

SimPL: A Framework for Web-based Materials Design Platform

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Thematic Materials Design Platforms @ KIST

nano.vfab.org: virtual nano fab

qcat.vfab.org: catalyst design platform

battery.vfab.org: battery materials design platform

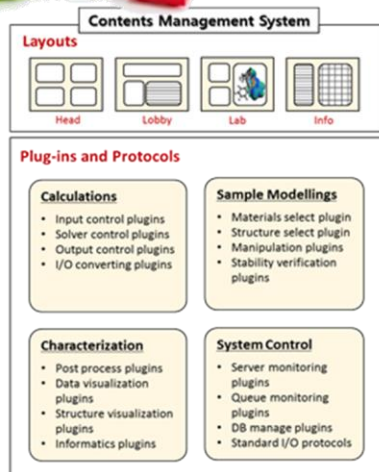
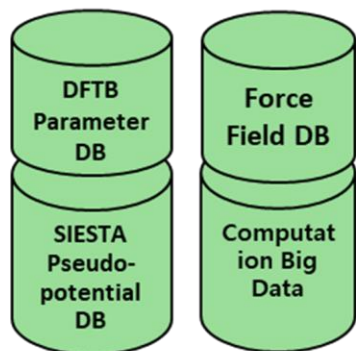


Simulation Platform Creator : *SimPL*

Functional Nano Particle Design Lab
qCAT/qBaandi

Nano Sensor System Design Lab
qFeel

Platforms for 3D Nano Device, Nano Fiber, etc



SimPL

Simulation Platform Creator

- **Contents Management System** for building web-based materials design platforms with great ease
- **Platform** for deploying developed computation codes
- **Database** of essential parameters integrated with computation environment

Simulation Platform Creator : *SimPL*


SimPL

Simulation Platform Creator

About Download Repository Showcase News

News

2nd SimPL Creator's workshop



2nd SimPL creator's workshop was held in KIST on Aug. 1, 2018.

In this workshop, SimPL v2.1 was released with officially released with several useful functions such as WYSIWYG Editor, Javascript function helper and DB

SimPL Developer Workshop


Update

Version	Date
2.2b	2018-07-09
2.1a	2018-02-20
1.0b	2017-12-15

Repository

Type	Title	Author
Page	kCmsdrawChart	Virtual Lab
Plugin	Get QE Energy	SimPL
Page	VLatoms to QE Format	SimPL
Page	Crystal Builder	SimPL
Page	Manipulator	SimPL

Supported by NRF of Korea through Nano Materials Technology Development Program



SimPL

About Download Repository Showcase News

GitHub

https://github.com/simpl-kist/SimPL_public

Download ZIP File

Download

Version	Release Note	Date
2.2b	<ul style="list-style-type: none">The following words can not be used as Page Alias: login, logout, verification, verification, repo, server, simulation, vlab, vportal, vplatform, vgenerator, vcalculator, veditor, vrepo, vupload.The argument of the Plugin built-in function getvalue has been changed from solvers to solvers's name. You can register the Solver with a name that already exists.You can back up the DB on the general tab of the admin page. You can also recover backed up data. The tables that can be backed up are as follows: Site, User, Job, User, Plugin, Page, Solver.The Repository can be used by users with less than Editor through the Front function kCms.uploadFile (repo, for users on server); file, callbak function: kCms.downloadFile (repo, for users on server); [tab of alias];WYSIWYG can be used to edit pages.Added option to run plugin on external site in general tab of admin page.If you use the plugin's attribute in plugin built-in function getdata, it loads the jobs saved in the plugin of the corresponding site. A property similar to plugin.If you use the plugin's property when you can update, the plugin will store the input value, not the id of the plugin.{pageURL, link} {parent} {plugin} allows users to change their own information.The elements displayed on the job tab of the admin page have changed. The elements that are displayed are ID, Plugin, Alias, Name, Status, Queue, ID, Time, Reason, Input, Output.The elements displayed in the Dashboard have changed.	2018-07-09
2.1a	<ul style="list-style-type: none">Full screen mode is available when editing the content of the Page and the Script of the Plugin. Pressing (Ctrl + Enter) switches to full screen mode and returns to its default size when you press (Ctrl + Enter) or (Esc).Added functionality to getdata in plugin in intrinsic function. You can use 'criteria' [array of search condition string]; 'order' [boolean: asc or desc]; 'limit' [integer: return limit]; in addition to existing 'id' (return only those columns values) and 'columns' [value] (returns only the value whose column value is 'value' as input value of getdata).The Repository has been split into for Web and for Server. For Web is used to update image files used for creating Page, and for Server website files to be used in Plugin with its structure file.A new function has been added to the plugin: getdataInfo() returns the information of the user who called the current plugin; getinfo() (only of an item or Repository for Server) returns the data of the file with the corresponding alias updated to the Repository for Server.File path, File name, File extension, File size, permission, File id, File type, File name, File...	2018-02-20

SimPL


About Download Repository Showcase News

Type: Name

1/16

Name	List	Author	Date	File Download
Template	Page kManipulator: Crystal Builder; VLatoms to QE Format; kCmsdrawChart Plugin Get QE Energy	SimPL, Virtual Lab	20180728 20180722 20180730 20181211	Web Server
XAS	Page Modeling: Crystal Builder; manipulator; Nav; Analysis Plugin XAS_run; pin in generator; inspect in generator; load job List; Load job	Yonsei Univ.	20180514	
OOB-QMHO	Page OOB-QMHO tuning; OOB-QMHO input parameters; Input Parameter; Nav; Nav; Analysis; wout_qt; Plugin	KAIST	20180702 20180504	
DFT+	Page DFT+; nav; DFT+; about; DFT+; modeling; DFT+; crystalbuilder; DFT+; manipulator; DFT+; simulation; DFT+; analysis Plugin DFT+; get qt; File from left by id; make Job; id; id; get; get; nav; angular_momentum; DFT+; save structure; DFT+; load; list; DFT+; load; list; get; list; from left by elements; DFT+; load; job; list; DFT+; load; job; get; to; of	KRIST	20180504	
Band gap Prediction	Page Bg; Modeling; Bg; CrystalBuilder; Bg; Manipulator Plugin predict_bandgap_run; predict_bandgap_code; Save; structure; Load; Structure; list; Load; Structure	KRICT	20180504	
SpecTAD	Page inspect; spectad; nav; spectad; analysis Plugin inspect; get; TAD; input; generator; get; file; list; get; job; list; get; structure; list; get; job; list; get; file; list	Minguo Kim, Art. E. Cho	20180503 20180504	
Postech 2IN MEAM	Page Job; calc; Plugin jobofcalc; make_script; run_jobs; def_order_element; def_job; job; readOutputFile; getMCJobList; make_PCC_particle	POSTECH	20180504	
qCal	Page qCal; Modeling; Navigation; qcal; Crystal Builder; qCal; Manipulator; RDF; Calc; explore; qcal; Reaction; for; file; Plugin; Enumerate; ORR; Structure; VASP; Input; Generator; Particily; Particily; esp; Particily; input; save; structure; load; structure; from; Modeling	SimPL Admin	20180222 20180722	

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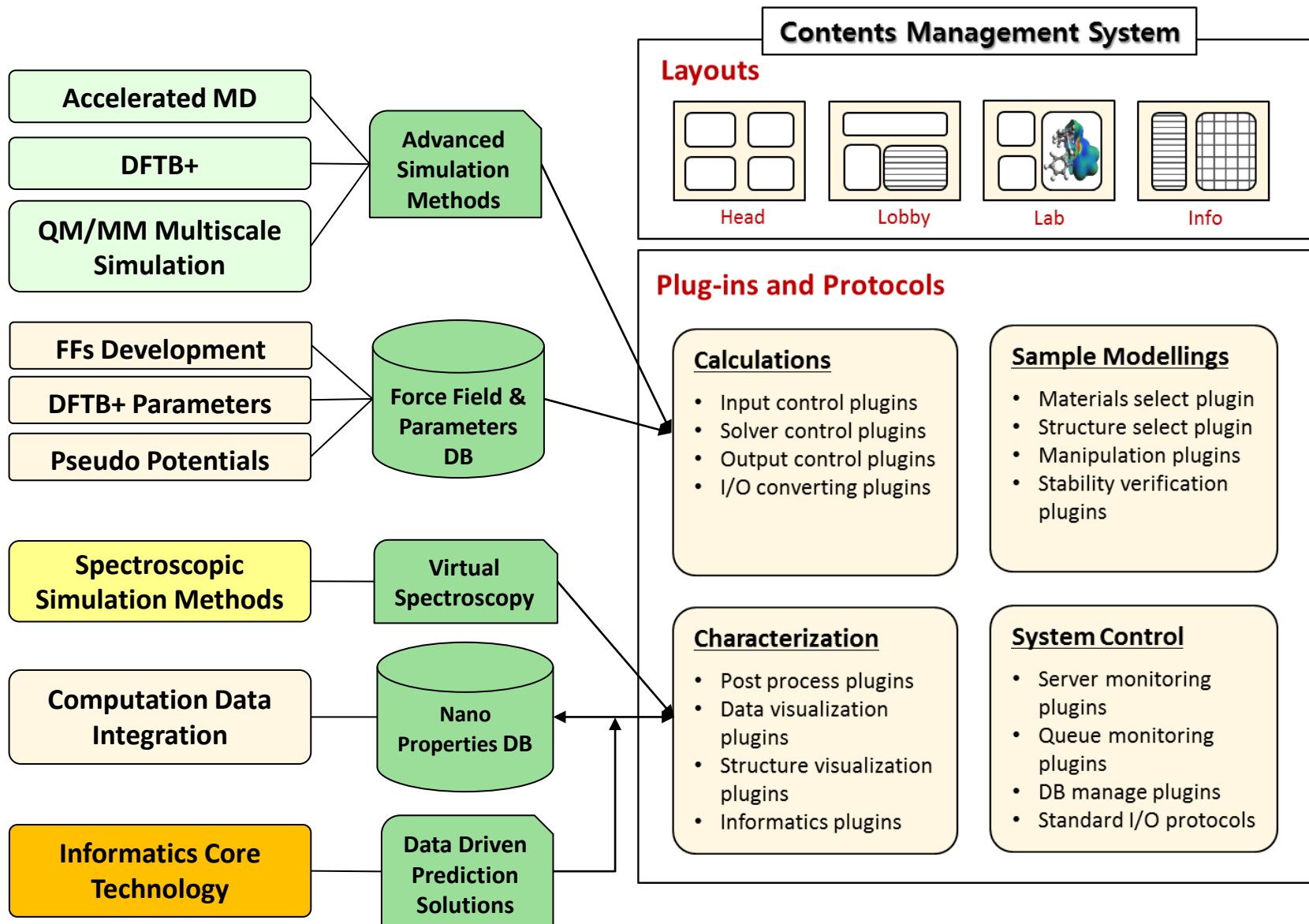


Version 2.2 is now available at <http://simpl.vfab.org/download> or https://github.com/simpl-kist/SimPL_public

SimPL docker is available at Docker Hub, [virtuallabs/simpl/simpl*](https://hub.docker.com/r/virtuallabs/simpl/simpl/)



Schematics of *SimPL* Framework



Platforms powered by *SimPL*

qCat
Lobby Modeling Lab Activity Lab Stability Lab Doc Logout

Load Sample
pt3In1_1nm

Surface Nano-Particle

Build Surface
a. From Crystal
Build Crystal Clear Surface
b. Preset
Composition Select Build

Save Sample
Name
pt3In1_1nm
Description
Periodic Boundary Condition
x: y: z:
Save

Thermal stabilizer
Temperature
Run

Structure Analyzer
Visualizer & Manipulator
PDF (for alloy)

Visualizer & Manipulator
Cell
STRAIN CLONE VACUUM CLEAR MERGE
Atom
SINGLE ATOM RECTANGULAR CIRCULAR HEXAGON ELEMENT SPHERE ADD ATOM MOVE/ROTATE CHANGE EDIT

DFTB Calculation of d-band center
KIST, Korea

Admin Logout

Number of Superoxides:16
Show Superoxide
Number of Ridge and Corner Sites:30
Show Ridge and Corner Sites
Show the Adsorbed Ca²⁺ Sites
Show Ca²⁺ Sites

Oxygen Adsorption Energy by Desorbing Oxygen One by One (PBE-U) (eV)

Choose File :CONTCAR
Current selected atoms :

Input Geometry Structure

Atom	Delete	x	y	z	z2	z1
175		32.356	37.738	32.370	1	1
180		29.643	37.735	32.370	1	1
184		29.667	37.722	29.683	1	1
188		26.906	35.062	32.382	1	1
191		29.610	35.067	32.372	1	1
192		29.639	35.042	35.042	1	1
193		26.905	35.055	29.603	1	1

Setting site type by coordination number
Element A :Ca
Element B :Ca
Coordination Number :4
Site type :2
Apply

Reaction List

Reaction 1 : 1=O(g)@gas + 4*=@surf + 2H+@surf

DFTB Calculation of d-band center
Uppsala U., Sweden

Platforms powered by *SimPL*

IIPS Ionic Interface Package for Sulfide

About Modeling Simulation Analysis Pre/After-Treat

Modeling Δ

Name: 303030

Volume: 27nm³ Density: 0.29910g/cm³

Cell: [Icons for Crystallographic Operations]

Atom: [Icons for Atomic Operations]

Atoms: 216
a,b,c (Å): 30.00, 30.00, 30.00

Polyhedral Template Matching Δ

Target Element: S RMSD cutoff: 0.5

Mark

ID	Structure	Count	Fraction
0	Other	27	25.0%
1	FCC	0	0.0%
2	HCP	0	0.0%
3	BCC	0	0.0%
4	ICO	0	0.0%
5	Simple Cubic	81	75.0%

RDF Δ

Cutoff: 3

Multiscale CAE Lab. Advanced Institute of Convergence Technology

Modeling Analysis Documentation

Job List

ID	Name	Owner	Applications	Total Layer	Status
12	6	Minho Lee	Bending Actuators	3	Finished
11	5	Minho Lee	Multilayer PZT Actuators	3	Finished
6	GaN-based HEMT Sensors [Example] Load 3-layer HEMT Sensor Example-M	Minho Lee	GaN-based HEMT Sensors	3	Finished
5	GaN-based HEMT Sensors [Example] Load 3-layer HEMT Sensor Example-A	Minho Lee	GaN-based HEMT Sensors	3	Finished

GaN-based HEMT Sensors [Example] Load 3-layer HEMT Sensor Example-M

Current layer: #3 (AlGa_N 20%) $\uparrow \downarrow$

Input

Application: GaN-based HEMT Sensors
Option: Example
Total Layer: 3

No.	Material	Thickness	Misfit 1(%)	Misfit 2(%)
1	AlN	2500nm	0	0
2	GaN	2500nm	-2.1	16.1
3	AlGa _N 20%	50nm	2.2	2.2

Plane: M-plane
Phi (φ): 0
Theta (θ): 0

Result

exx_N	eyy_N	Kkx	Kky	Ppx	Ppy
-0.01589078	0.075478	1669.594	42427.78	-1777.064	2821.48

Formula	5000nm	5050nm	
xxx_T (GPa)	-3475491.0* x^2 - 2.237854	-19.61531	-19.78908
yyy_T (GPa)	16721699.0* x^2 - 32.42076	5118769	52.02377
Ex_T (V/m)	2.000979e+9 - 3.427858e+14* x^2	287049800	269910500
Ey_T (V/m)	0	0	0
Ez_T (V/m)	-1.652725e-8	-1.652725e-8	-1.652725e-8

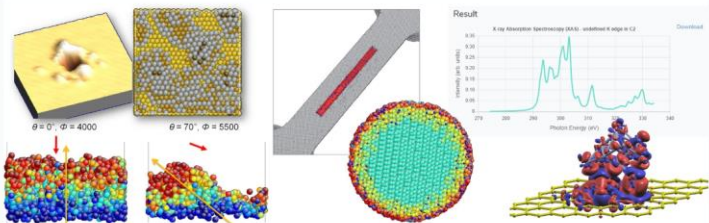
Multiscale CAE Lab.
(<http://www.multiscalecae.org>)
SUNY, USA

Ionic Interface Package for Sulfide
KIST, Korea



Platforms powered by *SimPL*

KIST Virtual Analysis Center



Spectrum

Simuloscope

- XAS
- XPS/UPS
- FTIR/RAMAN
- NMR
- IR/RS
- XRF
- EELS
- ISS
- XRD

- TEM
- AFM
- STM
- De Jureil Center

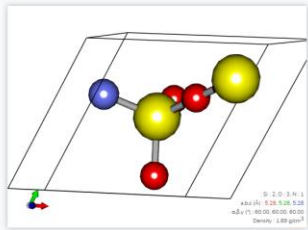
Contact : krlee@krist.re.kr
KRICT Computational Science Center

KIST Virtual Analysis Center

Kwang-Ryeol Lee(krlee@krist.re.kr)

XAS-MultiX

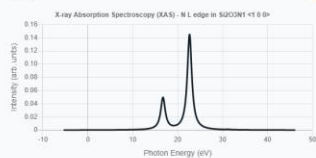
Structure



Input

Element: N
Edge: L
Polarization: <1 0 0>
Radius: 3 Å
Ground State: 2x2 2p3
Coulomb (0.7 - 1.8): 1.1
Crystal Field (0.7 - 1.8): 1.1
SO Coupling (0.7 - 1.8): 1.1
Broadening (0.5 - 1.3) eV: 0.6
Job name: SIZOIN1_XAS-MultiX_2

Result



Bandgap-ML

Dataset Manager ML Model Generation Prediction **Bandgap Predictor** KRICT

ML platform for novel material development
ML platform that can utilize own data
Bandgap-ML that predicts accurate band gap

Dataset Upload

Atomic Feature Generator

Dataset List

파일 선택 dataset_test20200506_01.csv Read 파일 선택 선택된 파일 없음 Gen test_test1.csv Load

My Dataset

sum_atomic_ratio	max_atomic_ratio	min_atomic_ratio	diff_atomic_ratio	sum_atomic_number	max_atomic_number	min_atomic_number	diff_atomic
2	1	0.13	0.87	166	82	34	48
1.15	1	0.15	0.85	134	83	51	32
2	1	0.17	0.83	166	82	34	48
2	1	0.25	0.75	166	82	34	48
2	1	0.36	0.74	164	83	34	33
3							

Bandgap-ML

Dataset Manager ML Model Generation Prediction **Bandgap Predictor** KRICT

ML platform for novel material development
ML platform that can utilize own data
Bandgap-ML that predicts accurate band gap

Dataset Name: dataset

Select Dataset for ML

20200630_dataset.csv Load

Set Features

- sum_atomic_ratio
- max_atomic_ratio
- min_atomic_ratio
- diff_atomic_ratio
- sum_atomic_number
- max_atomic_number
- min_atomic_number
- diff_atomic_number

Set Target

- sum_atomic_ratio
- max_atomic_ratio
- min_atomic_ratio
- diff_atomic_ratio
- sum_atomic_number
- max_atomic_number
- min_atomic_number
- diff_atomic_number
- sum_atomic_weight
- max_atomic_weight
- min_atomic_weight
- diff_atomic_weight
- Eg (eV)

Result data

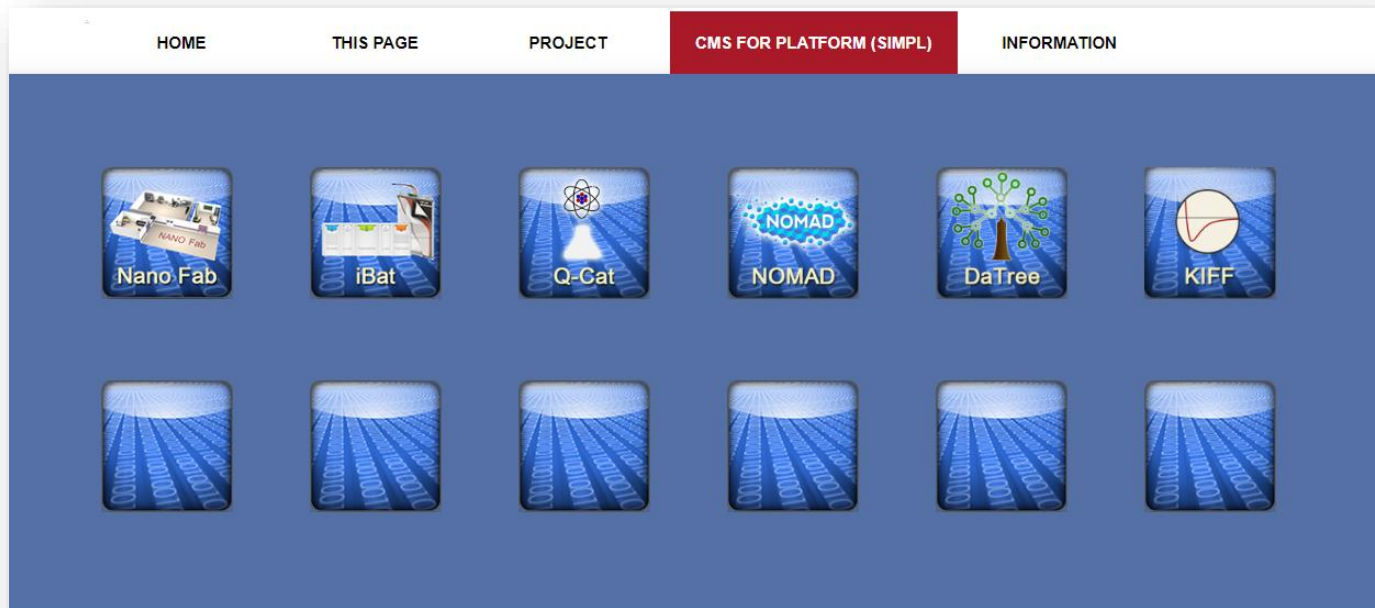
0.12049804671754188

KRICT
Korea Research Institute of Chemical Technology

BandGap Predictor
KRICT, Korea

Virtual Analysis Center, KRICT, Korea





NOTICE

(2018-07-05) 2nd SimPL Workshop (KIST, Aug.1, 2018)

The [2nd SimPL Workshop](#) will be held in KIST on August 1, 2018. In order to join the workshop, please send an e-mail to [Ms. Yerang Ryu](mailto:Ms_Yerang.Ryu) at Virtual Lab Co.

SimPL

Simulation Platform Creator a2.1

(2018-03-12) ACCMS-PRO will be launched in Nano Korea 2018

Asia Consortium on Computational Materials Science (ACCMS) will start its second phase activity with the name of ACCMS-PRO (Pre-real organization). KIST is to play a role of host for the ACCMS-PRO activities. A meeting to prepare the ACCMS-PRO activity will be held during [Nano Korea 2018 Symposium](#) (July 13, 2018) at KINTEX. Details are available [here](#).

