for critical facilities improvements coupled with added researcher training and awareness of laboratory and experimental standard operating procedures. In a similar vein, some exhaust systems appeared to have been installed without regard to current recommendations for materials to be used with snorkels that will be handling toxic or flammable organic solvents. Furthermore, to PhD-level researchers, the career path as a safety representative is not clear although the workload and the responsibilities of a safety representative are enormous. The reward system did not appear to align with the responsibilities of safety representatives. This misalignment does not encourage PhD scientists to serve as safety representatives in the division. Given the extensive Materials Science and Engineering Division relationships with industrial partners that were apparent during the assessment, the division would be advised to consider working with their industry partners to develop laboratory safety initiatives and programs to build a safety culture that aims for continuous improvement.

EFFECTIVENESS OF DISSEMINATION EFFORTS

The Materials Science and Engineering Division has a track record of engaging key stakeholders, including major industry players, for broad dissemination of knowledge and standards, to identify pressing national challenges, to formulate industry roadmaps, and to establish collaboration strategies.

In the past 3 years, the division has published 375 archival journals, 34 database publications, 16 NIST reports, 14 conference papers, and 6 book chapters. The division had strong engagements with key stakeholders as evidenced by 16 cooperative research and development agreements and hosting two

consortia (nSoft and Additive Manufacturing-Bench). It led or participated in 24 workshops in the past 3 years. Its researchers served on 96 standard committees and held 21 leadership positions in these organizations. Its engagements with leading players in the industry and standard organizations are broad, deep, and impactful. However, the division does not seem to track the long-term impacts of its work.

Recommendation 8-4: The Materials Science and Engineering Division should develop a plan to track the long-term, quantitative impact of its key programs and industrial engagements.

REFERENCE

NASEM (National Academies of Sciences, Engineering, and Medicine). 2023. *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology.* Washington, DC: The National Academies Press. https://doi.org/10.17226/26684.

9
Office of Data and Informatics

The Office of Data and Informatics is effectively meeting its mission to provide leadership and expertise to meet the data challenges and opportunities for the rest of the Material Measurement Laboratory (MML) and National Institute of Standards and Technology (NIST) research data infrastructure. Its mission also includes providing services to MML and to NIST through its expertise, guidance, and the resources it offers in order to enhance the discoverability, usability, and interoperability of data collected by other NIST laboratories and occasionally, outside sources. The office is similarly meeting this portion of its mission through programs that it offers, including creating data infrastructure workflows, modern and robust data repositories, and thought leadership for the use and dissemination of research data beyond the federal government (i.e., the Research Data Framework). There is potential for expansion and replication of these initiatives throughout MML and the rest of NIST.

Overall, the capabilities within the Office of Data and Informatics to increase the usability, interoperability, and discoverability of NIST's and MML's outputs are absolutely vital to meeting NIST's mission to "promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life" and MML's mission to "conduct measurement science research to benefit industries based in the chemical, biological and material sciences." Furthermore, these critical goals can only continue to be met if the initiatives and projects of the office are widely implemented across MML. Fortunately, this imperative is achievable owing to the foundations that have been laid over the past decade by the staff at the Office of Data and Informatics. Nevertheless, it will take concerted effort and planning to apply the lessons, tools, and workflows more broadly.

ASSESSMENT OF TECHNICAL PROGRAMS

The Office of Data and Informatics has a team that can bring consideration of experimental metadata early into every division. Experimental metadata describes the conditions under which the data were collected and allows later investigators to use that data for additional research or verification. This skill and perspective are too easily overlooked in common practice because many of the benefits are realized only in hindsight, by future users or projects or by external community members when accessing and making use of the results of past work. The fact that the benefits of high-quality metadata are being considered and implemented in the projects that this office spearheads will help to improve future reuse and may also improve research practice through the improved data management practices. These efforts benefit the wider scientific community and the nation because the data outputs from MML's work are preserved, curated, and disseminated allowing for others to reuse them and to increase the transparency, credibility, and impact of MML. This is enhanced by the consideration given to openness and transparency, which require technical skills to manage and to create workflows that enable both.

A major success has been the data pipeline created through the NexusLIMS[1] infrastructure. This networked system automatically captures scientific data as it is generated throughout the electron microscopy working groups and automatically applies relevant metadata. This benefits individual

[1] A LIMS is a laboratory information management system.

researchers, who are better able to access, store, manage, analyze, and retrieve the original experimental data. Colleagues and supervisors can see and support the research as it progresses and as results are generated. The automatic addition of important metadata and tags about the equipment, its settings, and the context in which the images were created addresses key shortcomings that affect reproducibility in scientific settings. The benefits to society grow exponentially as it feeds into a truly FAIR[2] pipeline that eventually allows for public discoverability through NIST's Public Data Repository, which allows for human and machine-readable data access.

This office's staff possess expertise in assessing technical solutions to determine if the reuse, modification, or creation of new custom tools is required. Prior to creating new software or workflows, the staff effectively evaluates commercial and open-source solutions for the degree of fit and an overall cost-benefit analysis. They possess the capability to create novel solutions that are effective and valuable where suitable commercial and open-source solutions do not exist.

The Materials Science and Engineering Division, with the support of the Office of Data and Informatics effectively uses virtual machines to increase the longevity of aging equipment that is controlled by computers running on obsolete operating systems (e.g., Windows XP or 2000). This increases and extends the return on investment that was made in the equipment in the first place.

The Office of Data and Informatics in collaboration with world experts helped to create the Research Data Framework. This framework is a useful tool for researchers, librarians, research support staff, and external stakeholders such as data repositories and scientific publishers because it provides specific recommendations for practices at each stage of the research process. Success in implementing this organizational infrastructure is establishing NIST's credibility and leadership in data information practices.

Recommendation 9-1: The Material Measurement Laboratory should periodically and frequently engage with industry and academia through activities such as workshops, meetings, conferences, and roundtables to standardize data management frameworks that fully support U.S. science advancement and industry competitiveness via open tools and instruments alike.

Recommendation 9-2: The Material Measurement Laboratory should disseminate broadly the Materials Science and Engineering Division's protocols for the use of virtual machines to increase the longevity of aging equipment controlled by obsolete computers, effectively empowering industry, academia, and government laboratories to extend the return on capital equipment investments.

ASSESSMENT OF SCIENTIFIC EXPERTISE

The Office of Data and Informatics has 23 total staff, comprising 14 scientists, 2 support staff, and 7 contract staff. Building, maintaining, and growing the capability to properly structure useful data repositories requires sufficient scientific expertise. This understanding is particularly important to be able to appropriately incorporate the needs of a broad technical community. These diverse communities at MML comprise fundamental and applied sciences like chemistry, physics, biology, materials, and engineering. The Office of Data and Informatics meets these requirements with a strong core team possessing scientific backgrounds in astrophysics, biology, and materials. Their ability to leverage other resources is exemplified through internal and external collaborations like their engagement with faculty from the University of North Florida. This relationship afforded a recent paper in *Nature* (Hanisch et al. 2022), in which staff from and peers of the Office of Data and Informatics call for machine readable units

[2] FAIR is a set of principles to ensure that data are findable, accessible, interoperable, and reusable; see GOFAIR, "FAIR Principles," https://www.go-fair.org/fair-principles, for more information.

of measurement and stands out as evidence of the strength and potential impacts these collaborations can have on the Office of Data and Informatics' ability to affect the NIST brand in a very positive manner.

The importance of incorporating internal scientific domain expertise from within MML into the Office of Data and Informatics is demonstrated from the significant impact made by a fully embedded material scientist who has extensive knowledge of electron microscopy. This inclusion of technical knowledge into the office's work provides the team with deep knowledge of the data requirements when using this critical tool for MML. Similarly, the epidemiological modeling work presented is another example of the impact domain experts have on the division's work as it grows its collaborations in data-intensive methodologies applied to biology (e.g., collaboration with the Jet Propulsion Laboratory). Despite these first-rate examples of collaborative efforts, a potential challenge in maintaining the necessary scientific breadth is conspicuously shallow, in some cases being only one person deep. For example, a significant capability gap would occur immediately within the Office of Data and Informatics if their only materials scientist were to pursue other career opportunities.

A home-grown capability described by the division's staff, and mentioned in several other assessment groups, was the development of virtual machines. This clever construct allows MML researchers to maintain instruments running proprietary software necessary for using equipment with proper security and technical support even after their original computers or operating systems are obsolete. This enables and extends the data capture that is instrumental for the Office of Data and Informatics. It is worth noting that the individual who built this capability is not officially a member of the office's staff. This situation demonstrates the team's ability to leverage resources available throughout MML and represents a kernel of an idea to scale up the office in a low-cost fashion while providing a significant opportunity for NIST's postdoctoral cohort as described below.

One possibility to bring additional resources to the Office of Data and Informatics in a way that will increase its sphere of influence and improve its ability to maintain the needed scientific breadth, is to develop a model that would create sustainable connections to the various laboratories. A hybrid of the two models described in the last two paragraphs would afford a sustainable solution: namely, 6-month rotations of postdocs from other groups through the office. It is possible that non-Office of Data and Informatics groups may find this idea to be a distraction to the postdoctoral cohort. However, this model would bring about several other tangible and impactful benefits to both the Office of Data and Informatics and postdocs such as:

- Providing more resources to work on data infrastructure without adding to the total number of Office of Data and Informatics staff, an important consideration owing to budgetary constraints.
- Creating and expanding a continuous stream of fresh domain knowledge from various MML groups into the office because the rotating postdocs would bring new perspectives from the various divisions in MML.
- Growing professional networks that could be leveraged during and after the postdocs' time at NIST.
- Expanding training opportunities for postdocs providing them with fungible skills such as data science; this would enrich the learning experience while postdocs are at NIST while providing a concrete benefit to MML and NIST through the additional expertise that it would provide.
- Embedding a data-driven culture into all of the divisions and research groups that participate in this model, encouraging the broader and faster adoption of a data mindset at NIST.
- Increasing publication opportunities because work with the Office of Data and Informatics would be published in a wider range of journals than those typically targeted by most MML researchers.

Conclusion 9-1: Embedding outside team members, such as postdocs from other groups rotating through the Office of Data and Informatics, to work on projects would benefit the divisions for which those researchers work. This would allow for technical expertise to be embedded with the workflow expertise in the office so that solutions for the MML divisions would be more specifically tailored to the language, tools, and other nuances of those divisions.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

The Office of Data and Informatics has a budget in fiscal year 2023 of $5.615 million, with $4.825 million coming from appropriations and $790,000 coming from providing standards reference data services. It has 23 staff, comprising 14 scientists, 2 support staff, and 7 contract staff.

MML's creation of the Office of Data and Informatics laboratory with world experts who are truly committed to data governance, FAIR data practices, and are regarded as leaders in scientific data management, is commendable. These experts are in a unique position to lead U.S. industry, government, and academic laboratories in establishing standardized best-in-class data practices. However, their impact could be increased if they were in a position to apply their expertise into additional laboratories within MML, or indeed across NIST where data infrastructure is also likely needed (though not directly assessed during this review process). As mentioned in previous sections on technical expertise, the Office of Data and Informatics is able to expand the useful life of existing equipment through the use of virtual machines and is able to increase research efficiency through the creation of high-quality data workflows. This efficiency gain has long term benefits for other laboratories that implement them by conducting more research on the same budget, although it requires an upfront investment to establish. A key example of this is the NexusLIMS that connects electron microscopy equipment to a centralized data management system. The investment that was made to create this system is worth replicating in additional research groups throughout MML.

Recommendation 9-3: To facilitate the deployment and adoption of state-of-the-art data practices in the Material Measurement Laboratory (MML) and across National Institute of Standards and Technology (NIST), the Office of Data and Informatics and MML should:

- **Institute a laboratory-wide policy requiring researchers to use automated data-handling workflows such as those demonstrated in NexusLIMS, and that output data that is easily disseminated through the Public Data Repository with rich meta-data. This will help to ensure that research data generated by MML comply with the FAIR principles of being findable, accessible, interoperable, and reusable. All MML researchers should also use the Public Data Repository so that their data are readily available internally and externally.**
- **Embed laboratory research personnel within the Office of Data and Informatics as a sabbatical or special assignment in order to spread awareness of the data workflows that they have developed and to help to generate new use cases for them under different laboratory conditions.**
- **Strengthen collaborations with the Information Technology Laboratory to help develop state of the art data practices and disseminate them across NIST.**

EFFECTIVENESS OF DISSEMINATION EFFORTS

The Office of Data and Informatics has evidenced a true commitment to its mission to be the premier, pioneering resource specializing in the large and information-rich data sets now common in many disciplines focusing on researchers and institutions in the life and physical sciences (i.e., biological, chemical, and materials sciences), areas that data science and informatics can support. The office's

research and implementation programs are driven by stakeholder needs both from within MML and from external constituencies such as users of the external-facing data repositories and patterns in the Research Data Framework, discussed in more detail below. As such, the NIST Public Data Repository[3] has been an innovative and effective mechanism for NIST researchers to disseminate their efforts since it allows others to explore or reuse data and the related tools and resources supporting science, engineering, and technology. Researchers in NIST labs communicated their excitement about how easy it is now to make their data public. This demonstrates that the Office of Data and Informatics does not solely provide service to other MML entities but across all of NIST. The NIST Public Data Repository includes fields for data set metrics that display usage statistics on total file downloads, total data set downloads, total bytes downloaded, total unique users, and last downloaded. Nine of 10 randomly selected data sets had only "Metrics not available" for the resource. The reader does not know if metrics cannot be counted for that data set (perhaps because it is hosted externally) or if there has been no usage of that data set.

Recommendation 9-4: The Material Measurement Laboratory should enter more information in the NIST Public Data Repository field to explain why data set metrics are not available where that is the case.

The NIST Alloy Data[4] application and the Metals Alloy User Interface are two examples of the quality and depth of the data in this public repository. In the past 3 years, the growth of data sets (now more than 30,000) and of the amount of data stored (now more than 20 TB) is a testament to the value of the repository to NIST scientists and to the public. Similarly, the Office of Data and Informatics has taken the leadership to create an open-source code repository, the NIST Opensource Contributions Portal.[5] This is a well-used hub for NIST open-source projects and has a full catalog that is updated regularly as repositories are added or modified. Its features include private or restricted access that enable data sharing with appropriate protections.

A new achievement has been the launch of the Research Data Framework version 1.5, which provides the research community with a structured approach to develop a customizable strategy for the management of research data. The State University of New York system's use of this framework is a testament to the awareness of and trust that large institutions have put in the NIST-led framework.

The Research Data Framework can become the data framework to guide NIST as a premier research organization in standards. Any other research and development organizations (in academia, industry, government, or other public or private institutes) can also rely on this framework as they become digitized and data centric. Its adoption will help standardize fragmented efforts, agree on a common data vocabulary, and provide necessary data governance and roles.

The Office of Data and Informatics' outreach includes working closely with world-class organizations on data science and engineering. For example, together with the Research Data Alliance, an external association of governments and researchers that promote best practices in data management, they now provide tools for data discovery within the Materials Resource Registry by using and providing a materials science metadata schema (Medina-Smith et al. 2021). Staff from this office are also active in the FAIR Digital Objects Forum Steering Group, the Committee on Data of the International Science Council Task Group, the Certified Information Privacy Manager Expert Group, and many others.

The Office of Data and Informatics has also taken leadership in the area of data models, tools, and infrastructure at the national level. As such, they are active in CENDI[6] focusing on improving the productivity of U.S. federal research and development efforts through collaborative agency participation, in the Department of Commerce Data Governance Board, and in the National Science Foundation Materials Research Data Alliance.

[3] See NIST, "Science Data Portal," https://data.nist.gov, for more information.
[4] See NIST, "NIST Alloy Data," https://www.nist.gov/mml/acmd/trc/nist-alloy-data, for more information.
[5] See the NIST Opensource Portal website at https://code.nist.gov for more information.
[6] See the CENDI website at https://www.cendi.gov for more information.

The Office of Data and Informatics also fosters strong collaborations with academia, notably with the NUANCE Center at Northwestern University, Johns Hopkins University, the City University of New York, and the University of Pennsylvania.

This office's staff have made efforts to include the private sector, for example, in 2023, in 3 conferences and 15 workshops. These efforts go beyond industry presence at meetings and could also include funded projects with lead companies within particular chemical or materials industrial sectors to adopt and implement standardized data repositories, tools, and approaches. Such projects can help to ensure the true adoption of data repositories or data management practices demonstrated by the Office of Data and Informatics. Efforts toward data standardization by equipment manufacturers and vendors of data solutions can be catalyzed by the Office of Data and Informatics' leadership. The basis of centralized data engineering, infrastructure, analytics methodologies, and tools have already been developed by office.

The Office of Data and Informatics has developed a common ecosystem for data management and sharing that has already been shown to be successful with the electron microscopy community in various sites and divisions as well with the additive manufacturing community. This ecosystem can be generalized to all MML divisions. This ecosystem can also be applied to any research organization in the physical sciences whether in industry, academia, or government.

Understanding the need for inspiring the next generation of data savvy researchers, the Office of Data and Informatics has created a NIST Educational STEM Resource Registry,[7] or NEST-R, which is used by students and teachers and serves as an additional mechanism for creating awareness of the work done in MML and at NIST more broadly.

The Office of Data and Informatics collects metrics that measure the use of all of the above programs. These metrics show an increase in their use in the past years. It also indicates that the adoption is limited. This could be enhanced by conducting use analysis jointly with key stakeholders.

Conclusion 9-2: The Office of Data and Informatics is positioned as a national and an international leader in data infrastructure and standardization because of its commitment to enabling open data, efficient data workflows, and because of its work with equipment manufacturers and vendors of data solutions. The office has already piloted and successfully demonstrated the usefulness of centralized data engineering, infrastructure, analytics methodologies, and tools.

Conclusion 9-3: The Office of Data and Informatics' efforts to inspire the next generation of physical scientists to be data natives is commendable. The office does this through the National Institute of Standards and Technology (NIST) Educational STEM Resource Registry or NEST-R while simultaneously creating awareness of the work done at the Material Measurement Laboratory and at NIST more broadly. The office is also uniquely positioned to offer NEST-R to all of the scientific community.

Recommendation 9-5: The Material Measurement Laboratory should strengthen its commitment to the Office of Data and Informatics by establishing clear data governance and data policies. It should establish the National Institute of Standards and Technology (NIST) Public Data Repository as the place to publish all open-source projects and take advantage of its restricted access functionality for any NIST confidential or internal project.

Recommendation 9-6: The Material Measurement Laboratory managers and researchers should adopt the materials science schema developed jointly with the Research Data Alliance.

[7] For more information, see the NIST Educational STEM Resource Registry (NEST-R) website at https://nestr.nist.gov.

Recommendation 9-7: The Office of Data and Informatics should collect and make more visible the usage metrics to measure the impact of its repositories. Numbers that report access, download, and reuse (although that is the hardest to measure) would showcase how data and teaching materials are used in and out of government.

REFERENCES

Hanisch, R., S. Chalk, R. Coulon, et al. 2022. "Stop Squandering Data: Make Units of Measurement Machine-Readable." *Nature* 605(7909):222–224. https://doi.org/10.1038/d41586-022-01233-w.

Medina-Smith, A., C.A. Becker, R.L. Plante, et al. 2021. "A Controlled Vocabulary and Metadata Schema for Materials Science Data Discovery." *Data Science Journal* 20:18. https://doi.org/10.5334/dsj-2021-018.

10
Office of Reference Materials

The Office of Reference Materials in the Material Measurement Laboratory (MML) serves a significant and prominent role in translation of measurement science at the National Institute of Standards and Technology (NIST) to stakeholders. The office's administrative activities include managing business operations, administrative oversight, product sales, and technical support for the NIST Standard Reference Material program. Through its responsibility for managing working capital and standards development funding, the office has strong influence in selecting and resourcing the technical work that is developed and disseminated.

The office is actively pursuing a modernization approach for their operations as part of its Measurement Services Modernization Strategy. Part of this effort involves close coordination with the Statistical Engineering Division to improve experimental design at an early stage of study. At the other end of the supply chain, the office is seeking to extend its distribution model by partnering with organizations possessing skills that complement its core capabilities. This strategic approach is designed to enhance the office's efficiency while allocating resources to alternative, high value-added activities.

The Office of Reference Materials effectively translates measurement services to a broad set of stakeholders and is the leading national metrology institute in doing so. Meeting that responsibility for more than 100 years has realized a portfolio of products that is dominated by legacy products; these products are impactful and touch many domains and many users. This office is presently in the position of maintaining this legacy catalog, with most of its resources devoted to that. The legacy catalog being maintained by the office has led to a product portfolio that appears to be balanced in a way that jeopardizes NIST's ability to support emerging needs and the industries of the future.

The Office of Reference Materials is fiscally incentivized by sales of units, with the legacy commodity products dominating the list of the highest-selling products, with only one recently developed product among the top 15 sellers. Revenue distribution is strongly skewed to the highest-selling products, with 4 percent of the catalog generating 50 percent of the office's annual revenue. The product portfolio is managed using the relative demand for each product, a fairly passive approach. It is not clear that this commodity sales-driven approach to product portfolio management is sufficiently active to best translate NIST measurement science to stakeholders.

The top grossing product in the past year has in fact been one of the newest and most innovative offerings, RM 8671 NISTmAb, Humanized IgG1κ Monoclonal Antibody. This is a commendable situation that shows the excellence that NIST is able to project to emerging industries, the impact of new product offerings, and their revenue potential.

ASSESSMENT OF TECHNICAL PROGRAMS

The Office of Reference Materials ships approximately 30,000 units from a catalog of 1,100 products, generating approximately $22 million in revenue. Accomplishing this within the confines of the laboratory is no small feat and speaks to the immense capability of the personnel that manage and implement the tasks.

This office functions as a stand-alone e-commerce business operating within the framework of a federal agency. This presents unique business, staffing, and technical constraints that are different from

other units within MML. The Office of Reference Materials is well aware of the nature of these challenges and has taken steps to address them, as mentioned above, in the development of service modification. This suggests the need to implement an enhanced portfolio governance process.

The portfolio of Office of Reference Materials products is not currently actively managed, in large part because there is no immediate need to do so. However, portfolio optimization would free resources (personnel, facilities, and dollars) for increasing the long-term value of the portfolio for U.S. industrial growth. In fiscal year (FY) 2023, renewals of existing products represent 81 percent of the investment for the future, leaving less than 20 percent for the difficult yet essential work of prosecuting new projects.

Portfolio optimization requires having insight into the value capture potential of the products in the catalog in light of the stakeholder value delivered. Active management of the portfolio would enable strategic decision-making across the whole of the catalog, both currently and in the future, as opposed to managing the portfolio on a program-by-program basis. Careful consideration of the entire portfolio would take the form of evaluating both the value proposition to the clients and the value capture potential for NIST. In that manner, all stakeholders can be served effectively. Value capture potential may take the form of understanding the economics of the offering, including opportunity cost, working capital and equipment requirements, resource allocation in preparation, sales effort, and opportunities for growth. Value proposition seeks to understand the offering in terms of the next best alternative to the customer base, with a keen eye toward looking at the relative value capture potential versus the value delivered relative to replacement options. For offerings with high value capture potential, active sales efforts would be advantageous. For those with low value capture or poor value propositions, exit or upgrade strategies would be implemented.

Recommendation 10-1: The Office of Reference Materials should develop and implement a portfolio management process based on the articulated measurement services modernization strategy. The full portfolio of products should be considered critically and monitored on a periodic basis for (1) each offering's utility and impact, (2) the resource commitment needed to maintain the product, and (3) effectiveness and performance of translation. Each existing product should have a maintenance and sustaining plan, and a plan to either perpetuate or discontinue products through transition to alternative products or obsolescence. A plan should be developed for every new product proposed or being developed that includes projection of these characteristics, with emphasis on life-cycle analysis, value proposition for stakeholders and value capture for the National Institute of Standards and Technology.

PORTFOLIO OF SCIENTIFIC EXPERTISE

The portfolio of expertise of the Office of Reference Materials is aligned with its mission as a stand-alone business unit and does not lend itself to direct comparison to other MML divisions. Of the 31 staff members, 12 are scientists, 7 are technicians, and 12 provide administrative or other program support. The scientific and technical staff collaborate with peers in the research divisions to produce and document existing standard reference materials and perform the necessary research and measurements to create new standard reference material products as they are needed by industrial customers.

BUDGET, FACILITIES, EQUIPMENT, AND HUMAN RESOURCES

In FY 2023 the budget for the Office of Reference Materials was $12.332 million. Of this, $1.170 million was appropriated by Congress and $11.161 million came from services and a working capital fund. For comparison, in FY 2020 the numbers were $9.471 million, with $870,000 appropriated and $8.601 million coming from services and a working capital fund. This represents approximately an 8.5

percent increase. This predominantly fee-based funding model incentivizes commodity in favor of innovation. The fee-based budget gives rise to facilities that are optimized for the wrong things, and there is insufficient investment in maintaining them to be safe and of high integrity. The office has 31 staff, comprising 12 scientists, 7 technicians, 10 administrative personnel, 1 support person, and 1 associate.

The Office of Reference Materials relies on the analytical and research facilities in other divisions outside of MML to make appropriate measurements in support of mission delivery. It has facilities and equipment that enable standard reference materials preparation, packaging, and shipping. The office is allocated a 20,000-square foot building for storage, sample preparation, and shipping operations. Some products require controlled temperatures while stored, and the office maintains close to sixty –80°C freezers, seven walk-in –20°C freezers, and four walk-in 4°C refrigerators. Much of the infrastructure, both buildings and equipment, has exceeded its expected life, leading to the potential that time is spent inefficiently compensating for the reduced capabilities of old equipment and facilities compared to the capabilities of state-of-the-art equipment, which could greatly enhance work efficiency.

Many of the Office of Reference Materials' backend activities, such as order fulfillment, warehousing, and shipping, can be accomplished better by outside vendors who have both the experience and automation to reduce errors and increase efficiency. Outsourcing selected tasks can provide more time for value-added work by Office of Reference Materials staff and create products with updated capabilities without the need for expensive capital equipment, some of which will not be used on a regular basis within ORM.

Recommendation 10-2: The Office of Reference Materials (ORM) should benchmark its tasks and the capabilities required to accomplish them against best-of-class capabilities that exist in the private sector. Tasks that are deemed to be better done by outside vendors should be targeted for outsourcing and staffing within ORM should be reallocated accordingly.

Aged infrastructure and equipment can have an impact on the safety mentality of the staff. While it is not necessarily true that modern buildings lead to positive safety performance, it is often true that old facilities in disrepair result in poor safety awareness. The laboratory tour indicated that the Office of Reference Materials runs the risk of safety incidents in the near future as a result of a perception that the risks in those facilities are minimal. This attitude allows the persistence of unsafe conditions that form the base of the safety pyramid and can ultimately result in injury or even fatality.

Unsafe conditions also have the potential to impact performance of the products. As facilities degrade, the organization may not recognize the risk of microbes and other contaminants can have on the packaging and integrity of the products. The importance of management involvement in fostering a safety culture is discussed in more detail in Chapter 2. Safety and excellence go together.

Key Recommendation 2: Safety is as much a line management responsibility as an individual one. Leaders should recognize that every task can be done safely, and every task has inherent risks. That attitude needs to be transmitted down the line in order for each individual to take responsibility for maintaining the safety of their environment and the environments of those around them. The Office of Reference Materials should maintain statistics of leading indicators of safety risks and facilities dangers that represent the base of the safety pyramid. These statistics should be socialized within the organization in such a way that the safety environment is uplifted, ultimately resulting in a revised safety culture. It may be desirable to enlist an experienced industrial partner who can bring a fresh perspective on the safety risks as a way of providing an unbiased and fresh pair of eyes to the situation.

EFFECTIVENESS OF DISSEMINATION OF OUTPUTS

Dissemination of NIST work is the essence of the Office of Reference Materials; however, it appears that there is no dissemination of their portfolio management and performance outside of informal internal assessment. There have been reports on the dissemination function and aspirations in the past.[1] Such reporting on a periodic basis would serve both NIST planning and inform key NIST stakeholders. In years past, NIST published SRM Spotlight,[2] a newsletter with the goal of providing information about the offerings and new reference materials.

Such tools are an opportunity to disseminate the portfolio and engage stakeholders in best taking advantage of NIST measurement science tools. Feedback and dialog with stakeholders triggered by this marketing approach can lead to a virtuous cycle that encourages active and responsive management of the portfolio, with leading indicators and market knowledge supporting decision-making.

Recommendation 10-3: The Office of Reference Materials (ORM) has done an excellent job in managing and distributing product stock, however the marketing effort that leads to sales most often relies on an outside-in approach, in which a potential customer makes a request for a standard. As part of the input for Recommendation 10-1, ORM should initiate an inside-out marketing effort to determine the current value add of each offering in the standard reference material catalogue. This active marketing can increase uptake of languishing products, and at the same time reveal products in the portfolio of limited value proposition. This effort would be expected to increase ORM revenue.

REFERENCES

Gills, T.E., S. Dittman, J.R. Rumble, Jr., C.S. Brickenkamp, G.L. Harris, and N.M. Trahey. 2001. "NIST Mechanisms for Disseminating Measurements." *Journal of Research of the National Institute of Standards and Technology* 106(1):315–340.

Montgomery, R.R., ed. 2011. *SRM Spotlight*. March. https://www.nist.gov/publications/srm-spotlight-1.

[1] See, for example, Gills et al. (2001).

[2] See, for example, Montgomery (2011).

11
Material Measurement Laboratory's Responses to the Findings and Recommendations of the Fiscal Year 2020 Assessment Report

This chapter presents the Material Measurement Laboratory's (MML's) responses to the findings and recommendations made in the previous review by the National Academies of Sciences, Engineering, and Medicine in *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020* (NASEM 2021; hereafter "the FY 2020 Assessment."). The sections below are verbatim MML's responses (NIST 2023). The panel recognizes and appreciates the actions taken by MML in response to the FY 2020 Assessment.

Across the MML divisions, the FY 2020 Assessment found the following common core attributes: a high technical quality of the research, excellence of the scientific staff, strong customer outreach and scientific collaboration, and strong publication and dissemination activities. It was clear that MML digested the FY 2020 Assessment and enacted real change in response. The panel concluded that MML is in high demand by external stakeholders, its relevant technologies are leading edge and dynamically changing, and there is competition for individuals with the expertise required of its staff. MML therefore faces challenges with respect to achieving an effective balance between maintaining its success in ongoing efforts and initiating new efforts that represent appropriate investment of MML resources in niches that will produce the best impact. These include appropriately allocating the resources of its staff, who are stretched thin in several areas; utilizing MML's network of former postdocs as brand ambassadors; devising succession plans in anticipation of staff who will leave; maintaining an equipment infrastructure by applying make/buy/borrow/share strategies that provide state-of-the-art capabilities within cost constraints; and ensuring that the mission priorities of MML scientists and the National Institute of Standards and Technology's (NIST's) administrative and legal staff are aligned with respect to purchasing of equipment and other resources. Detailed responses to the FY 2020 Assessment recommendations can be found below.

OFFICE OF REFERENCE MATERIALS

Recommendation 3-1: The Office of Reference Materials (ORM) should plan and host a series of topic-focused workshops with participation from industry, academia, and other government organizations to benchmark and identify state-of-the-art business practices, ecommerce tools/platforms, marketing and sales operations, packaging, and other areas critical to its operations. As part of such an undertaking, ORM should assess the appropriateness and feasibility of outsourcing portions of its operations or the expanded use of public-private partnerships to increase efficiency of its operations including standard reference material fabrication, storage (inventory control), packaging, and other critical operations.

MML Response to Recommendation 3-1:

ORM has licensed non-exclusive distribution agreements with Laboratory of the Government Chemist (LGC) and Millipore Sigma. LGC is the private business arm of the UK national

metrology laboratory. Millipore/Sigma is one of the largest for-profit certified reference material producers (Our relationship prior to 2020 was limited to distribution of our products through their supply chain. Currently (FY 2022) nearly 21% of our sales are handled by these two businesses, up from 11% approximately 7 years ago. As of 2020, ORM has been in discussions to increase our utilization of the capabilities of each of these two CRM producers. We are providing them with advanced marketing materials for new and renewal products and advanced information regarding products in our pipeline.

We've met with LGC and Millipore leadership to discuss expanding our relationships. Given that both have significant manufacturing, packaging and certification capabilities as well as secure supply chains (from warehouse to customer) it behooves ORM to learn and partner with these entities. Currently NIST (ORM) makes no distinction between selling to an end user, a licensed distributor, or a reseller. This was never a problem for our "20th" century products, i.e., cements, metals, organic solutions and industrial materials. Now however our portfolio is evolving to include protein biologics, health and clinical materials, and cells, all of which require exquisite handling and storage to ensure the integrity of our certified reference materials. In the next FY we will be exploring the practice of pre-positioning NIST SRM products in accredited warehouses for both LGC and Millipore to ensure adequate care of our products for our foreign customers. We anticipate prepositioning product in both the EU (Germany) and Asia (Singapore). In addition, the ORM director is in discussion with both regarding advanced packaging, processing and distribution of NIST products, perhaps under a co-label. The ORM director is also engaged internally and externally to determine the feasibility of expanding the NIST Traceable Reference Materials (NTRM) beyond our SRM gas program. Implementation of this program could ensure adequate supply of our products to our stakeholders, expand upon the offerings of our SRM program, and relieve our laboratorians of time-consuming support work related to SRM support (i.e., stability monitoring, homogeneity assessment etc.).

Workshop on Digital NIST in September 2022. Over 450 participants were in attendance at this virtual conference. Included were discussions on digital reference material certificates. Worked with industry, academia and government to gauge interest in developing a digital alternative to the current SRM paper and PDF certificates. A white paper was published and efforts are underway to implement these new certificates. This will be a much more technically challenging task than creating digital calibration certificates as SRMS have many more and different measurands and SRM certificates have a diversity of formats.

E-commerce. ORM IT team implemented and transitioned all measurement services from custom in-house software business systems to *the* NIST store front. Now all measurement services are on one common platform serviced and aided by ORM's implementation of Sales Force customer relationship management system.

Development of Research Grade Test Materials Concept. Originally developed from a strategic plan eight years ago to fully realized in FY22 to improve evaluation of candidate materials for RM/SRM development. ORM is currently developing the infrastructure to assist in all phases of implementation of the RGTM process to include support for SDS authoring, shipping and packaging expertise, and ecommerce implementation (document retention) to support in excess of 20 interlaboratory studies per year. Expanding service to possibly all of NIST.

NTRM. Started discussions with external CRM producers to support joint efforts on making and supporting RM's that are out of stock and/or need external manufacturing capability.

Other NMIs. Actively *engaged* with NMIA and JRC Geel to discuss business models and share best practices.

Recommendation 3-2: The Office of Reference Materials should develop processes and procedures to strategically select and prioritize the use of working capital funds toward high demand products, which can maximize the throughput and return value; and examine methods to accelerate and evaluate the development of these new standard reference material products. The evaluation can be used to further promote and/or incentivize the MML division-level SRM development.

MML Response to Recommendation 3-2:

ORM has modified our process for evaluation of service development projects. We utilize the RGTM process that includes an interlaboratory study to gauge stakeholder interest and engagement and feedback on proposed projects. With regard to ongoing production projects, we do, in collaboration with the participating division, prioritize development and renewal of high demand SRM's over less in-demand products, to maximize our ROI from the WCF.

Recommendation 3-3: The Office of Reference Materials (ORM) should conduct informational symposia and workshops to better communicate the vital role that ORM plays in the mission of NIST and to highlight success stories. The office should also provide more systematic evaluation feedback and greater incentives for MML division staff to more effectively and efficiently develop new standard reference materials that are aligned with the needs of industry.

MML Response to Recommendation 3-3:

In FY 22 the ORM director gave three internal talks on education and improvement for SD projects and the new RGTM process to MML specific and NIST general audiences. In FY 21 the ORM director gave four division level internal talks to discuss the "Guide to SRM Development" and the impact of several of our newer products. The ORM director and staff regularly meet one on one and in groups to discuss all aspects of measurement service development from origination of ideas to funding, to stakeholder engagement and outreach. Beginning in April of FY 23 ORM will host SD projects presentations to the NIST audience to encourage participation from those unfamiliar with SRMs and to share the very excellent science and metrology of the supported projects.

OFFICE OF DATA AND INFORMATICS

Recommendation 4-1: The Material Measurement Laboratory management should promote the concept of "data as an asset" and its associated culture within the Laboratory. With that understanding, management can be expected to advocate and support its adoption throughout the organization, resulting in increased professionalism within NIST, higher quality of output by NIST, increased impact of NIST products on the STEM world, and public perception of NIST as a leader.

MML Response to Recommendation 4-1:

Since the 2020 NASEM assessment, MML has developed complementary efforts aimed at leveraging Data as an Asset, driven initially by elements of the MML strategic plan for Next Generation Data. These efforts included establishment of Laboratory Information Management Systems (LIMS), a data infrastructure development and deployment effort referred to as Data Plumbing, and work to support development of sound Artificial Intelligence (AI) and Machine Learning (ML) tools.

In 2020, led by the Office of Data and Informatics (ODI), MML assembled a team of representatives from across MML to establish a LIMS Community of Interest (COI). This team prioritized projects from each division, which were used to develop and prototype LIMS capabilities. These projects factored in lessons learned from early LIMS adopters such as MML's NIST Center for Automotive Lightweighting. In recent years, this effort has produced several successful and hi-impact LIMS, including the NexusLIMS which serves electron microscopy facilities across MML and NIST. To spread LIMS further, core shared services and infrastructure and specialized tools for research were developed, supported in large part by the Data Plumbing effort, discussed next. These capabilities, and related best practices, were developed in consultation with research subject matter experts and Data Science experts from both within and outside of NIST. In 2021, the MML LIMS COI published a roadmap for MML that serves as a key guide to ongoing development of LIMS capacity.

The Data Plumbing effort has been highly successful establishing infrastructure needed to automate and orchestrate data movement from instruments laboratories, through local network storage to newly deployed centralized storage. In partnership with the NIST Office of Information Systems Management, MML purchased a modern EMC Isilon 1.25 Petabyte storage array for centralized storage of research data. This highly redundant, highly available storage ensures that MML's valuable data is both protected and accessible. This new enterprise class storage array provides key capabilities for MML researchers to store and access large datasets from across the NIST network and to integrate data for machine learning and other advanced analyses. In addition, the Data Plumbing project has deployed infrastructure to automate data transfers from laboratory instruments to central storage. Data files are stored in a structure that identifies originating instrument, creation date, and in some cases instrument operator. Files are read-only to preserve data integrity and are broadly accessible to NIST researchers. Storing data in a secure, defined, broadly accessible location is seen as the foundation for all future data management efforts. To date, approximately 95 instruments have been "plumbed" for automated data transfer.

Deployment of AI/ML capabilities have been widespread across NIST, and research data is the critical component to the development of algorithms and validation of solutions. To leverage its own data, MML Established the MML AI/ML working group, which has identified data and code assets to benchmark and demonstrate AI/ML in the research mission space.

In addition, the MML ODI continues to work with the NIST Special Programs Office and NIST Library services to provide Data Management Planning tooling and Data Publication services critical to establishing data as an asset for the organization. More details are specified in Division 641 NASEM report chapter. It is notable the MML continues to lead efforts in critical exercises for data management planning, documentation and support across NIST. Exercises are underway to expand practice and use of planning tools, within the context of individual areas of research.

Recommendation 4-2: The Office of Data and Informatics (ODI) should build out structures for enhancing divisional interactions. One concrete mechanism for this is to create tightly integrated multidisciplinary teams, which include ODI domain expertise as an integral part of a research team. The concept of "research software engineering" has been advocated as one such mechanism for creating research teams that can respond to the centrality of data and computation in a research activity.

MML Response to Recommendation 4-2:

ODI has made greater use of detail assignments from other divisions in MML to broaden both our capacity and our footprint in the laboratory. We also have less formal liaison agreements with MML staff from other divisions who regularly participate in group and division meetings. Detailees and liaison staff have joined ODI from divisions 642, 643, 646, and 647, and we have worked closely with 642 on the AMBench platform and 644 on the deployment of LIMS for biosciences. We also have close collaborations with the NIST Library (data curation and publication, Research Data Framework).

Finding: Postdoctoral fellows are being used effectively in other organizational units within the MML, however within ODI their use is limited. This is understandable given the service-oriented nature of their mission. However, even within these confines, postdocs could be used effectively to both to advance the direct goals of ODI, but more importantly to act as agents of culture change across the laboratory toward an awareness of data as a product. ODI is already engaged in training with its programs in "software carpentry."

MML Response to Finding:

Widely used methods for recruitment of postdocs at NIST are not amenable ODI. For example, the NRC postdoc competition does not focus on data science. We have made some efforts to build stronger connections with MML postdocs whose research relies on data science and AI/ML.

Recommendation 4-3: The "software carpentry" program should be expanded to include rotations of postdocs through ODI for more extensive, hands-on guidance. In addition, identifying postdocs in the MML divisions with an understanding of the importance of sound computational techniques and establishing joint mentorship programs with those divisions and ODI would be beneficial.

MML Response to Recommendation 4-3:

This is an excellent suggestion. Due to competing priorities, ODI has not yet been able to expand the software carpentry program. As noted in Response 4.2, ODI has expanded its efforts to interact with division staff in ways that include mentorship and other guidance on sound computational techniques.

Recommendation 4-4: The Material Measurement Laboratory should enhance engagement with creation/integration of reference materials.

MML Response to Recommendation 4-4:

Development of reference materials occurs in MML's technical divisions, with the MML ORM coordinating seed funding, scale up, packaging, sales and distribution. Respectfully, is unclear what this recommendation suggests ODI or MML do or change with respect to reference materials development.

MATERIALS SCIENCE AND ENGINEERING DIVISION

Finding: The computational work of the Thermodynamics and Kinetics group is well ahead of many other entities outside of NIST.

Recommendation 5-1: The Materials Science and Engineering Division (MSED) should consider investment in additional high-performance computing resources to continue the comparative advantage the Thermodynamics and Kinetics group holds. In making such investments, MSED should maintain balance with empirical approaches.

MML Response to Recommendation 5-1:

MSED operates the Center for Theoretical and Computational Materials Science (CTCMS), a high-performance computing (HPC) resource supporting computational research in MSED (and other MML divisions), including the efforts within the Thermodynamics and Kinetics Group. MSED makes annual investments of approximately $200K that largely maintain current capabilities as computing hardware technologies advance. MSED similarly provides approximately $100K annually to support another HPC resource at NIST (Raritan, operated by OISM on behalf of participating labs) in addition to the annual use-based charges (≈$150K). Beyond these annual investments, there have been a few recent targeted investments that support specific use cases / projects in MSED and in other MML divisions, some of which have increased CTCMS capabilities to provide value to other users (e.g., GPU resources, additional nodes and storage). Additionally, many of the MGI-supported efforts in MSED involve data repositories that depend on the NIST Configurable Data Curation System (CDCS) as their data infrastructure, such that MSED invests in contract support for the associated CDCS instances. MSED does not currently have the resources to invest beyond these largely maintenance level support costs. Strategic investment and associated NIST-level commitment is needed (and is the subject of NIST HPC planning efforts) to support the broader NIST community in this regard.

These limited investments reflect the current resource constrained environment and an effort to balance investment needs across our portfolio, including experimental capabilities that support empirical approaches. Recent examples specific to the Thermodynamics and Kinetics Group

include a gas-cooled vacuum furnace (replaces 20+ year old system, procurement underway), a lab-scale directed energy deposition (DED) additive manufacturing capability (procurements underway), and electron microscopy upgrades that included a broad-beam ion mill and new XEDS/EBSD detectors for our JEOL 7100 SEM (procurements complete).

Recommendation 5-2: The Materials Science and Engineering Division should develop a clear articulation of a broad-based strategic plan of the division and state how that plan reflects the overarching strategic plan of the Material Measurement Laboratory.

MML Response to Recommendation 5-2:

MSED has developed a new strategic plan. Strategic planning activities commenced in FY2021 following the 2020 NASEM review, culminating in a living strategic plan that is being used to prioritize investments during this period of intense resource constraints. This plan includes prioritization of scientific staff / expertise and investments in equipment, computational / data resources, and associated facilities. Three strategic goals were established to support state-of-the-art core competencies that provide unique value and impacts for our stakeholders and for addressing national initiatives (Goal 1), to modernize and sustain critical measurement services and standards efforts (Goal 2), and to expand capabilities in lab automation, high-throughput computation, and AI/ML methods to seed new capabilities in support of specific stakeholder needs in data and informatics (Goal 3). These goals support NIST Strategic Goal 1: Position NIST to Advance U.S. Science and Innovation, NIST Strategic Goal 2: Maximize NIST's Stakeholder Impact through High-Value Service Delivery as well as several current Administration initiatives. In terms of the 2015 MML Strategic Plan, MSED Goal 1 aligns with MML Goal 1: Measurement Science Excellence; MSED Goal 2 aligns with MML Goal 2: Measurement Service Excellence; and MSED Goal 3 aligns with MML Goal 3: Data Science and Data Management Capabilities. Additionally, MSED Goal 1 supports MML Goal 4: Strategic Partnering and Customer Engagement.

Recommendation 5-3: The Material Measurement Laboratory (MML) should evaluate how it budgets new equipment purchases and how this figure into the resource management in its divisions. The MML should further remain aware of the damage to equipment due to flooding and other problems with buildings and facilities.

MML Response to Recommendation 5-3:

MML to respond and may consider including the following information. Due to continued resource limitations brought on by increasing labor costs, overhead rates, renovation costs, equipment maintenance costs, etc., MSED has chosen to reduce its division overhead rate to a level just above the minimum required based on the Invested Equipment (IE) loan model that is part of the NIST WCF. That minimum level supports only a very limited set of annual equipment purchases and is often needed to upgrade or replace aging equipment across the division. Likewise, MML's IE allocation is very limited relative to the needs across the lab.

MML Leadership has helped influence NIST-level changes to WCF / OH policies / management of high-dollar (shared) equipment needed to enable some new equipment purchases. While more movement is needed from NIST, MML was successful in arguing that purchases made with other agency funds be treated to a much lower OH rate.

Recommendation 5-4: The Material Measurement Laboratory should increase its activities aimed at communicating its accomplishments to its customers, collaborators, and audiences. This should include greater effort at highlighting results from the primary work of the laboratory. This could be accomplished using forms of media such as YouTube and improving the effectiveness of the NIST website by adding specific examples of unique and transformative contributions.

MML Response to Recommendation 5-4:

MSED has limited resources and capabilities for using multiple forms of media to communicate research achievements. We have focused efforts on revamping our external website over the past year, working within the constraints of Drupal, which governs the available webpage formats. MSED has also partnered on several occasions with NIST PAO to highlight division research efforts. Links to recent examples are found on our external webpage and include:

- Spotlight: Mimicking Our Own Senses to Detect Ovarian Cancer
- Spotlight: Blood Vessels on a Chip for Dental Research and More
- With Fuzzy Nanoparticles, Researchers Reveal a Way to Design Tougher Ballistic Materials
- Spotlight: The Behavior of Polymers in Our Recycled Plastics
- Thermal MagIC: New NIST Project to Build Nano-Thermometers Could Revolutionize Temperature Imaging

In-person, virtual, and hybrid workshops and meetings have been used to engage with customers and collaborators over the last several years.

MATERIALS MEASUREMENT SCIENCE DIVISION

Finding: The development, fabrication, and sale of standard reference materials and documentary standards are central to the mission of MMSD. MMSD has a broad client base for SRMs etc., but contacts are handled by other groups.

Recommendation 6-1: The Materials Measurement Science Division (MMSD) should increase the degree to which it utilizes its customers for feedback on new products and information with regard to emerging opportunities. To this end, the Material Measurement Laboratory should utilize a process for obtaining feedback. MMSD should increase its interaction with the offices managing sales of such products at NIST.

MML Response to Recommendation 6-1:

MMSD has a close relationship with the Office of Reference Materials (ORM), who manages the inventory and sales of new physical reference materials. For example, the MMSD Division Quality Manager reviews all customer inquiries received by ORM [at https://shop.nist.gov] to determine areas where MMSD should explore new reference materials projects and/or consider reissuing discontinued reference materials due to customer demand. This sharing of inquiry data is automated through ORM's purchase of a Salesforce CRM (customer relationship management) software. To this end, MMSD is planning a workshop in 2023 aimed at obtaining feedback from the X-ray user community on the needs and uses of various Standards Reference Materials. MMSD will use this information to inform future production, staffing levels, and timely availability of products to the community.

Finding: In 2017, MMSD initiated a new effort focusing on the separation, characterization, and quantification of nanoscale soft materials (including plastics) by adopting previously developed methods and by investigating new approaches.

Finding: The shift in emphasis toward nanoscale soft materials is an excellent area for growth but may require new equipment and expertise, because the group was previously focused primarily on hard materials.

Finding: The group name for the Materials for Energy and Sustainable Development Group seems to be outdated. While there is research on energy materials, the increasing focus of the group appears to be in the area of high-throughput materials, materials data, and autonomous materials science.

Recommendation 6-2: The Materials Measurement Science Division should evaluate whether to move some of the work of the Materials for Energy and Sustainable Development group (e.g., X-ray Metrology) to another group (e.g., Materials Structure and Data Group) and refocus the former group's efforts on materials data and artificial intelligence approaches.

MML Response to Recommendation 6-2:

In 2021, MMSD began a reorganization process to better support the programmatic focus areas. Researchers working on the X-ray Metrology project are now a part of the 'Nanomechanical Properties Group' where they continue to collaborate and coordinate the production of X-ray Metrology related SRMs. The Data and AI-Driven Materials Science Group (formerly known as the Materials for Energy and Sustainable Development Group) has realigned to conduct research, develop, and disseminates measurement science, data, models, workflows, and technologies pertaining to AI-driven materials science and data infrastructure operations related to materials and measurement science.

Recommendation 6-3: The Materials Measurement Science Division should conduct additional intra-divisional collaboration, which might be exploited to add fundamental understanding for the benefit of the research component of the work going forward.

MML Response to Recommendation 6-3:

Since 2020, MMSD has identified six focus areas representing the division programmatic priorities. The focus area goals leverage core competencies across groups thereby promoting the assembly of diverse and agile research teams within the division.

Further recognizing the importance of supporting intra-division collaboration, the division has begun removing operational and/or cultural barriers to collaborative science. As a catalyst for more impactful intra-division collaboration, the division has had numerous cross-group/division-wide discussions and technical "showcases" targeted our priority programs towards elevating all staffs' awareness of resources and technical efforts within the division.

Recommendation 6-4: The management of the Materials Measurement Science Division will need to continue to evaluate and understand the impact of the change in staff numbers and redistribution of workloads. Specifically, there needs to be a shared understanding of the division mission that justifies staff numbers.

MML Response to Recommendation 6-4:

The Division is constantly evaluating the impact of staff numbers on programmatic focus and impact. We have recently adopted a "single point of failure" analysis for several projects, which involves understanding what research efforts or relationships would be substantially impaired should a single staff member cease their activity, and continually evaluate staff motivation, engagement, and growth through the life of a given project. Since the beginning of the global pandemic (early 2020), the Division Office has held Division-wide meetings twice a month to communicate the Division's mission, purpose, core competencies, and focus areas. The Division also strives for transparency about new hires, promotions, and equipment upgrades/purchases to help reinforce communication about Division priorities.

Finding: The MMSD has the lowest female/male ratio compared with other divisions in the Material Measurement Laboratory.

Recommendation 6-5: The Materials Measurement Science Division (MMSD) should examine ways to recruit and retain greater numbers of female scientific staff. MMSD staff should all work to enhance the visibility of NIST as a career option through technical meeting/society activities

and university interactions. All team members should ensure inclusiveness and assist with career development of the diverse workforce, including the careers of associates and post docs.

MML Response to Recommendation 6-5:

Hiring: Since 2020, MMSD has implemented MML's best hiring practices aimed at increasing transparency and fairness in the hiring process thus promoting a more diverse pool of qualified applicants. Two management vacancy positions (Deputy Division Chief and Group Leader) were competed, attracting strong diverse candidates. The selection process included input from diverse sources such as management, technical, and administrative staff. This process resulted in two female applicants being identified as best qualified for the needs of the organization and now serve in the Division management team.

Promotions: Since 2020, three female scientists were promoted to ZP V, the highest pay band level for NIST in recognition of their outstanding technical leadership and impact in their field.

Recruitment: MMSD launched the MMSD Academic Showcase Seminar aimed at inviting guest academic speakers to exchange ideas, identify areas of potential collaboration, and promote MMSD's programs to future NRC/post-doctoral candidates. Furthermore, MMSD now utilizes LinkedIn to promote the division and its staff scientific achievements to a broad audience and LinkedIn Recruiter as a tool to attract a diverse applicant pool to opportunities within the division.

Retain: MMSD has recommitted its internal efforts to have an engaged and inclusive work environment. In 2022, MMSD held a 'People' off-site where all staff, including associates and post-docs were invited to participate, provide feedback, and develop a strategic plan on how to improve the division. Initiatives such as improved onboarding for incoming staff, internal events that promote staff engagement and launching an informal mentoring group for early career staff are being led by two internal working groups.

Finding: MMSD recognizes the need for sustainable funding for higher-cost instrumentation (>$2 million) as a division priority. The Synchrotron Science Group has recently developed beam lines at NSLS-II supported by division funds. NIST policies that add cost to purchases increases the burden. Other needs are to address aging buildings and facility requirements for special instrumentation. (See Recommendation 5-3.)

Finding: The work of the MMSD is extremely dependent on access to state-of-the-art instrumentation. There were areas in which current new technologies are needed as a group moves into exciting new areas such as soft materials. Other instrumentation is aging and will need replacement in the near future (e.g., 3D atom probe instrumentation and electron microscopes). NIST extensively uses national user facilities beyond MMSD, particularly when instrument development is not a part of the project.

Recommendation 6-6: The Materials Measurement Science Division should prioritize the division's needs for upgrading/replacement of equipment.

MML Response to Recommendation 6-6:

The Materials Measurement Science Division is continually assessing all resources, including equipment, instrumentation, facilities, and personnel. There is a formal assessment at the beginning of each fiscal year, with a subsequent prioritization and process for funding consideration. Prioritization is based on many factors, including, but not limited to, strengthening the Division's core competencies, growing programmatic focus areas, and succession planning. Where possible, the Division attempts to leverage the servicing of existing and purchase of new instrumentation and throughout both the Division, MML, and NIST. For example, the Division shares several electron microscopy service contracts with other MML Divisions and another Laboratory. More recently, the Division has purchased several new instruments through a cost-sharing relationship with other Divisions and the MML Lab Office. Such equipment purchases would have otherwise proved insurmountable for our Division alone, but MML staff and management are always seeking ways to collaborate, and the MML Lab Office has remained quite supportive for our programmatic needs.

BIOSYSTEMS AND BIOMATERIALS DIVISION

Finding: BBD has built an exceptionally strong network of collaborators and stakeholders comprised of government entities, academic institutions, and industry, which has allowed for strong technical programs and scientific capability. The challenge will be to continue to build these assets sustainably and further to enable agility as U.S. economic factors shift.

Recommendation 7-1: The Biosystems and Biomaterials Division (BBD) should (1) with creativity, develop a business strategy that focuses on BBD's unique products that may include licensing and further consortia for use of BBD products, services, and expertise; (2) strategically place BBD postdoctoral fellows into industry, academia, and other government positions to improve connectivity with outside current and future collaborators and stakeholders; (3) hire or contract with a communications person with YouTube and other media expertise to reach individuals who are searching for BBD-type expertise, products, and research services; and (4) determine how to connect with quality and manufacturing personnel at small and medium-sized companies in targeted industries. Emphasizing NIST BBD leadership, with thoughtfulness and quantification, in BBD program areas should be addressed by BBD leadership and staff to further enhance leadership with collaborators and stakeholders.

MML Response to Recommendation 7-1:

(1) Since the 2020 panel review, the BBD has established two new NIST-led consortia, the Rapid Microbial Testing Methods Consortium (launched in June 2020) and the Flow Cytometry Standards Consortium (launched in Dec. 2020) that leverage NIST technology and standards expertise to address critical pre-competitive needs of the Regenerative Medicine and Advanced Therapies (RMAT) stakeholder community. As of December 2022, we have established over 170 formal agreements (CRADAs, MTAs, etc.) with companies and other organizations to collaborate on joint research, technology, and standards development projects that advance BBD's core capabilities, technologies, and measurement science expertise.

(2) We collaborate closely with industry, other federal agencies, and academic labs to enable novel and robust technologies and tools to support stakeholder needs. We leverage the strategic placement of our postdocs in outside labs to transfer NIST knowledge and expertise in measurement science, standards, and technology development. Some recent examples include:

- One NIST postdoctoral fellow in engineering biology used his NIST experience to launch a position as a senior scientist in protein engineering with Absci in Portland, Oregon.
- One NIST postdoctoral fellow in engineering biology transitioned from NIST to a successful consulting position for DARPA's Biological Technologies Office with Booze Allen Hamilton.

(3) We have been working closely with communications experts (e.g., science writers, social media writer/editors, graphic designers) in the NIST Public Affairs Office and leveraging their expertise and tools to develop news articles, podcasts, blog posts, graphics/artwork, and tweets to inform the public and NIST stakeholders about BBD's technical outputs such as high impact publications, standards, workshops, and product releases. Recent examples of high-performing content include:

- News article on implementing systems thinking/data in training the regenerative medicine workforce (January 12, 2023). LinkedIn
- News article related to the updated human genome (March 31, 2022). Facebook, Twitter, LinkedIn, Reddit.
- New article related to the development of biological computers that could potentially persist inside cells. (March 23, 2022). Facebook, Twitter, LinkedIn, Reddit.
- Feature-style post about taking a closer look at the human gut's interactions with nanoplastics (January 18, 2022). Facebook, Twitter, LinkedIn, Instagram.

(4) Our Consortia are designed to be inclusive, including small and medium size companies. Examples include Slinshot Biosciences, Spherotech, and BioLegend, Inc. We continue technical

expertise to the NIST Manufacturing Extension Program (MEP) program, a program dedicated to serving small and medium-sized businesses.

Recommendation 7-2: The Biosystems and Biomaterials Division should improve awareness of its products and capabilities, especially within small to medium-size enterprises and companies that are not currently stakeholders because they are in different industries (e.g., agriculture).

MML Response to Recommendation 7-2:

Our multidisciplinary team of scientists and engineers develop foundational measurement science and capabilities that serve a number of applications and different sectors of the bioeconomy. Our programs are designed to be agile and address the most pressing needs in various emerging industrial applications. For example, we have recently recruited a postdoc to our Engineering Biology Program, who brings expertise in culturing environmental microbes, such as those found in soil. She is transferring protocols and knowledge on measuring differential gene expression in microbes exposed to environmental pollutants, through RNA sequencing including the bioinformatics pipeline for the associated data. Another recent postdoc recruit brings expertise in yeast microbiology, especially engineering GPCR protein sensors for therapeutic applications. He also brings experience with ML/AI tools for protein engineering and library design for directed evolution. The NIST Genome Editing Consortium is focused on addressing the measurements and standards needed to increase confidence and lower the risk of utilizing genome editing technologies in research and commercial products mainly in the advanced therapies sector. However, the measurements and standards developed are applicable to other sectors such as agriculture.

Recommendation 7-3: The Material Measurement Laboratory should evaluate whether the square footage assigned the Biosystems and Biomaterials Division is commensurate with the division's current size and mission.

MML Response to Recommendation 7-3:

Since the 2020 Panel review, the BBD has established multiple measurement capabilities to support the National priority areas of Engineering Biology, Microbiome, and RMAT. Additional space is urgently needed to continue to grow these emerging programs, but our laboratory spaces in buildings 227 and 224 are at full capacity. To address our pressing space needs, we have been working closely with MML leadership to identify space currently occupied by the ADA in building 224. As of January 2023, MML has agreed to provide 5 additional laboratory modules to help alleviate our pressing microbial program space needs in the short term. Access to additional space will also improve laboratory safety by reducing unnecessary exposure to potential hazards due to overcrowding and clutter (e.g., tripping hazards and storing heavy items high up) and providing sufficient bench space to safely work in the labs and ensure our laboratories are aligned with our Quality Management System. We continue to work with MML to initiate formal evaluation to determine whether the square footage assigned the BBD is commensurate with the division's current size and mission.

Recommendation 7-4: The Biosystems and Biomaterials Division should provide additional resources in thermodynamics, fluid mechanics, colloidal science, virology, immunology, microbiology, and bioinformatics in a manner commensurate with the increasing importance of these specialties.

MML Response to Recommendation 7-4:

Since the 2020 panel review, the BBD has established new programs in virology (e.g., viral and non-viral vectors), immunology (e.g., serology and neutralization assays for SARS-CoV-2), microbiology (e.g., Mpox Research Grade Test Material 10223), and bioinformatics (e.g., genomic cybersecurity, LIMS/data infrastructure for managing data/metadata in collaboration with

NASA/JPL). We were able to obtain additional funding to expand into adjacent disciplines related to material science and have strengthened partnership with other parts of NIST with deep domain expertise in thermodynamics, and colloidal science.

Recommendation 7-5: The Biosystems and Biomaterials Division should analyze underserved minority representation among its staff and develop an action plan to address findings both from such study and from NIST's equity disparity studies.

MML Response to Recommendation 7-5:

BBD is actively contributing to the broader NIST DEIA efforts. We consider underserved minority representation in our hiring practices. Through a partnership with Morgan State University, we provide paid internship opportunities to two graduate students. We have asked appropriate NIST offices with the proper authority to collect data related the BBD's ethnic and diversity composition so that we can conduct analysis and develop appropriate action plans.

Recommendation 7-6: The Biosystems and Biomaterials Division should develop a plan for outplacing long-tenured postdoctoral fellows into synergistic positions in industry, academia, or government. This plan should include an assessment of what shortfall, if any, this might create in its staffing plans.

MML Response to Recommendation 7-6:

The BBD did not have any long-tenured postdoctoral fellows at the time of the 2020 review or during the current review period. The BBD benefits greatly from the contributions of our postdocs in terms of carrying out our mission, building alliances and bridges to other organizations, and mentoring students. We greatly support the career goals of each of our postdocs and in addition to the research and training opportunities that are available to them at NIST, they have the opportunity to meet and connect with NIST stakeholders through workshops, consortia, and other collaborative efforts that are relevant to their research and future career goals. For example, we have joined the Global Biofoundry Alliance (GBA), where we placed a postdoc, who was engineering protein sensors with our automated workflows. This provided the necessary experience for the postdoc and enabled him to take a position with the bio foundry at the Concordia Genome Foundry at Concordia University in Montreal, Canada.

Recommendation 7-7: The Biosystems and Biomaterials Division leadership should implement cross-training of staff with intent during each year to mitigate the effects of loss of key staff and ensure continuity.

MML Response to Recommendation 7-7:

We work to ensure that protocols important to our workflows are shared across the BBD (e.g., between technicians and from postdocs to technicians), to help guard against the loss of this knowledge in the Division. Our staff have also implemented electronic resources (e-notebooks, LIMS) that are shared across the groups and Division, to ensure access to protocols, data, and metadata associated with measurements and laboratory operations.

BIOMOLECULAR MEASUREMENT DIVISION

Finding: The applications of artificial intelligence (AI) and machine learning (ML) have now permeated the science and engineering fields, enabling discoveries and insights not previously possible. Indeed, these methods have now become common and indispensable components of virtually all analytical or measurement methods. The list of BMD applications includes MS spectra/databases, NMR library contours, retention index analyses, forensics, and others. An

AI/ML expert would likely provide novel insights into the embedding of these methods throughout the division as well as playing an educational role.

Recommendation 8-1: The Biological Measurement Division (BMD) should evaluate its portfolio of expertise of staff with expertise in artificial intelligence and machine learning as applied to the measurement tools specifically in BMD. BMD might want to consider a joint hire with another division to leverage additional expertise and resources, or develop a more centralized collaboration model (i.e., community of practice) to make enhanced use of AI/ML expertise.

MML Response to Recommendation 8-1:

The BMD has taken several steps to address this recommendation. First, the BMD evaluated its portfolio of staff expertise and projects in AI/ML. It was found that the BMD's activities in AI/ML fall into two broad categories: 1) the application of AI/ML approaches to advance biomolecular measurement science and tools, and 2) the development of reference materials and test data sets to advance AI/ML approaches applied to biomolecular measurement systems. Second, the BMD formed an AI/ML working group with a representative from each group to provide updates on AI/ML related projects in the division, exchange ideas, and to promote collaborations. A BMD staff member also represented MML on the NIST AI Community of Interest group, which helped the division to stay abreast of AI/ML activities and expertise across NIST and to raise the visibility of the BMD's activities. Third, the BMD actively sought to leverage expertise and resources both inside and outside of NIST to expand its portfolio of AI/ML-related projects. Examples of new collaborative AI/ML-related projects are given below.

A new collaboration between scientists in the BMD's Mass Spectrometry Data Center Group, the Biosystems and Biomaterials Division, and NIST's Information Technology Laboratory (ITL) was initiated to use and develop artificial intelligence and other machine learning methods for a new class of genomics Standard Reference Materials and proteomics Standard Reference Data. The project was funded by ITL through a Use-Inspired proposal competition. The Mass Spectrometry Data Center Group developed neural networks to predict peptide spectra from their sequences and potential modifications. The models were trained on well-characterized NIST mass spectral libraries using over one million MS2 peptide spectra. The models were able to predict spectra and to evaluate over the collision energy range over which predictions are valid. One paper has been submitted on the topic of using AI predictions to improve mass spectral library searching. Two additional papers are in preparation, one on spectral prediction of proteins with post-translational modifications, and another on creating reliable mass spectral datasets for AI.

The Bioprocess Measurements Group collaborates with researchers from the University of Colorado, the FDA, and Ursa Analytics, Inc. in the development of convolutional neural networks (CNNs) to analyze flow imaging microscopic images of protein particles. The presence of protein particles in formulated protein therapeutics and their potential impact on safety and efficacy are of great concern to the biopharmaceutical industry and regulators. A resulting publication demonstrates that CNN analysis of microscopy images was able to determine distinguishing "fingerprint" features for different preparations and materials and that NIST particle reference materials can be used as a repeatable, quantitative control for image acquisition and analysis. The approach is promising for quality control applications such as the detection of manufacturing deviations (DOI: 10.1007/s11095-021-03130-9).

The Biomolecular Structure and Function Group collaborates with researchers from ITL, Brown University, George Mason University, and the University of Pennsylvania to develop ML methods for analyzing cryo-electron microscopy images of mRNA-Lipid Nanoparticle (LNP) structures. The structures of mRNA-LNP vaccines and therapeutics are complex containing a range of diameters, water-filled pockets of different sizes with RNA present or absent in cores or pockets. Cryo-EM is a promising tool for characterizing this heterogeneity; however, the tracing of large numbers of LNPs by hand is intractable and simple algorithms for finding particles perform poorly due to low contrast. Two approaches are being evaluated: 1) the training of ML models on manually-annotated micrographs using "Cellpose", a deep-learning segmentation method designed for segmenting cells and 2) "U-net", which uses simulated images.

The BMD machine learning portfolio also includes collaborations between NMR spectroscopy groups at IBBR, computational scientists in ITL, and collaborators at the Network for Advanced NMR, sited jointly at UCONN, UGA, and UW. Nearly all interpretation of biomolecular NMR in two dimensions and higher is performed by interactive inspection of 2D contour plots by experts, and identifying peaks is a required step in most every NMR workflow, both for biomolecular data and small molecules. The goal of this project has been to use machine learning and other methods to build a system that can identify and characterize peaks as effectively as a human analyst can. The method must be able to identify partially resolved peaks, discriminate true signals from artifacts, and make high-quality decisions about whether two peaks are related. In a first approach, a UNET convolutional neural network architecture has been used to identify peaks in contour plot images via segmentation. The project benefits from the nature of NMR data, which allows realistic training spectra to be constructed completely synthetically from mathematical models, or semi-synthetically, by combining individual signals from measured spectra.

Finding: The majority of BMD's application areas are human based, that is forensics, biotherapeutics, Chimeric antigen receptor T cells (CAR T cells), and so forth. Significant opportunities may be present in areas beyond that applied to humans; these include agriculture, veterinary science, biocatalysis, and environmental and marine research areas.

Recommendation 8-2: The Biological Measurement Division (BMD) should develop a strategy to assess agriculture, veterinary science, biocatalysis, and environmental and marine research areas as possible opportunities for growth and sources of additional collaborations and funding.

MML Response to Recommendation 8-2:

Since the Panel's recommendation in 2020, the BMD has initiated several projects in other biotechnology sector areas:

The development of LC/MS approaches to screen and identifying plastic degrading enzymes. This project was supported by a new NIST Circular Economy Initiative.

The development of a mass spectral library of plasticisers in high volume, commodity polymers with applications towards plastics recycling – a project also supported by the Circular Economy Initiative.

In collaboration with the Chemical Sciences Division, the development of tree nut reference materials — hazelnut and almond flours — that will help ensure accurate and consistent results for test kits that regulators and food manufacturers can use to detect tree nut allergens.

In direct response to this recommendation, the BMD has also taken several actions to develop a programmatic strategy to assess measurements and standards needs of other biotechnology sectors so that we are positioned for future collaborations, funding opportunities, and growth. First, we have been engaging stakeholders to learn and assess current and emerging measurement and standards needs in these other sectors. We have found BioMade, a Manufacturing Innovation Institute (MII) founded in Oct. 2020, to be a useful resource. BioMade's goal is to advance sustainable and reliable bioindustrial manufacturing technologies for a wide array of products including chemicals, detergents, polymers, electronic films, fabrics, agricultural products (e.g., feedstock), crop protection solutions, food additives, fragrances, and flavors. Interactions with BioMade have been facilitated through the detail of a BMD staff member in NIST's Advanced Manufacturing National Program Office which coordinates Manufacturing USA, the network of MIIs across the country that includes the biotechnology MIIs NIIMBL, BioMade and the ARMI/BioFab. Second, BMD management team and staff have also attended numerous conferences and workshops that have dealt with biotechnology applications for industrial chemistry, agricultural, energy, or climate including a recent Oct. 2022 NASEM workshop "Successes and Challenges in Biomanufacturing". Third, we have played an active role in internal MML/NIST and interagency discussions on expanding the NIST biotechnology and biomanufacturing programs to advance key societal goals outlined by the Administration's recent Executive Order "Advancing Biotechnology and Biomanufacturing Innovation for a Sustainable, Safe, and Secure American Bioeconomy": (https://www.whitehouse.gov/briefing-

room/presidential-actions/2022/09/12/executive-order-on-advancing-biotechnology-and-biomanufacturing-innovation-for-a-sustainable-safe-and-secure-american-bioeconomy/).

Through these interactions and discussions we see the BMD and NIST playing important roles in providing measurement science and standards to support a wide array of emerging biomanufacturing technologies and products. Most biotechnology processes involve an upstream, cell culture operation where process analytical technologies (PAT) are used to generate real time data for monitoring and predicting process trajectories and ensuring the quality of products. Biomanufacturing facilities of the future will use PAT data combined with advanced, big data analytics including AI/ML to achieve consistent quality, higher yields, lower costs, and reduced waste – important goals for all bio-based production. Critical to the implementation of PAT will be the availability of robust measurement technologies with understood measurement uncertainty, the development of new measurement technologies, and platform standards to drive adoption of new manufacturing technologies. The BMD has initiated several efforts in upstream process measurement including the use of dielectric measurements for measuring live cell concentration, the use of NMR for on-line measurements of cell metabolites, and the use of LC/MS methods for at-line measurements of product attributes. These measurement approaches are general and applicable to any biomanufacturing process.

CHEMICAL SCIENCES DIVISION

Recommendation 9-1: The Chemical Sciences Division (CSD) should consider administrative changes to give greater definition to connectivity among the Division's scientists, including binning the teams in CSD to make commonalities with other groups more apparent; and, as warranted, splitting larger divisions and aggregating the groups into new divisions where similarities are strongest.

MML Response to Recommendation 9-1:

One of the strengths of the Chemical Sciences Division is the connection and interactions between members from different groups to provide metrological support to NIST stakeholders in the chemical sciences. The strength of these collaborations and synergies have significantly increased in recent years given the multidisciplinary nature of some of the grand challenge problems tackled by the Division. As an example, members from the Organic Chemical Metrology Group, Chemical Informatics Group, and the Biochemical and Exposure Science Group (in Charleston, SC) have been working together with scientists from the Engineering Laboratory in the development of a metrological framework aimed at the identification, characterization, and quantitation of PFAS in water, firefighter gear, sea food, and marine organisms.

Finding: The appropriated funds out of general taxpayer revenues (the STRS is one such account) is for the purposes of performing research and preparing and maintaining standards. Bureaucratic processes can unnecessarily impede mission progress. Cost-benefit analysis that values time devoted to research can elucidate this. A survey of how staff spend their time could assist management in quantifying this loss.

Recommendation 9-2: The Chemical Sciences Division should evaluate its portfolio to determine the fit to Material Measurement Laboratory's (MML's) strategy with a view toward adoption of a "steady state" economic model in which new costs are paid for by pruning existing operations. Alternatively, MML could adopt a "pay as you go" model in which they would add new programs, instrumentation, employees, and so forth as new funds become available, or by intentionally pursuing external funding in strategic areas.

MML Response to Recommendation 9-2:

For the most part, the Chemical Sciences Division does not have control over the allocation of NIST appropriated STRS funds. Once the STRS has been allocated to the Division, the proper

resources are dedicated in support of the programs and technical activities within the groups based on a diverse set of drivers, including stakeholder needs, NIST mission, MML mission, and Division mission. In addition, the research and measurement service delivery needs are also driven by the following focus areas:

- Develop and maintain *state-of-the-art* chemical measurement capabilities.
- Generate, gather, curate and disseminate critically evaluated data.
- Develop, implement and validate accurate theoretical models and reliable chemical informatic tools.
- Conduct research concerning the qualitative and quantitative determination of chemical composition.
- Provide measurement service delivery activities based on focus area needs.
- Disseminate tools for measurement traceability and quality assurance (such as reference materials and other services).
- Demonstrate international comparability of U.S. standards for chemical measurements.

In recent years, the Division has been working with MML management to delineate a plan leading to a more sustainable and forward-looking funding model to support the development of our SRM programs and to modernize the Division's measurement services. NIST management has taken the suggestions of this plan and have included or are planning on including a line item in future NIST budgets to address these issues. Additionally, the Division management and the staff have been extremely active (and successful) at procuring additional funding from other agencies to support work in impactful programs that requires the technical excellence and expertise provided by the Division in Chemical Metrology.

Recommendation 9-3: The MML should create an instrumentation strategic plan as a useful mechanism to define the current status of instruments via a census (item, age, location, status, responsible person, availability) and prioritization of new instrumentation, as well as identify internal and external support (funds). The MML should also consider developing a plan for maintenance and eventual instrument replacement (where needed) as well as a means of relocating or repurposing underutilized resources.

MML Response to Recommendation 9-3:

The Division has appointed Kevin Huncik, from the Biochemical and Exposure Science Group, the Division Instrumentation Officer. One of his duties is to maintain a list of the instrumentation around the Division (including information regarding location, age, users, programs associated with the instruments, etc.), and advice the Division Chief in matters of repairs, maintenance, and acquisition of instruments.

Recommendation 9-4: The Chemical Sciences Division (CSD) should remain in contact with postdoctoral (NRC and Associate) and other categories of associates who have left CSD as a way of collecting input on emerging areas of concern, problems of note, and feedback on the adoption and implementation of CSD and Material Measurement Laboratory efforts.

MML Response to Recommendation 9-4:

In addition to exit interviews, CSD is actively keeping contact (whenever possible) with postdoctoral fellows that find employment outside NIST. In addition to help the Division obtain invaluable input regarding new opportunities, these interactions have also provided CSD a very efficient vehicle to reach out to other young scientists that might be willing to come and work in our division.

APPLIED CHEMICALS AND MATERIALS DIVISION

Recommendation 10-1: The Applied Chemicals and Materials Division should create a capital equipment replacement plan that considers also the requirements for space and ongoing maintenance.

MML Response to Recommendation 10-1:

The ever-present need for investing in new capabilities requiring substantial capital equipment, replacing aging capital equipment where capabilities are still needed and the ongoing need to maintain capital equipment via service contracts requires financial resources that are beyond those strictly available within the Applied Chemical and Materials Division (ACMD). Accordingly, ACMD uses a multifaceted approach to addressing this need. First, at NIST, each division can have an Invested Equipment account which is roughly analogous to a capped home equity loan which can be used in the present for purchases and then paid back in the future. In addition, we can, and do, partner with the MML Lab Office to share costs on major equipment purchases and maintenance contracts. For example, in FY22, the Lab Office financed the purchase of a new Focused Ion Beam (FIB) tool to be located in MML Boulder lab space that will broadly support ACMD materials research. Much of the maintenance contracts expenses that ACMD incurs are associated with microscopy equipment in the NIST-Boulder Precision Imaging Facility (PIF). Increasing concern in recent years about these costs (as well as issues with user access) have resulted in a reorganization of PIF management where it is being organizationally incorporated into the Boulder Microfabrication Facility (BMF), an entity which reports directly to the Physical Measurement Laboratory (PML) Director. This new PIF subunit is now co-lead by one PML and one MML scientist to ensure access and operational concerns of both user groups are addressed. Further, the equipment maintenance costs are now handled at the Laboratory level. In addition to the above mechanisms for financing capital equipment purchases, ACMD keeps an active eye on the availability of suitable equipment on the Federal Government Excess Equipment list and the second-hand market. This can be especially useful when an equipment capability is needed in a more supporting role, but does not have to be state-of-the-art. For example, in FY22, ACMD acquired a lightly used laboratory scale x-ray diffraction system for just the cost of shipping and installation. In an ideal world, such looking for bargains would not be needed, but in the real world where research resources are always finite, such prudent purchasing results in additional funds for conducting research. On the topic of obtaining sufficient suitable laboratory space to enable optimal performance of capital equipment, that is generally beyond the control of an individual division. That said, ACMD will be getting five new on-grade laboratories in Building 1 Wing 4 once it is renovated (2024/2025) and NIST has begun the planning process to replace Buildings 2 and 24, which are two of the older research buildings on the Boulder campus.

Recommendation 10-2: The Applied Chemicals and Materials Division should take steps to realize the true value of standard reference data and standard reference materials thereby enabling revenue for growth of new programs.

MML Response to Recommendation 10-2:

The Applied Chemicals and Materials Division (ACMD) has two primary revenue generating standard reference programs which are the Charpy Standard Reference Materials (SRM) and the Thermodynamic Research Center Standard Reference Data (SRD) products exemplified by ThermoDynamic Engine (TDE). As originally authorized in the 1968 Standard Reference Data Act and amended in the 2017 American Innovation and Competitiveness Act, prices for SRM/SRD products sold or licensed by NIST shall be set to reflect the cost of producing and selling the product. Hence, the revenue to ACMD gained through the sales of SRM and SRD can, at most, only cover the costs associated with those specific programs. They cannot be a source of revenue for the growth of new programs. That said, ACMD is continuing to modernize and upgrade the SRM and SRD products and business models ACMD provides. Specifically, the Charpy SRM program brings in ~ $3.4M per year in sales. In addition to covering the full

production costs of the Charpy SRM's, this also covers the two ACMD staff who work full time on the Charpy program. To improve Charpy program customer service, the viability of using customer-provided electronic images of post-testing Charpy reference specimens was evaluated and a new online/e-mail based service was added to the Charpy verification program. This has been highly successful and was the basis for two ACMD staff receiving the NIST 2022 Judson C. French award for outstanding customer service by creating a digital verification program for Charpy standards involving >1900 customers per year in 60 countries. The resultant ever-increasing collection of post-test Charpy specimen images and associated data is now being used to develop an AI-based image evaluation tool with the expectation to be able to provide user-initiated on-demand evaluation and interpretation of Charpy specimen images. In general, such SRM capability development work is funded the NIST Standards Development (SD) program of the Office of Reference Materials. In short, both the current day operations and the forward-looking improvement of the Charpy SRM Program is self-financed. For the Thermodynamic Research Center SRD program, the annual revenue from SRD sales, subscriptions and consortium memberships is ~$600K, which covers roughly half the annual cost for providing these SRD services. Similarly, SRD sales of REFPROP bring in about $500K/year to ACMD which again covers about half the cost of producing, maintaining and distributing REFPROP. Both to potentially increase revenue and to serve more customers (stakeholders), the TRC is currently working with the Office of Data and Informatics to implement sales of *data extractions* (ie, customer-defined targeted subsets of the full TRC data and model collection) as there has been a dramatic increase in the demand for such a service due to researcher's interest in well curated data sets for training AI models. ACMD is also hiring a full-time application programmer to modernize the front end of both TDE and REFPROP, which will both improve their utility for customers and enable new sales modalities aimed at broadening the customer base for these SRD products.

Recommendation 10-3: MML should (1) clearly define the Applied Chemicals and Materials Division's (ACMD's) mission and how ACMD aligns within the Material Measurement Laboratory mission; and (2) integrate teams more closely with corresponding efforts in NIST Gaithersburg facilities.

MML Response to Recommendation 10-3:

The mission of the Applied Chemicals and Materials Division (ACMD) is *to characterize the properties and structures of industrially important fluids and materials, thereby providing a diverse stakeholder community with innovative measurements and models and dissemination of critically evaluated data, leading to improved processes and better products, as well as new and improved standards*. This mission is very well aligned with the higher-level mission of NIST *To promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.* "Applied" is part of the ACMD division name because of the ACMD focus on serving external stakeholders interests and needs in areas of chemical production including new greener chemical processes, reducing climate change through identification of alternate chemicals/processes, improving domestic manufacturing by advancing additive manufacturing, developing metrologies to advance the US semiconductor industry, developing robust breath analysis metrologies for public safety and human health and advancing metallurgy and metals metrology to enable meeting future infrastructure needs for new energy sources and/or mitigating climate change. While all but one ACMD staff member are located at NIST-Boulder, ACMD actively engages with NIST-Gaithersburg based staff and research groups to bring the best NIST resources and researchers together to address any specific challenge. At the present time, ACMD staff are engaged in 20 distinct cross-campus research collaborations of which 13 are not just cross-campus, but also involve collaborations with NIST staff outside of MML. One such project is a joint PML/MML effort on Semiconductor Gas Flow Metrology which is one of the five projects selected across NIST to receive FY22 funding as a NIST internal CHIPS Act quick start project. ACMD's very productive and increasing engagement in collaborative research with NIST-Gaithersburg stems in part from a 2019.

ACMD Leadership decision to be more actively engaged with NIST-Gaithersburg. Accordingly, greater attention was put on ensuring that ACMD subject matter experts attended relevant Gaithersburg based meetings and workshops and improved teleconferencing capabilities were established at ACMD in Boulder pre-COVID to facilitate high-quality remote meetings. The broader adoption of virtual meeting technologies and practices during the work-from-home period (2020 – 2022) has further reduced the barriers to facile cross-campus communication. With business travel returning to near pre-COVID levels, ACMD is once again sending staff to Gaithersburg as appropriate to ensure the continuation of effective collaborations. Finally, ACMD provides space for five MML HQ staff based at NIST-Boulder. This arrangement further improves ACMD communications with the MML Lab Office and Leadership.

Recommendation 10-4: The Applied Chemicals and Materials Division should continue to increase the number of high-risk projects.

MML Response to Recommendation 10-4:

In line with the Applied Chemicals and Materials Division (ACMD), MML and NIST missions, ACMD maintains a balance of providing (and modernizing) external stakeholder serving services and high-risk high-reward research projects to advance the state-of-the-art metrology in ACMD research domains. At NIST, one funding source for high-risk high-reward research is the internal NIST Innovations in Measurement Sciences (IMS) program. Each year, only two or three new projects are selected for funding NIST-wide and projects generally run for five years. ACMD is part of three active IMS research projects, *Measuring Intermolecular Interactions with Electric-Acoustic Spectroscopy* (started FY21), *Getting From Qubit to Mega-Qubit Quantum Computers with RF Calibrations* (started FY21) and *Metrology to Enable Hot Qubits* (started FY23). The selection process for new FY24 projects is underway and ACMD is leading one and part of three proposals that are still in contention after an initial 50% down-selection, although there is still a long way to go before specific proposals are selected for FY24 project starts. The 2022 CHIPS Act is also creating opportunities for new research at NIST. More specifically, ACMD submitted 13 new project ideas on advancing semiconductor materials metrology to the internal NIST Metrology R&D Program's recent initial call for ideas. Outside of the NIST IMS and CHIPS programs, ACMD staff are pursuing high-risk research projects in the areas of machine learning for predicting thermophysical properties of mixtures; re-inventing viscosity-liquid-equilibrium (VLE) measurements of mixtures through both NMR and microwave methods; entropy scaling to predict transport (dynamic) properties from equations of state (equilibrium properties); development of human breath metrology (breathomics) for public safety and public health needs; applications of NMR to quantifying CO2 sequestration in building materials; growth and grain-boundary metrology of engineered metallic bi-crystals to advance material property predictions; 3D printing of composite materials for biological and medical applications; and applications of nanoscale topological features in 2D materials to biological, filtering and sensing challenges among others. In summary, ACMD continues to be very actively engaged in advancing the state-of-the-art in science and metrology areas within the NIST mission and our scope of expertise.

REFERENCE

NASEM (National Academies of Sciences, Engineering, and Medicine). 2021. *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020.* Washington, DC: The National Academies Press. https://doi.org/10.17226/26048.

NIST (National Institute of Standards and Technology). 2023. "Read-Ahead Material for NASEM Assessment of MML." Received May 1 from Callie Higgins, Material Measurement Laboratory, NIST.

12
Overarching Themes, Key Recommendations, and Chapter-Specific Recommendations from This Assessment

OVERARCHING THEMES AND KEY RECOMMENDATIONS

Adequacy of Facilities and Equipment

As highlighted in the fiscal year (FY) 2020 National Academies of Sciences, Engineering, and Medicine assessment of the Material Measurement Laboratory (MML) (NASEM 2021) and more recently in the 2023 National Academies' report *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology* (NASEM 2023), aging facilities and infrastructure present significant handicaps. Notably, the report found that NIST research staff spent from 10 to 40 percent of their time working around facility shortcomings, with the typical reported values being 20 percent. (NASEM 2023) As direct consequence of these limitations, at NIST generally and specific to this report, MML researchers are left to mitigate these limitations through repeating their work or implementing workarounds with limited research budgets.

The MML laboratories in Boulder, Colorado, and Gaithersburg, Maryland, laboratories are negatively affected by poor temperature and humidity control, in addition to inadequate air flow in their laboratories, which are not compatible with state-of-the-art measurements and instrumentation. On the Gaithersburg campus, in 2022, aging infrastructure led to serious flooding of MML research laboratories, resulting in a loss of millions of dollars of equipment and lost time. The facilities are in general inadequate for the performance of modern materials chemistry related processes. Much of the infrastructure, both buildings and equipment, has exceeded its expected life, leading to time spent inefficiently compared to the capabilities of state-of-the-art facilities and equipment in academic and industry laboratories and at metrology institutes around the world. While MML research efforts are world-leading, aging facilities and infrastructure are such that MML is at the cusp of losing its world-leading position and its ability to continue to attract new generations of world-leading researchers.

> **Key Recommendation 1: The Material Measurement Laboratory (MML) and the National Institute of Standards and Technology Office of Facilities and Property Management should work together to identify and document critical laboratory infrastructure issues. They should collaborate to prioritize items that need to be addressed and create a plan with an associated timeline to address those needs. MML should actively encourage its researchers to document facilities issues and all associated time lost repeating experiments, and the portion of the research budget spent on working around facility issues.**

The identified infrastructure issues also represent safety issues: floods can easily lead to sparks that can in turn initiate fires; inadequate exhaust will lead to contaminated laboratory air that can negatively impact research product quality and in the long term can impact the health of research staff. As

a whole, aged infrastructure and equipment can have an impact on the overall attitude of the staff toward safety.

Safety involves an entire organization, including and particularly line management. Managers set the tone and monitor the progress against metrics. They participate in safety inspections. They lead investigations of incidents and near misses. In so doing they create the environment that ultimately grows into a safety culture. Safety is not a grassroots effort, and management needs to do more than establish the objectives; managers at all levels needs to recognize their responsibility and accountability for what happens at the same organizational intensity level as revenue and productivity targets. Participation in the Occupational Safety and Health Administration's Voluntary Protection Programs might be a useful way to approach safety at MML.[1]

Key Recommendation 2: Safety is as much a line management responsibility as an individual one. Leaders should recognize that every task can be done safely, and every task has inherent risks. That attitude needs to be transmitted down the line in order for each individual to take responsibility for not only maintaining but also improving the safety of their environment and the environments of those around them. The Material Measurement Laboratory (MML) should maintain statistics of leading indicators of safety risks and facilities dangers that represent the base of the safety pyramid. These statistics should be socialized within the organization in such a way that a safe and safety-conscious environment is created that results in a safety culture that supports continuous improvement. MML should consider engaging with experienced industrial partners who can bring a fresh perspective on the safety risks as a way of providing an unbiased and fresh pair of eyes to the situation.

Adequacy of Scientific and Technical Expertise

MML conducts research at a very high level. It has formal arrangements with renowned institutions such as Brookhaven National Laboratory and the Institute for Bioscience and Biotechnology Research, a joint institute with the University of Maryland, College Park, and the University of Maryland, Baltimore, two campuses of the University of Maryland system. MML has primary responsibility within NIST for producing and curating standard reference materials (SRM) and standard reference data (SRD). In addition to maintaining critical SRM and SRD, MML has developed these products in newer areas standards products based on biology. The balance of maintaining legacy SRM versus repurposing those redirecting limited resources toward producing SRM and SRD in new and emerging areas presents both a challenge and an opportunity. MML notes that areas of new opportunities include the bioeconomy and engineering biology, data science and engineering, and artificial intelligence, and the circular economy.

The robustness of MML's program against retirements or unforeseen departures could be improved. In some places there needs to be more systematic succession planning to prevent gaps from occurring. Cross-training to provide backup coverage in case the primary cognizant scientist leaves is a further way to protect against disruption. In other instances, retraining staff to take on emerging issues requiring different disciplinary knowledge was lacking.

Pandemic restrictions limited onboarding and other processes that contribute to a cohesive work culture, which has been recognized by the MML leadership team. The lack of cohesion negatively impacts an organization or culture where career mentoring and professional development for the population of term-limited scientific appointees becomes uneven.

Key Recommendation 3: The Material Measurement Laboratory (MML) should work with National Institute of Standards and Technology human resources to develop effective

[1] More information about the Voluntary Protection Programs and how to participate can be found at Occupational Safety and Health Administration, "Voluntary Protection Programs," https://www.osha.gov/vpp.

processes and procedures for hiring and career development of staff. Processes to ensure timely support to MML in hiring and onboarding of postdocs, term, and permanent employees should be developed and implemented.

Key Recommendation 4: The Material Measurement Laboratory (MML) should require mentorship training for all research staff within the laboratory to ensure quality vertical mentorship and sponsorship in order to increase the impact of the postdoc and early career population both within MML and later in industry, academia, or government positions. MML should increase the number of employees who have formal leadership training to standardize mentoring and onboarding of new personnel. The training should include a formalization of clear mentor and mentee expectations in terms of work, in-person meetings, and supervision. MML should consider a standard message about the processes of transitioning from a postdoc or term appointee to a permanent staff member, and the probability thereof so as to minimize the uncertainty around this process.

Data Management and Data Infrastructure

Data science represents an increasingly important part of MML's work to meet its mission. Within MML, the Office of Data and Informatics is a dedicated, service-oriented data resource for physical sciences with domain expertise in biological, chemical, and materials sciences, specializing in large and information-rich data sets.

Across MML, data collection, storage, analysis, and movement appear to be handled by multiple, fragmented platforms, and computational data does not appear to be managed in a centralized platform. In addition, not all the experimental measurement systems have a consolidated and automated data infrastructure, which results in a fragmented data infrastructure that, unfortunately, leads to discrete, inefficient, and stovepiped experimental data infrastructure across MML. These observations lead to opportunities to unify all computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management.

Key Recommendation 5: To the extent possible, the Material Measurement Laboratory should launch an initiative to unify all computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management. This data science initiative could be applied to machine learning deployment and expand capabilities in laboratory automation, high-performance computing, and artificial intelligence. Computing infrastructure should, to the extent possible, be updated to meet current laboratory standards.

CHAPTER-SPECIFIC RECOMMENDATIONS

In addition to the major themes and key recommendations above, the panel developed division- and office-specific recommendations in each chapter. Some of these are unique to a given division or office. Others form the basis for the overarching themes of this assessment that led to the key recommendations.

Applied Chemicals and Materials Division

Recommendation 3-1: The Applied Chemicals and Materials Division should develop a process to evaluate the maturity and current and future importance of ongoing projects relative to new opportunities to help decide which programs could be cut in effort or retired completely.

Recommendation 3-2: The Applied Chemicals and Materials Division, and the Material Measurement Laboratory broadly, should have a streamlined and standardized mentoring plan with suitable evaluation of the mentors.

Recommendation 3-3: To maximize outcomes from the use of external funds, the Applied Chemicals and Materials Division should make greater use of technicians for maintaining legacy projects and provide adequate staff time for new initiatives.

Recommendation 3-4: The Applied Chemicals and Materials Division should carry out a detailed market assessment to assess and maximize the return on the long-term investment in generating and maintaining Material Measurement Laboratory's data-based products.

Biosystems and Biomaterials Division

Recommendation 4-1: Owing to increasing demands on the unit resulting from new bioeconomy initiatives, the Material Measurement Laboratory should prioritize allocations to the Biosystems and Biomaterials Division within budgetary constraints to ensure adequate support and the Biosystems and Biomaterials Division should continue to prioritize its efforts mindful of its limited budget.

Recommendation 4-2: The Material Measurement Laboratory leadership should evaluate space allocations to co-locate the Biosystems and Biomaterials Division in a single building with adequate temperature, humidity, and power control for continuous instrument function.

Recommendation 4-3: The Biosystems and Biomaterials Division leadership should require mentorship training for all laboratory employees and increase the number of employees who have formal leadership training to standardize mentoring and onboarding of new personnel and to make career development opportunities more uniform.

Biomolecular Measurement Division

Recommendation 5-1: The Biomolecular Measurement Division should work with the Material Measurement Laboratory (MML) leadership and the National Institute of Standards and Technology's headquarters human resources personnel to develop effective procedures for the hiring and career development of staff. Internally, MML should improve their mentorship of postdoctoral fellows to address career development planning.

Recommendation 5-2: The Biomolecular Measurement Division (BMD) should work with Material Measurement Laboratory leadership and the National Institute of Standards and Technology to identify, as soon as possible, laboratory facilities with the level of temperature and humidity control, and space required by BMD to perform its work safely and at a world-class level. A move of BMD to the Institute for Bioscience and Biotechnology Research could be part of this solution.

Recommendation 5-3*:* The Biomolecular Measurement Division should increase laboratory automation to support critical steps in production of standard products and processes.

Recommendation 5-4: The Biomolecular Measurement Division (BMD) should increase engagement with communities focused on workforce development and forensics analysis, and compile data on how often their resource materials are used. For biomanufacturing workforce development activities, instructional information related to using BMD standards and standard processes could be provided to educational and professional groups providing training for biomanufacturing. Dissemination of information about how often BMD's published validation studies, research findings, and standard reference materials are used by the stakeholders in forensic activities could increase the appreciation of the value they provide to the legal community.

Chemical Sciences Division

Recommendation 6-1: The Chemical Sciences Division should look for ways to add new scientist- and technician-level staff to continue to service the existing array of standard reference materials (SRMs) and free up staff resources to pursue development of new SRMs. In addition, the division should continue to emphasize staff cross training to ensure functional redundancy. The Chemical Sciences Division should continue to prioritize internal and external collaboration as a solution to maintaining the significant breadth and depth of expertise.

Materials Measurement Science Division

Recommendation 7-1: The Materials Measurement Science Division should consider leveraging its focus area and core competency and capabilities matrix structure to manage the challenge of balancing ongoing base work with the needs of critical emergent initiatives, such as the CHIPS and Science Act of 2022.

Recommendation 7-2: The Materials Measurement Science Division should develop or leverage outside expertise in life-cycle assessment and techno-economic analysis in order to guide and focus its research in the climate mitigation focus area. Likewise, where complex measurement complements complex chemistry (e.g., catalysis, active materials and separations, and sustainable cement), the division should support a more substantial effort in the corresponding chemistries or leverage outside expertise to do so. This could include having a world-class catalyst chemist and metal-organic framework expert working side by side with the division's materials measurement scientists.

Recommendation 7-3: The Materials Measurement Science Division should consider reallocating budget and staff support to facilitate refurbishment of the division facilities; purchasing of new equipment; increasing the number of technicians, especially in strategic areas or in areas where considerable routine laboratory work is required; and improving the response time and bandwidth of formal Human Resources activities.

Recommendation 7-4: Materials Measurement Science Division management and postdoc advisors should consider a standard message about the chances and processes of transitioning from a postdoc to a permanent staff member to minimize the uncertainty around this process.

Recommendation 7-5: The Materials Measurement Science Division should consider, perhaps in collaboration with other divisions in the Material Measurement Laboratory, establishing a managed data repository, or at least a common data management plan, to aggregate the division's

data; facilitate sharing across program teams, National Institute of Standards and Technology divisions, and external users; and facilitate data analysis.

Recommendation 7-6: Where appropriate, the Materials Measurement Science Division's program staff should partner with measurement equipment manufacturers and vendors to facilitate the development and implementation of National Institute of Standards and Technology measurements and standards; this could improve the impact of a range of programs and help identify the quantitative impact of the Division's work.

Materials Science and Engineering Division

Recommendation 8-1: The Materials Science and Engineering Division should develop more coordinated technical and stakeholder engagement plans for its effort in carbon dioxide capture and the circular economy of plastics and track the long-term impacts of the division's programs on the nation's economy and related innovations.

Recommendation 8-2: The Materials Science and Engineering Division should launch an initiative to unify its computational systems, data formats, and data transmission protocols into a single, uniform platform for more efficient and effective data curation, storage, processing, transmission, and security management. This data science initiative could be applied to machine learning deployment and expand capabilities in laboratory automation, high-throughput computation, and artificial intelligence and machine learning methods.

Recommendation 8-3: The Materials Science and Engineering Division should hire more scientists skilled in artificial intelligence, machine learning, and data science to build internal capabilities and capitalize on the growing, diverse sets of data the division has handled.

Recommendation 8-4: The Materials Science and Engineering Division should develop a plan to track the long-term, quantitative impact of its key programs and industrial engagements.

Office of Data and Informatics

Recommendation 9-1: The Material Measurement Laboratory should periodically and frequently engage with industry and academia through activities such as workshops, meetings, conferences, and roundtables to standardize data management frameworks that fully support U.S. science advancement and industry competitiveness via open tools and instruments alike.

Recommendation 9-2: The Material Measurement Laboratory should disseminate broadly the Materials Science and Engineering Division's protocols for the use of virtual machines to increase the longevity of aging equipment controlled by obsolete computers, effectively empowering industry, academia, and government laboratories to extend the return on capital equipment investments.

Recommendation 9-3: To facilitate the deployment and adoption of state-of-the-art data practices in the Material Measurement Laboratory (MML) and across National Institute of Standards and Technology (NIST), the Office of Data and Informatics and MML should:

- **Institute a laboratory-wide policy requiring researchers to use automated data-handling workflows such as those demonstrated in NexusLIMS, and that output data that is easily disseminated through the Public Data Repository with rich meta-data. This will help to ensure that research data generated by MML comply with the FAIR principles of being**

findable, accessible, interoperable, and reusable. All MML researchers should also use the Public Data Repository so that their data are readily available internally and externally.

- **Embed laboratory research personnel within the Office of Data and Informatics as a sabbatical or special assignment in order to spread awareness of the data workflows that they have developed and to help to generate new use cases for them under different laboratory conditions.**
- **Strengthen collaborations with the Information Technology Laboratory to help develop state of the art data practices and disseminate them across NIST.**

Recommendation 9-4: The Material Measurement Laboratory should enter more information in the NIST Public Data Repository field to explain why data set metrics are not available where that is the case.

Recommendation 9-5: The Material Measurement Laboratory should strengthen its commitment to the Office of Data and Informatics by establishing clear data governance and data policies. It should establish the National Institute of Standards and Technology (NIST) Public Data Repository as the place to publish all open-source projects and take advantage of its restricted access functionality for any NIST confidential or internal project.

Recommendation 9-6: The Material Measurement Laboratory managers and researchers should adopt the materials science schema developed jointly with the Research Data Alliance.

Recommendation 9-7: The Office of Data and Informatics should collect and make more visible the usage metrics to measure the impact of its repositories. Numbers that report access, download, and reuse (although that is the hardest to measure) would showcase how data and teaching materials are used in and out of government.

Office of Reference Materials

Recommendation 10-1: The Office of Reference Materials should develop and implement a portfolio management process based on the articulated measurement services modernization strategy. The full portfolio of products should be considered critically and monitored on a periodic basis for: (1) each offering's utility and impact, (2) the resource commitment needed to maintain the product, and (3) effectiveness and performance of translation. Each existing product should have a maintenance and sustaining plan, and a plan to either perpetuate or discontinue products through transition to alternative products or obsolescence. A plan should be developed for every new product proposed or being developed that includes projection of these characteristics, with emphasis on life-cycle analysis, value proposition for stakeholders and value capture for the National Institute of Standards and Technology.

Recommendation 10-2: The Office of Reference Materials (ORM) should benchmark its tasks and the capabilities required to accomplish them against best-of-class capabilities that exist in the private sector. Tasks that are deemed to be better done by outside vendors should be targeted for outsourcing and staffing within ORM should be reallocated accordingly.

Recommendation 10-3: The Office of Reference Materials (ORM) has done an excellent job in managing and distributing product stock, however the marketing effort that leads to sales most often relies on an outside-in approach, in which a potential customer makes a request for a standard. As part of the input for Recommendation 10-1, ORM should initiate an inside-out marketing effort to determine the current value add of each offering in the standard reference

material catalog. This active marketing can increase uptake of languishing products, and at the same time reveal products in the portfolio of limited value proposition. This effort would be expected to increase ORM revenue.

REFERENCES

NASEM (National Academies of Sciences, Engineering, and Medicine). 2021. *An Assessment of the Material Measurement Laboratory at the National Institute of Standards and Technology: Fiscal Year 2020.* Washington, DC: The National Academies Press. https://doi.org/10.17226/26048.

NASEM. 2023. *Technical Assessment of the Capital Facility Needs of the National Institute of Standards and Technology.* Washington, DC: The National Academies Press. https://doi.org/10.17226/26684.

Appendixes

A
Acronyms and Abbreviations

2D	two dimensional
ACMD	Applied Chemical and Materials Division
AI	artificial intelligence
ARMI	Advanced Regenerative Manufacturing Institute
BBD	Biosystems and Biomaterials Division
BMD	Biomolecular Measurement Division
BMF	Boulder Microfabrication Facility
CAR T	chimeric antigen receptor T cell
CDCS	Configurable Data Curation System
ChiMad	Center for Hierarchical Materials Design
CMR	Construction and Major Renovations
CNN	convolutional neural network
COI	community of interest
CRADA	Cooperative Research and Development Agreement
CRF	Construction of Research Facilities
CRM	certified reference material; customer relationship management
CRISPR	Clustered Regularly Interspaced Short Palindromic Repeats
cryo-EM	cryo-electron microscopy
CSD	Chemical Sciences Division
CTCMS	Center for Theoretical and Computational Materials Science
DARPA	Defense Advanced Research Projects Agency
DED	directed energy deposition
DEIA	diversity, equity, inclusion, and accessibility
EBSD	electron backscatter diffraction
EU	European Union
FDA	Food and Drug Administration
FIB	focused ion beam
FY	fiscal year
GBA	Global Biofoundry Alliance
GPCR	G protein-coupled receptor
HPC	high-performance computing
HQ	headquarters

IBBR	Institute for Bioscience and Biotechnology Research
IE	invested equipment
IMS	Innovations in Measurement Sciences
ISO	International Organization for Standardization
IT	information technology
ITL	Information Technology Laboratory
JPL	Jet Propulsion Laboratory
LC/MS	liquid chromatography/mass spectrometry
LGC	Laboratory of the Government Chemist
LIMS	Laboratory Information Management Systems
LNP	lipid nanoparticle
MEP	Manufacturing Extension Program
MGI	Materials Genome Initiative
MII	Manufacturing Innovation Institute
ML	machine learning
MML	Materials Measurement Laboratory
MMSD	Materials Measurement Science Division
MSED	Materials Science and Engineering Division
MTA	material transfer agreement
NASEM	National Academies of Sciences, Engineering, and Medicine
NEST-R	NIST Educational STEM Resource Registry
NIST	National Institute of Standards and Technology
NIIMBL	National Institute for Innovation in Manufacturing Biopharmaceuticals
NMR	nuclear magnetic resonance
NOAA	National Oceanic and Atmospheric Administration
NRC	National Research Council
NSLS-II	National Synchrotron Light Source II
NTRM	NIST traceable reference material
ODI	Office of Data and Informatics
OFPM	Office of Facilities and Property Management
OH	overhead
OISM	Office of Information Systems Management
ORM	Office of Reference Materials
PAO	Public Affairs Office
PAT	process analytical technology
PFAS	polyfluoroalkyl substance
PIF	Precision Imaging Facility (Boulder)
PML	Physical Measurement Laboratory
R&D	research and development
REFPROP	Reference Fluid Thermodynamic and Transport Properties Database
RGTM	research grade test material
RM	reference material
RMAT	Regenerative Medicine and Advanced Therapies

ROI	return on investment
SCMMR	Safety, Capacity, Maintenance, and Major Repairs
SD	Standards Development (program)
SEM	scanning-electron microscopy
SRD	standard reference data
SRM	standard reference material
SRMS	
STRS	Scientific and Technical Research and Services
TDE	ThermoDynamic Engine
TRC	Thermodynamic Research Center
UCONN	University of Connecticut
UGA	University of Georgia
UK	United Kingdom
UW	University of Wisconsin
VLE	viscosity-liquid-equilibrium
WCF	Working Capital Fund
XEDS	X-ray energy dispersive spectrometer

B
Panel Biographical Sketches

ELSA REICHMANIS, *Chair*, is professor and Carl Robert Anderson Chair in Chemical Engineering in the Department of Chemical and Biomolecular Engineering at Lehigh University. Prior to joining Lehigh, she was professor and Pete Silas Chair in Chemical Engineering in the School of Chemical and Biomolecular Engineering at the Georgia Institute of Technology (Georgia Tech). She started her independent career at Bell Labs where she was Bell Labs Fellow and director of the Materials Research Department. She received her PhD and BS in chemistry from Syracuse University. Her research, at the interface of chemical engineering, chemistry, materials science, optics, and electronics, spans from fundamental concept to technology development and implementation, with particular focus on polymeric and nanostructured materials for advanced technologies. Dr. Reichmanis was elected to the National Academy of Engineering in 1995 and has participated in several National Academies of Sciences, Engineering, and Medicine activities. She was elected fellow of the National Academy of Inventors in 2021; was an elected member of the Bureau of the International Union for Pure and Applied Chemistry (IUPAC); has been active in the American Chemical Society (ACS) throughout her career, having served as 2003 president of the society; and is currently a member of the board of the American Institute of Chemical Engineers (AIChE). She is the recipient of several awards, including the 2022 John M. Prausnitz AIChE Institute Lecture Award, 2018 AIChE Margaret H. Rousseau Pioneer Award for Lifetime Achievement by a Woman Chemical Engineer, ACS Award in the Chemistry of Materials (2018), ACS Award in Applied Polymer Science (1999), the IUPAC Distinguished Woman in Chemistry and Chemical Engineering Award (2013), the ASM International Engineering Materials Achievement Award (1996), and the Society of Chemical Industry's Perkin Medal (2001). She is a fellow of the American Association for the Advancement of Science (AAAS), the ACS, the AIChE, the Materials Research Society, and the Royal Society of Chemistry. In other service, she is executive editor of the ACS journal *Chemistry of Materials*.

ROBERT ARLEY BEVER is serving as senior scientist and forensic laboratory director at Bode Technology. He has 34 years of experience in directing research and operations for three accredited forensic and parentage testing DNA laboratories. He has 15 years of experience directing and managing government research contracts associated with the development and optimization of advanced molecular techniques for detecting and analyzing human and bacterial DNA. His current research interests are developing and implementing next generation sequencing for human identification and for forensic investigative genetic genealogy. He has provided expert testimony in more than 160 civil and criminal trials and has served as a subject-matter expert to the Department of Defense (DoD) and Intelligence Community in biodefense and forensic science. Dr. Bever is certified forensic laboratory director for the New York State Department of Health and is a member of the American Academy of Forensic Science and the American Association of Blood Banks and was a member of the American Society of Microbiology. He earned his PhD in microbiology from the University of Maryland and performed postdoctoral research in molecular pathogenesis at the Oregon Health & Science University and the University of Rochester School of Medicine.

AUGUST W. BOSSE is currently senior principal scientist, hydrocarbon and materials science, at ExxonMobil Technology and Engineering Company. While at ExxonMobil, Dr. Bosse has had a range of positions, including new hydrocarbon products program leader, section head of polymer and hydrocarbon science, and various research team lead positions. Before coming to ExxonMobil, he was a postdoc, a National Research Council postdoctoral research associate, and a member of the permanent staff in the Polymer Division at the National Institute of Standards and Technology (NIST). Dr. Bosse's research has

focused on the theory and simulation of block copolymer phase behavior to enable critical dimension metrology, polyolefin crystallization, polymer blends, polymer interfaces, composites, and random copolymers. His primary research interests are rooted in statistical field theories of heterogeneous systems, especially soft materials. Dr. Bosse received a BS in physics from the University of California, Davis, and an MA and a PhD in physics from the University of California, Santa Barbara.

KENNETH M. CALDERONE is an advanced workflow specialist supporting confocal microscopy applications with Leica Microsystems. He is responsible for teaching and training research scientists on the appropriate applications of advanced microscopy, with a focus on laser scanning systems. Prior to his career at Leica, he gained 12 years of experience in microscopy as a research technician at the University of Michigan. At Michigan, he became a research laboratory technician lead by developing microscopy techniques and training scientists on proper microscopy protocols. During his career at Michigan, he focused on developing techniques to stain thick biological samples and image them using multiphoton microscopy. He also gained extensive experience in staining biological samples using immunofluorescent and chemical techniques, developing widefield microscopy protocols, and 2D and 3D image data analysis. He graduated from Western Michigan University with a BS in biomedical sciences and a minor in chemistry.

IULIANA CERNĂTESCU is senior technical fellow of material characterization and applications for Pratt & Whitney (P&W). In her role, she provides technical leadership for materials characterization field at P&, including identification, development, and championing of characterization technologies that enables agile engineering development, increased efficiencies, and inspection and measurement capabilities at each stage of the jet engine life cycle. Furthermore, Dr. Cernătescu identifies and develops external partnerships to enhance P&W material characterization and inspection technologies that align with P&W business-critical strategic and tactical goals. She serves as the P&W materials characterization expert internally to P&W, other RTX divisions, and within external technical communities. She is actively engaged in recruitment, training, mentoring, and development of talent. Dr. Cernătescu has more than 20 years of industrial experience in materials characterization. She joined P&W in 2011 as an X-ray analytical methods subject-matter expert, and later became discipline chief for materials characterization and subsequently manager of the materials characterization group and laboratories where in addition to leading the technical and strategic direction for the discipline, she modernized the laboratory facilities and developed new partnerships, expanding P&W's material characterization capabilities. Prior to joining P&W, she worked at two major companies that produced material characterization systems, where she served as technical leader for new methods and systems development and implementation. Dr. Cernătescu holds a master's degree in physics and a PhD in materials and solid state physics from Eötvös Loránd University of Science, Budapest, Hungary. She is the author of 8 patents and more than 25 peer-reviewed technical publications.

STEVEN C. FREILICH is currently executive-in-residence at the Princeton University Andlinger Center for Energy and Environment and holds a similar position in the Joint Institute for Strategic Energy Analysis at National Renewable Energy Laboratory (NREL), having recently retired from DuPont after a 33-year career. While at DuPont, he served as director of materials science. In that role, Dr. Freilich was responsible for developing and implementing technology growth strategies in rapidly moving areas such as materials for energy, displays, and biomedical applications. He used his experience to impact corporate innovation through leadership at the interface of technology and markets. During his tenure as director of materials science, Dr. Freilich held the additional position of chief technology officer of DuPont Electronics and Communication and was appointed as chief technology advocate for north Asia. He has served on the boards of the United States Display Consortium, the DuPont-MIT Alliance, and was vice chair of both the advisory panel for the Center for Revolutionary Solar Photoconversion and the advisory committee for the Clean Energy Manufacturing Analysis Center in the Department of Energy. He has also

served on the advisory boards for Sandia National Laboratories, NREL, and the National Research Council of Canada.

GARY S. GROENEWOLD is a recently retired scientist with 35 years of service at the Idaho National Laboratory. During this span, Dr. Groenewold's broad research interests involved investigations of reactivity and measurement of molecular and atomic species of importance in military, nuclear, and industrial enterprises. His research emphasized analysis of material surfaces, focusing on adsorbed organic and inorganic species in ambient environments. He specialized in mass spectrometry, and many studies utilized secondary ion mass spectrometry for surface characterization. He has authored approximately 150 peer-reviewed publications in these diverse areas, a significant fraction of which address surface analysis. Dr. Groenewold holds a PhD in chemistry from the University of Nebraska and completed a postdoctoral fellowship at Oak Ridge National Laboratory (ORNL). Dr. Groenewold has co-authored six National Academies reports in the area of chemical demilitarization and served as chair of the Committee on Chemical Demilitarization from 2013 to 2017. He is a national associate of the National Academies.

MINKI HONG is senior manager of Kyulux North America. He is responsible for developing a web-based materials informatics platform for OLED (organic light-emitting diode) applications. The platform includes a high-throughput virtual screening system, a computational job managing system, and a data management system. Dr. Hong supervises scientific research on molecular discovery and machine learning prediction models, as well as software and system development for the platform. Prior to joining Kyulux North America, Dr. Hong worked as a postdoc at the King Abdullah University of Science and Technology and Georgia Tech. His postdoctoral research focused on the degradation mechanism of organic materials. Dr. Hong earned his PhD in materials science and engineering from the University of Florida and has more than 10 years of experience in computational materials science of various materials, including oxides, nitrides, and organic materials. He possesses a broad knowledge of first principles calculation methods and related software packages, as well as experience in lattice and molecular dynamics. Dr. Hong is also trained as an experimentalist and is well versed in inorganic thin-film growth for optoelectronic devices. Thus, he is familiar with ultra-high vacuum technology and related characterization methods.

MOHAMMAD A. KHALEEL is associate laboratory director (ALD) of ORNL for National Security Sciences and oversees capabilities in protection of nuclear materials, defense materials and manufacturing, cyber-physical security, and human security. He previously served as ORNL's deputy director for science and technology (interim) and ORNL's deputy director for projects. He was ALD for energy and environmental science and oversaw a broad portfolio in biological and environmental sciences, and energy efficient transportation, building, and manufacturing. He was executive director of the Qatar Environmental and Energy Research Institute from 2013 to 2015. Dr. Khaleel held several technical and senior managerial positions at Pacific Northwest National Laboratory where he was a laboratory fellow (highest scientific rank by promotion) and led the Computational Sciences and Mathematics Division from 2003 to 2013. Dr. Khaleel received his PhD in structural engineering and mechanics from Washington State University and his MBA from University of Washington. He has extensive multidisciplinary research experience with more than 250 technical papers and three patents. His research interests have been in electrocatalytic materials and systems, superplasticity, dislocation dynamics, and lightweight materials. He is currently adjunct professor in the School of Materials Science and Engineering at Georgia Tech, a member of the Washington State Academy of Sciences, and a fellow of the American Society of Mechanical Engineers, the American Society of Civil Engineers, and the AAAS.

RICHARD A. LESAR has served as materials science and engineering professor at Iowa State University since 2006. Prior to that, Dr. LeSar worked at Los Alamos National Laboratory, as a postdoctoral fellow,

as a research scientist, and in management. His research uses computational modeling to study the properties of materials, with a long-term interest in multiscale models and work spanning from electronic structure methods to theoretical mechanics. His current work is focused primarily on developing and applying polycrystal plasticity calculations (based in part on discrete dislocation mechanics), developing multiscale simulations of additive manufacturing, and an increasing focus on developing new computational strategies for multiscale design. Dr. LeSar is a fellow of the American Physical Society and the AAAS. He served on the scientific advisory board (SAB) for the U.S. Air Force (2005–2009) and SAB science and technology review panels for the Air Force Research Laboratory Materials and Manufacturing Directorate, the Air Vehicles Directorate, and the Office of Scientific Research. He received his BS in chemistry from the University of Michigan (1975) and an AM in physics (1977) and a PhD in chemical physics (1981) from Harvard University. In 2006–2008, Dr. LeSar served on the National Academies' study panel on integrated computational materials engineering.

FRANCES S. LIGLER is Eppright Chair and professor of biomedical engineering at Texas A&M University. From 2013 to 2022, she was Ross Lampe Distinguished Professor of Biomedical Engineering at North Carolina State University and University of North Carolina at Chapel Hill. Before 2013, she was at the Naval Research Laboratory for 28 years, during the last 18 of which she was the U.S. Navy senior scientist for biosensors and biomaterials. She earned a BS from Furman University and both a DPhil and a DSc from Oxford University. She has more than 450 full-length publications and patents, which have led to 11 commercial biosensor products and generated an H = 85 (Google Scholar). She was elected an SPIE fellow in 2000, a member of the National Academy of Engineering in 2005 (2020 winner of the Ramo Founders Award), a fellow of the AIMBE in 2011, a fellow of the AAAS in 2013, a fellow of the National Academy of Inventors in 2016, and an honorary member of the Hellenic Society for Nanotechnology in Health Sciences in 2017. In 2003, she was awarded the Presidential Rank of Distinguished Senior Professional by President Bush. In 2012, she was awarded the Presidential Rank of Meritorious Senior Professional by President Obama. In 2014 and 2018, she was awarded honorary doctorates from the Agricultural University of Athens, Greece, and Furman University, respectively. She is a 2017 inductee of the U.S. National Inventors Hall of Fame, honored for her invention of portable optical biosensors. In 2015, Dr. Ligler chaired the review panel for the assessment of the NIST Material Measurement Laboratory.

QUINGHUANG LIN is president of Linktech International, LLC. Linktech is a consulting firm for the semiconductor and materials industries focusing on semiconductor technology, materials, wafer fabrication and testing equipment, workforce development, supply chain management, and sustainability. It aims to enable clients to innovate to meet customer's needs for an increasingly digitized, interconnected and knowledge-centric economy and for the betterment of people's lives. Dr. Lin was previously the director of advanced technology development at Lam Research in Fremont, California. He is an SPIE fellow, an ACS fellow, a PMSE fellow, and a POLY fellow. For more than 15 years, he has held technical and executive positions in photoresist development, advanced lithography, BEOL materials and integration, 3D integration, semiconductor equipment, and semiconductor technology strategy for several nodes of CMOS technology research and development at Lam Research, IBM, and ASML. He holds more than 120 U.S. patents and is author and co-author of more than 100 technical papers. Dr. Lin is the recipient of the Industrial Polymer Scientist Award (2018), Roy W. Tess Award (2020), E.V. Murphree Award (2023), and several IBM awards. He is co-chair of SPIE Advanced Lithography and Patterning (2021–2023) and serves as associate editor of the *Journal of Micro/Nanopatterning, Materials, and Metrology*. Dr. Lin received a PhD in materials science and engineering from the University of Michigan, Ann Arbor, and an MS and a BE from Tsinghua University, China.

DAVID MELLOR leads the policy and incentive programs at the Center for Open Science as director of policy. These initiatives seek reward increased transparency and reduced bias in scientific research and are covered in the transparency and openness promotion guidelines (TOP, https://www.cos.io/top.). His

research background and professional training include behavioral ecology, citizen science, and research methods and policy. Dr. Mellor received his PhD in ecology and evolution from Rutgers University.

NICOLA POHL is professor of chemistry, Joan and Marvin Carmack Chair in Bioorganic Chemistry, and associate dean of natural and mathematical sciences and research for the College of Arts and Sciences at Indiana University Bloomington. She was professor of chemistry and chemical and biological engineering and held the Wilkinson Professor of Interdisciplinary Engineering at Iowa State University before moving to Indiana University. The Pohl research group works to find new ways to make and analyze sugars to dissect their important roles in plant, animal, and human biology and to design therapeutics. One major long-term goal of the group is to develop rational designs of therapeutic interventions, such as vaccines and glycoproteins, on the basis of a deeper knowledge of the role of carbohydrates. Her research group created the first automated solution-phase method for readily synthesizing oligosaccharides and is now working to expand the scope of those methods to tackle the equal challenge of providing building blocks to feed their automated oligosaccharide synthesis machines. Dr. Pohl received her PhD in chemistry from the University of Wisconsin–Madison and completed a National Institutes of Health postdoctoral fellowship in the Department of Chemical Engineering at Stanford University.

JAYAKANTH RAVICHANDRAN is associate professor in the Mork Family Department of Chemical Engineering and Materials Science with courtesy appointment in Ming Hsieh Department of Electrical and Computer Engineering at the University of Southern California (USC). He holds the Philip and Cayley MacDonald Endowed Early Career Chair. His research interests are in materials design, synthesis, characterization, and physical properties of complex materials for electronic, photonic, and energy applications. His honors include the 2020 TMS Young Leader Professional Development Award and 2017 Early Career Scholar in Materials Science by the *Journal of Materials Research*. He received his PhD from the University of California, Berkeley, in 2011. He performed postdoctoral research at Columbia University and briefly at Harvard University, before joining USC in 2015 as an assistant professor.

JAMES W. RINGER is currently president of Innovative Process Solutions, LLC, where he provides consulting expertise in research, manufacturing, and business strategies. His professional experience includes the following: president of technology and new business development for Innovative Process Solutions, LLC (2021–2023); strategic leadership of large organizations (design and leadership development); innovation strategies to drive value capture, value generation strategies (implementation of new innovation concepts and continuous improvement programs), and technology portfolio strategies (pipeline development, portfolio optimization, and technology solutions); and active ingredient process development and bioprocessing and bioengineering research and development (R&D) leader at Corteva (2017–2019). He led new technology identification and development for both chemistry and fermentation process, delivery of financial impact through implementation of new R&D processes into commercial operations, and identification of external partnerships (academic and industry). At the Dow Chemical Company in Midland, Michigan, he was director of engineering and process sciences (2010–2017). He led the organization of 160 personnel for new technology development and implementation of new R&D processes into commercial operations for multiple Dow businesses (more than 20 business units including electronic materials, polymers, agrichemicals, coatings, etc.) and development and execution of more than 20 university projects. Dr. Ringer graduated from Purdue University (BS in chemistry) and University of Wisconsin (PhD in organic chemistry). He authored or co-authored 15 granted patents with more than 25 patent applications. He was a recipient of TDCC Michigan Scientists Organization Excellence in Science Award, received the DAS “Increase the Slope Award” in 1994 and 1999, a TDCC WRAP award, multiple Awards for manufacturing improvements, and the 2013 Noland Poffenberger Award from AIChE. He is currently a member of the ACS.

GEORGE RODRIGUEZ is computational chief scientist at ExxonMobil Technology and Engineering. He obtained undergraduate degrees in chemistry and mathematics from State University of New York (SUNY) Geneseo. Upon joining Exxon in 1997 with a PhD in inorganic chemistry from the University of Rochester, he completed a master's degree in statistics from the University of Houston-Clear Lake, focusing on the application of statistical design of experiments to understand workflows in high throughout experimentation. Dr. Rodriguez has worked in organometallics, polymers, computational chemistry, chemometris, and cheminformatics. He recently led teams at ExxonMobil who were using quantum chemistry, soft matter physics, and data science to accelerate the discovery pipeline of homogeneous catalysts and polymers. He was involved with researchers at the University of North Texas-Denton to explore computational chemistry and statistical learning in the development of organometallic catalysts and is a co-investigator in a DMREF/GOALI program with researchers at the Massachusetts Institute of Technology to design additives that control polymer morphology and performance. He is a member of the ACS and the American Statistical Association (statistical learning and data science section).

JAMES E. SAAL is director of external research programs at Citrine Informatics, where he manages Citrine's government-funded research programs, advancing the state of the art in materials informatics with collaborators. Before joining Citrine in 2018, he was manager of technology at QuesTek Innovations, leading programs in alloy design and integrated computational materials engineering (ICME) methods development. Dr. Saal earned his BS in materials science and engineering from Rice University in 2005 and his PhD in material science and engineering from The Pennsylvania State University in 2010, where he focused on the integration of density functional theory with CALPHAD. He continued his postdoctoral study at Northwestern University, developing a high-throughput materials property database and studying Mg- and Co-based alloys. Since then, Dr. Saal has specialized in computational simulation of process-structure-property relationships, ICME design of new materials, and the use of data-driven methods in materials science. His research has included alloys, ceramics, and polymers, and diverse properties such as corrosion, additive manufacturing printability, and thermoelectric performance. Dr. Saal is author of more than 50 peer-reviewed publications, several patents on designed alloys, and co-edited the book *Computational Materials System Design*. He currently serves as a trustee of ASM International and chair of the TMS ICME committee.

MARC SALIT is a measurement scientist who has worked in chemistry, physics, and biology over a career in the public, private, and academic sectors. He realized significant advances in these fields in more than 28 years of work at NIST. He contributed to the modernization of chemical metrology and developed world's-best measurement capability to support calibration of elemental analysis, broadband ultraviolet-visible wavelength metrology, and the world's first standard materials for the human genome. He has contributed 97 papers to the scientific literature. While at NIST, he established a partnership among Stanford University, NIST, and the SLAC National Accelerator Laboratory to form a Joint Initiative for Metrology in Biology. To seed this, he moved half of his research group to Stanford University from NIST in 2013 and established academic partnerships across the engineering and medical schools. His recent research interests have been focused on innovation and development of measurement science, standards, methods, and tools for biology. Such tools are at the foundation of our ability to generate and sustain scientific advance by enabling sharing of reproducible data, results, and materials; distribution of labor by supporting accurate, low-friction transactions; confidence in technologies permitting regulated applications; and access to quantitative measurement of previously inaccessible phenomena—all through systematic application of the principles of metrology. He is at MITRE as a fellow.

ISAAC C. SANCHEZ is professor of chemical engineering and William (Bill) J. Murray, Jr. Endowed Chair in Engineering at The University of Texas at Austin. Dr. Sanchez is an expert in the properties of polymer liquids, solutions, and blends. He attempts to solve problems in polymer science and engineering

by studying polymer interfacial phenomena, and how changes in temperature, pressure, and volume affect polymers. He develops models and uses computer simulations to understand polymer solubility and conformation and to understand the role of water in polymer processes. He received his PhD in physical chemistry from the University of Delaware.

ALIX L. SCHMIDT is senior data scientist at Dow Chemical leading programs in predictive formulation and machine learning model deployment strategy. Her previous roles in Dow and Dow Corning include process research for silicone-organic copolymer production, high-throughput research for catalyst discovery, and manufacturing chemometrics for operations troubleshooting. She is an expert in statistics and machine learning as applied to chemicals and materials, and through her roles has been involved in all phases of the data life cycle—experimental design, data generation and collection, data storage, data cleaning, and data analysis and modeling. Dr. Schmidt is an expertise leader in Dow's Citizen Data Science training program, developing and delivering foundational training on data stewardship and programming to researchers. She is a member of the AIChE and has chaired conference sessions on data analytics at the spring meetings since 2017. She has a BS in chemical engineering from University of Illinois at Urbana-Champaign and an MS in predictive analytics from Northwestern University.

JESSE C. SEEGMILLER is a board-certified clinical chemist in the Division of Clinical Chemistry at the University of Minnesota. He focuses his research activities on esoteric testing where he primarily employs mass spectrometry to analyze and develop methods for biological samples in the Advanced Research and Diagnostics Laboratory. He also oversees clinical laboratories at M Health Fairview, including the Drug Analysis Laboratory and Acute Care Laboratory. Dr. Seegmiller also serves as the medical director for the M Health Fairview Maple Grove Laboratory. Before his fellowship and faculty appointment, Dr. Seegmiller worked in industry for a mass spectrometry company as a product applications specialist in clinical applications. Dr. Seegmiller earned a PhD in chemistry from the University of Wyoming and a BS in chemistry from the University of Minnesota, Duluth (2000).

JOHNNA S. TEMENOFF is Carol Ann and David D. Flanagan Professor in the Coulter Department of Biomedical Engineering at Georgia Tech/Emory University. Dr. Temenoff is also currently deputy director of the National Science Foundation (NSF) Engineering Research Center in Cell Manufacturing Technologies (CMaT). Scientifically, she develops new biomaterials for use in cell manufacturing and regenerative medicine applications. At CMaT, she co-leads a center that spans more than eight research institutions throughout the United States, with more than 200 researchers working to develop new manufacturing technologies for emerging biologic therapies. Dr. Temenoff has received the NSF CAREER Award and was named to the College of Fellows of the American Institute for Medical and Biological Engineers, as a fellow of the Biomedical Engineering Society, and as a fellow of Biomaterials Science and Engineering, International Union of Societies for Biomaterials Science and Engineering. She was recently awarded the Clemson Award for Contributions to the Literature from the Society for Biomaterials. Dr. Temenoff received a BS in biomedical engineering and a BA in French from Case Western Reserve University (1998). She was then granted a PhD in bioengineering from Rice University in 2005.

CRISTINA U. THOMAS has more than 34 years of technical and leadership experience in research and development organizations including in the Venezuelan oil industry, IBM (New York), and 3M (Minnesota). She has undergraduate degrees in chemistry and mathematics and a PhD in chemical engineering. She is currently 3M's senior director for Global R&D Services and R&D GPO and has had prior assignments as strategy manager, laboratory manager, commercialization manager, Design for Six Sigma technical black belt, and group leader of materials modeling. She became an early leader in chemical engineering's molecular and materials modeling community, led the reinvention of the 3M window-film product platform, the design and implementation of new product introduction processes, and the incorporation of digital technologies in new connected safety platform. She is a co-inventor in more

than 25 patents and is recognized for persistently nurturing team high performance to deliver innovative ideas that move new technologies into markets. She is an industry expert and leader in knowledge discovery and analytics, materials modeling and simulation, advanced materials design, electronic laboratory environments, and laboratory information management systems. Dr. Thomas has a passion for institutions that focus on education of underrepresented students and women in science and engineering. She is a board member at Crito Rey Jesuit Twin Cities High School and at Project Scientist. She leads 3M Science Encouragement Programs and is a member of the AIChE Corporate Council & Industry Leader's and the Government-University-Industry Research Roundtable of the National Academies of Sciences, Engineering, and Medicine. She received the 2019 AIChE Industry Leadership Award, the 2019 AICHE Management Division Award, and is an ACS fellow, an ACS PMSE fellow, and an AIChE fellow.

OCKERT J. VAN DER SCHIJFF is principal engineer in Exponent's Materials and Corrosion Engineering practice. He is a chemical and metallurgical engineer with almost four decades of experience in the materials engineering field. He specializes in aqueous corrosion of materials in industrial applications and materials failure analysis in utility, manufacturing, and chemical processing environments. He has managed and participated in a wide variety of forensic investigations, failure analyses, and condition assessments on individual above-ground and buried components such as piping, valves, pumps, tanks, presses, fire protection systems, reactors, bearings, medical devices, and manufacturing machinery to determine the root cause for in-service failures. Dr. Van Der Schijff is a recognized industry expert on corrosion and microbiologically influenced corrosion of fire protection systems and the use of nitrogen as a supervisory gas in dry and preaction fire protection systems. He also provides consulting services in the fields of corrosion of metals, microbiologically influenced corrosion, medical device corrosion and failure, materials selection, alloy development, and AC and DC electrochemical techniques for investigation of corrosion mechanisms of metal alloys. Since 2001, Dr. Van Der Schijff has served as an expert witness on a number of diverse litigation cases dealing with corrosion of river going barges; corrosion failure of home heating furnaces; internal corrosion of wet, dry, and preaction fire protection systems; corrosion of buried fuel and gas piping; corrosion resulting from defective drywall; caustic cracking of refinery components; stress corrosion cracking of dairy processing equipment; pinhole leaks in domestic copper piping; and premature corrosion and/or failure of brass, copper, and stainless steel plumbing components. Prior to joining Exponent, Dr. Van Der Schijff founded CorrConsult, LLC, a consultancy providing consulting and litigation support services in the areas of corrosion engineering, metallurgy, forensic science, and failure analysis. Earlier, he was employed at Altran Corporation for a period of 9 years from 1995 through 2003. In his position as principal engineer, he was responsible for business development, project management, failure analysis, and contract research in the materials science disciplines. From 1984 to 1996, Dr. Van Der Schijff was associate professor in the Department of Metallurgical Engineering at the Potchefstroom University in South Africa. In addition to teaching undergraduate courses in materials science, corrosion, pyrometallurgy, and thermodynamics, he conducted research in the field of corrosion. During this time, he also consulted widely to industry in the fields of chemical engineering, materials science, metallurgical engineering, corrosion, and wear. Previously, Dr. Van Der Schijff was employed by the Council for Mineral Technology in South Africa as a contract researcher where he conducted research into the plasma smelting of directly reduced iron. This led to a master's degree in metallurgical engineering from The University of Pretoria in 1986. Dr. Van Der Schijff completed a PhD in metallurgy at the University of Connecticut in 1990 where he worked in the Institute of Materials Science under the advisorship of Professor Owen Devereux. In 2001, he was awarded an MBA from the Potchefstroom Business School at North–West University.