Diffusion of quantum liquids in bulk and confinement: A neutron scattering investigation

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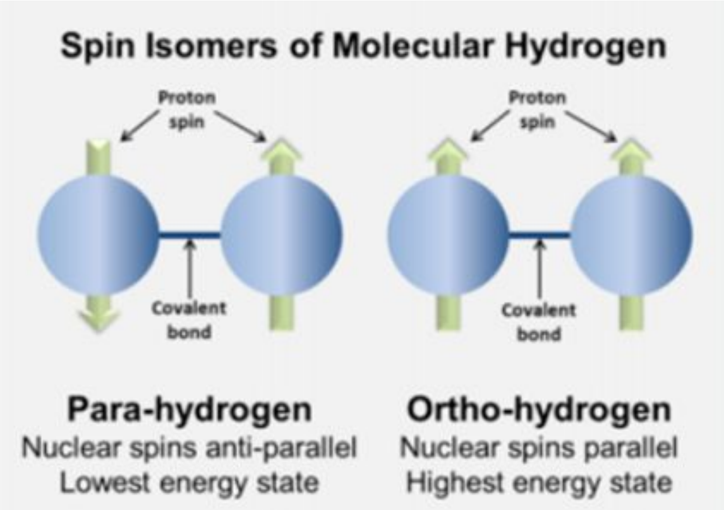
Outline of presentation

- Refinement of last years experiment: Diffusion of bulk liquid normal H_2
- Dynamics of confined liquid hydrogen deuteride
- Applications of research to high school physics

Why H_2 and HD?

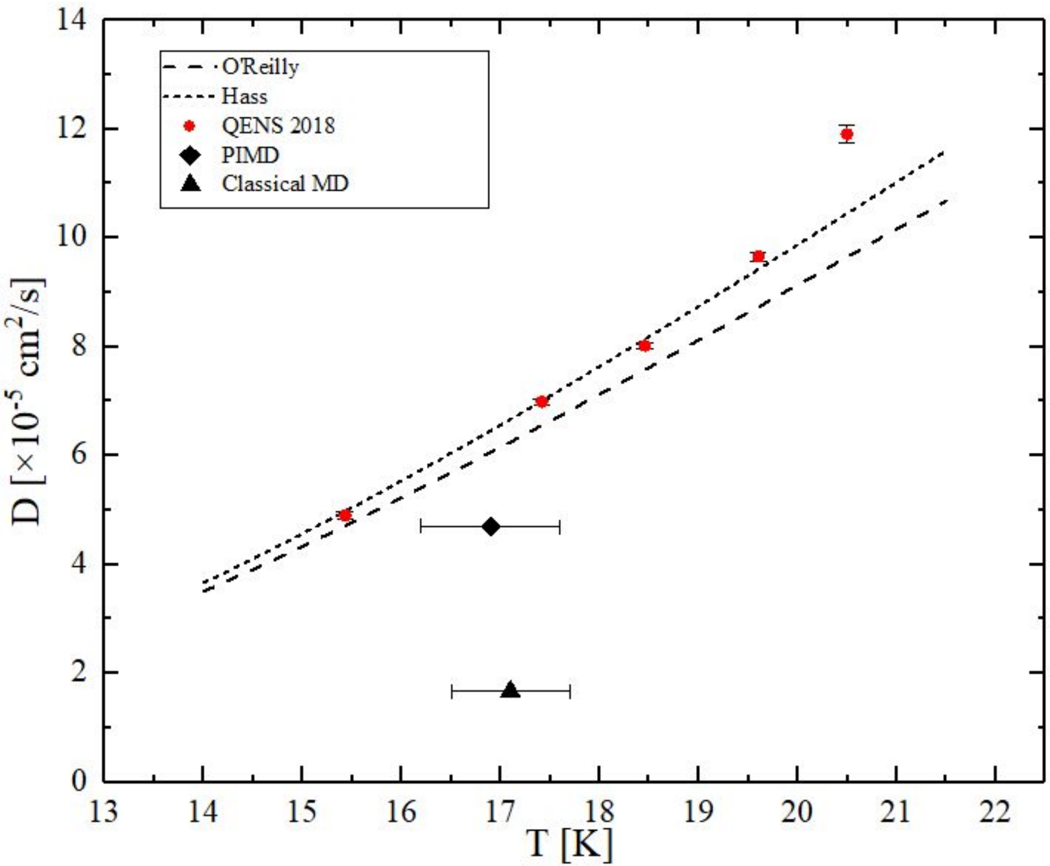
- They form a quantum fluid and solid in nature
- They can be modeled from first principles
- H_2 vs. HD - spin properties



https://hub.wsu.edu/ise/design/vortex-tube/

Motivation for the study of liquid H_2 diffusion

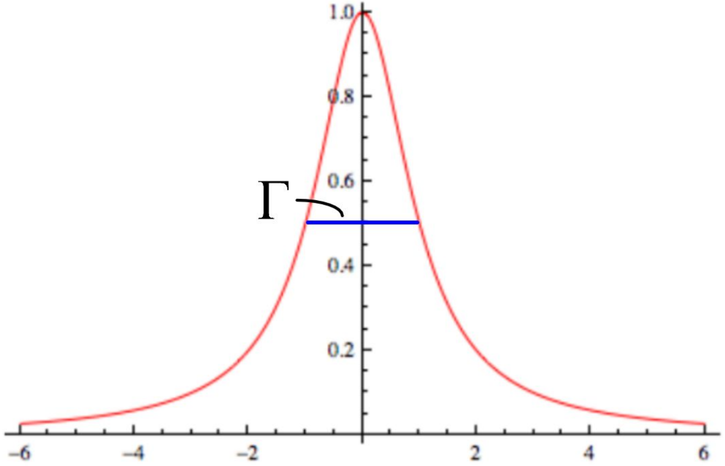
- Large zero-point energy contribution
- Better statistics at lower resolution will refine our results
- A smaller counting time will allow more temperature measurements.



Neutron Scattering and Diffusive Dynamics of Low Temperature Hydrogen

Lorentzian Structure Factor

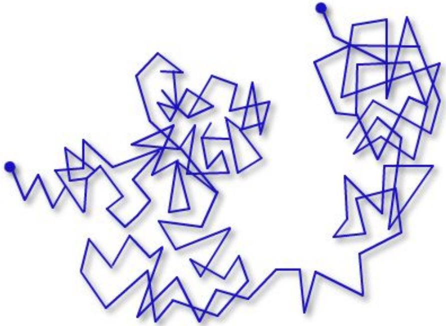
$$S_{inc}(Q,w) = \left(\frac{A}{\pi}\right)\frac{\Gamma_{fwhm}/2}{w^2 + (\Gamma_{fwhm}/2)^2}$$



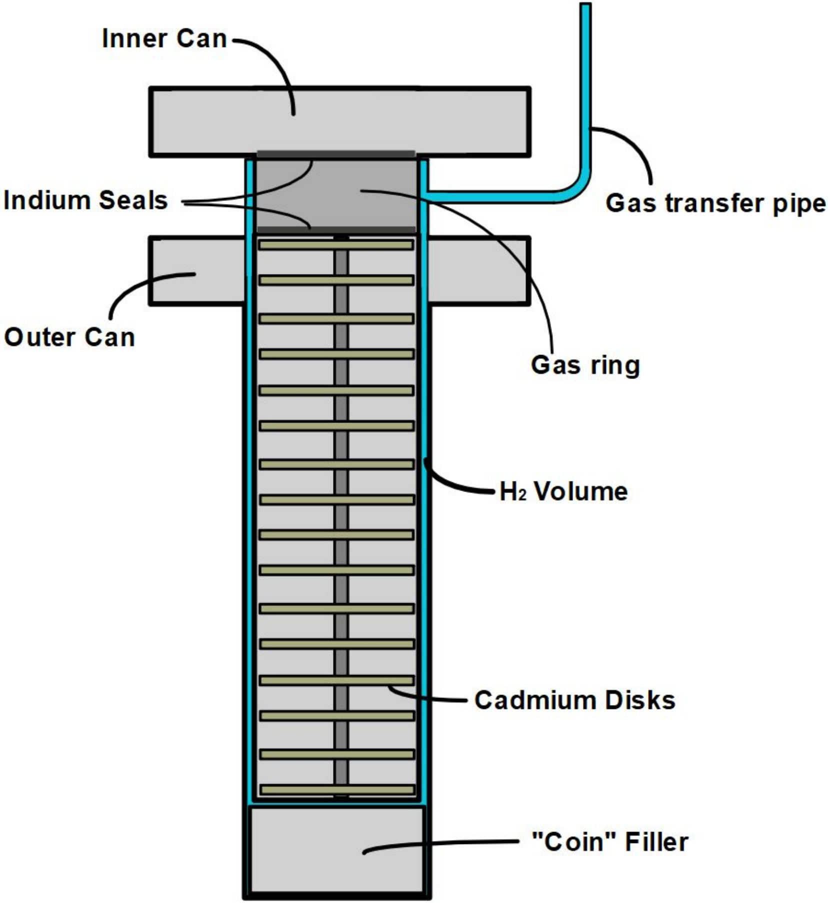
Jump Diffusion Width Model

$$\Gamma_{fwhm} = \frac{2}{\tau_0}\left(1 - \frac{1}{1+(Ql_0)^2}\right)$$

$$\boxed{D = \frac{l_0^2}{\tau_0}}$$



Sample Environment



- Annular radius around 0.1mm for 10% scattering.
- We collected data for 8 different temperatures between 14.5 K and 20.5 K.
- We also performed measurements of the empty can background, and vanadium resolution.

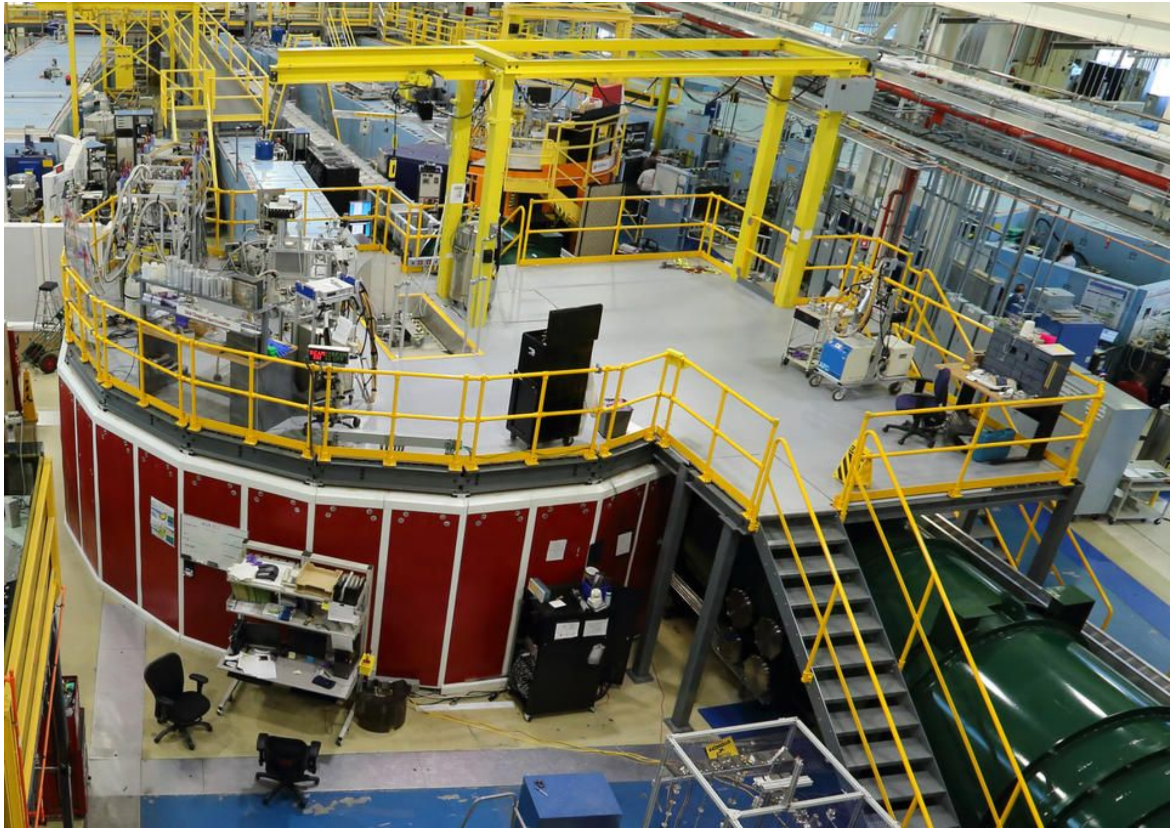
Our instrument: The disk chopper spectrometer (DCS)

Diffusive time scales: $\sim 10^{-12}$s

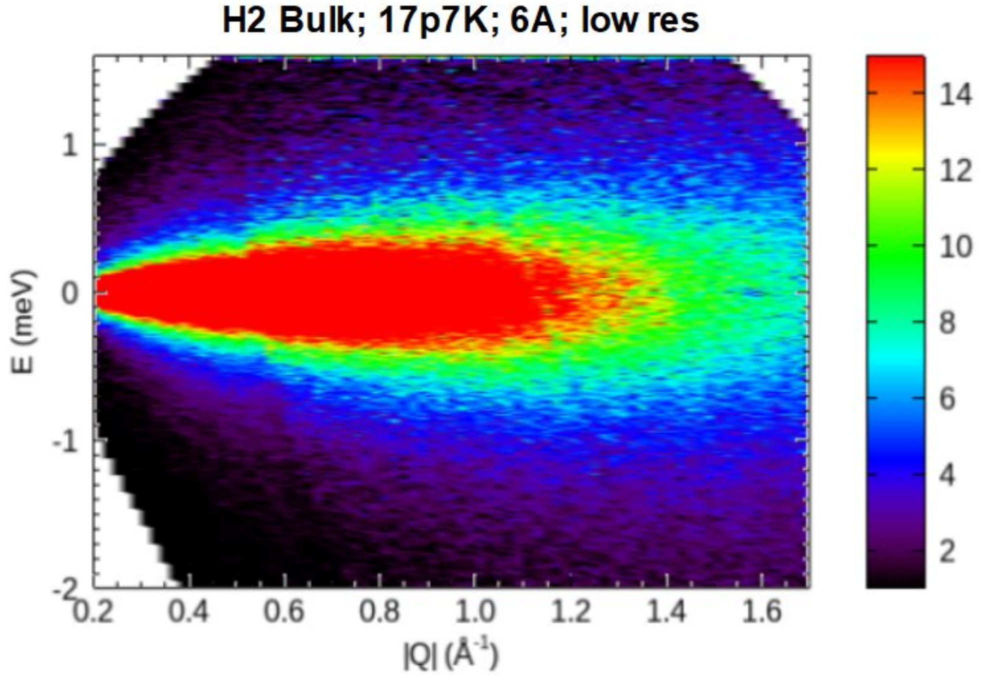
$\lambda_{incident} = 6.0$ Å

Resolution: ~60 μeV

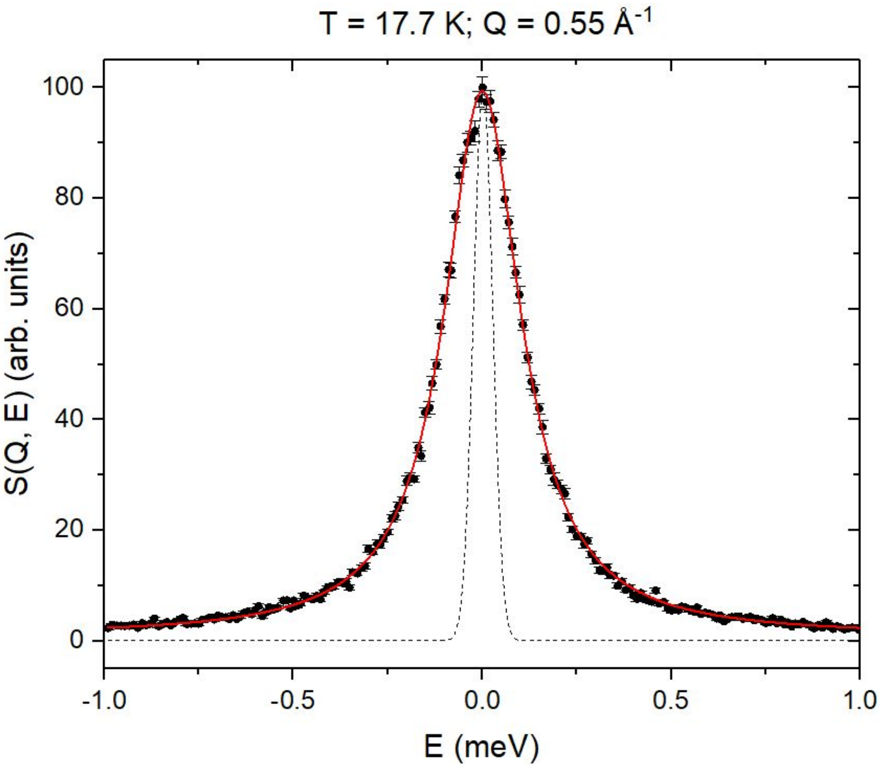
Temperatures between 14.5 K and 20.5 K.



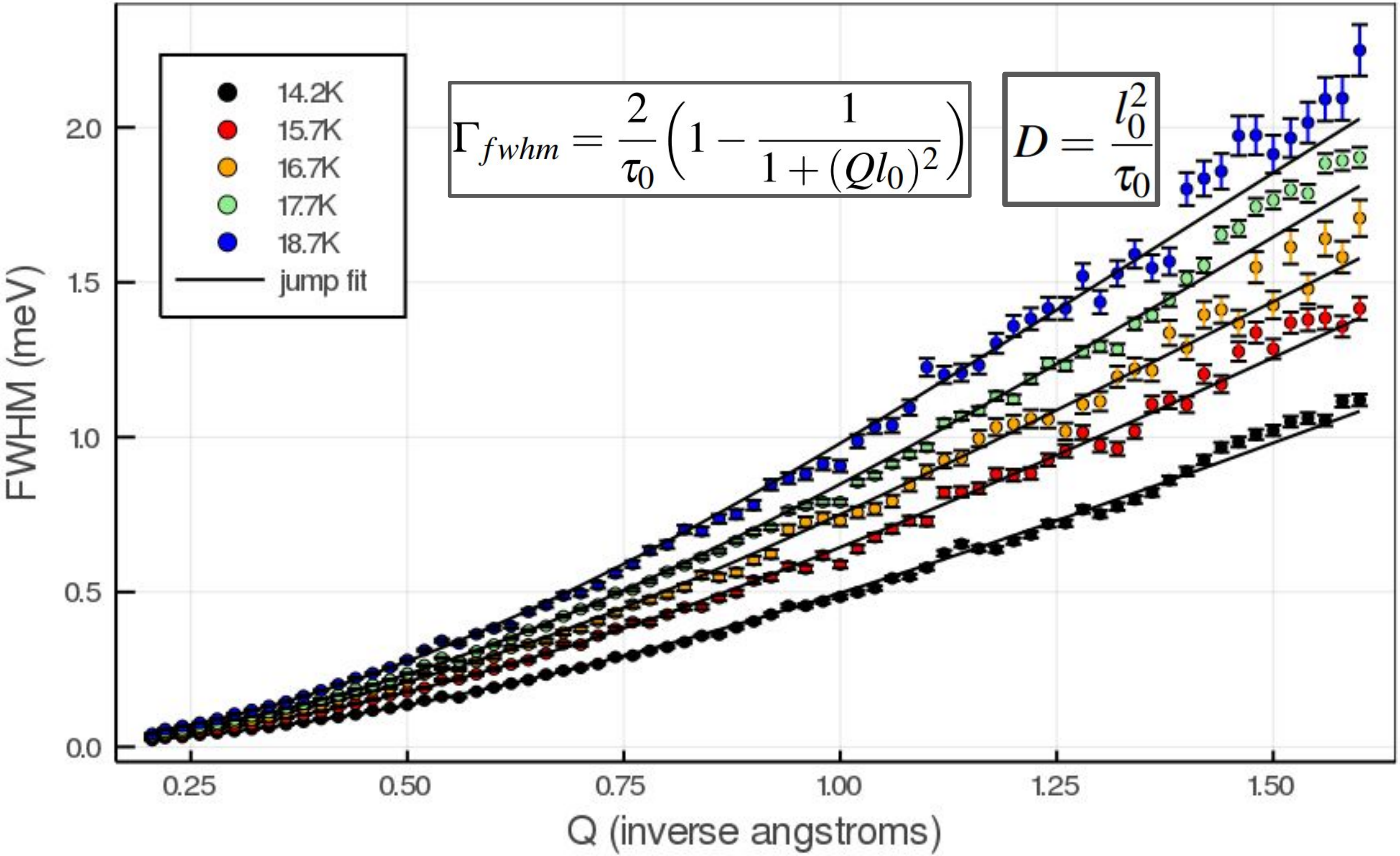
Modeling quasielastic broadening



$$S_{inc}(Q,w) = \left(\frac{A}{\pi}\right)\frac{\Gamma_{fwhm}/2}{w^2+(\Gamma_{fwhm}/2)^2}$$



Lorentz width as a function of Q

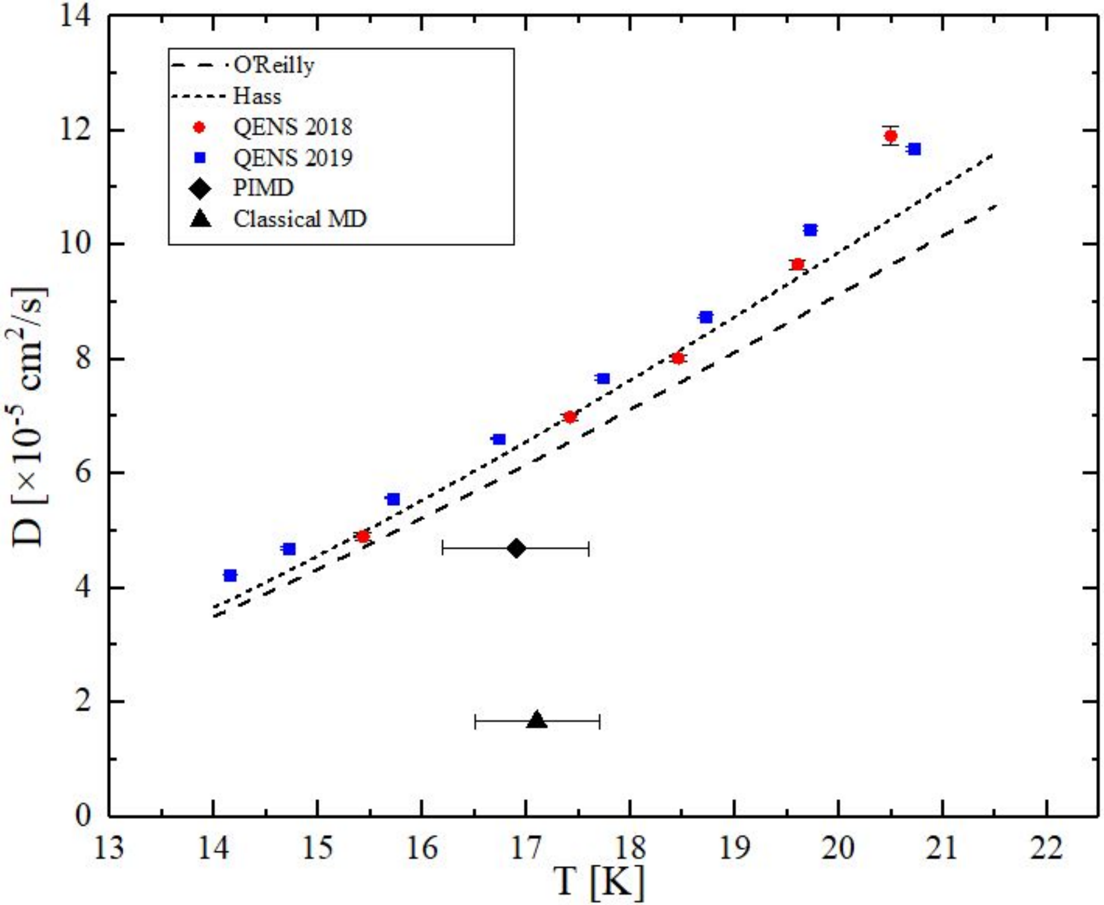


Modeling Temperature Dependence and Conclusion

- Our results provide independent experimental confirmation

- Quantitative Agreement: Activation Energy
  Q_{exp} = 3.864 +/- 0.118 meV
  Q_{lit} = 3.85941 meV [1]

$$D = D_o \exp\left(-\frac{Q}{RT}\right)$$



Motivation for studying the dynamics of confined HD

- Effects of confinement
  - Increase of liquid viscosity
  - Suppression of freezing temperature. Supercooling.
- Why HD and not H_2?
  - Adsorption dependence on ortho H_2 content
  - H_2 ortho to para conversion

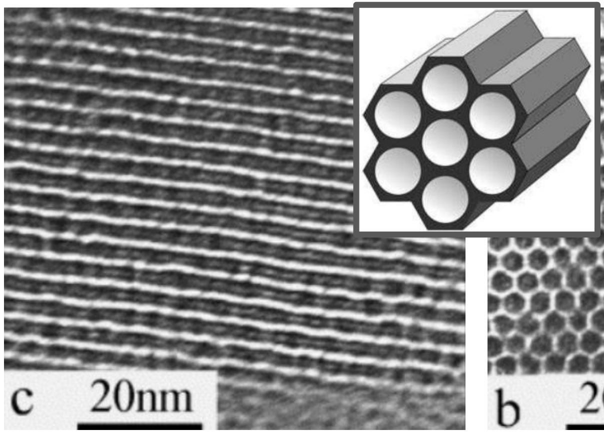
Sample Characterization

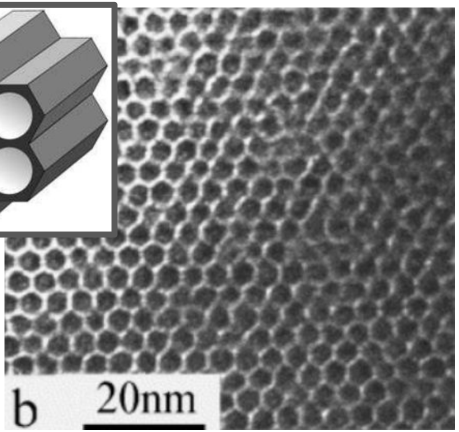
Thank you Taner!

MCM-41 Powder - SiO2 Hexagonal Pore Structure

Pore Size: ~3-5nm

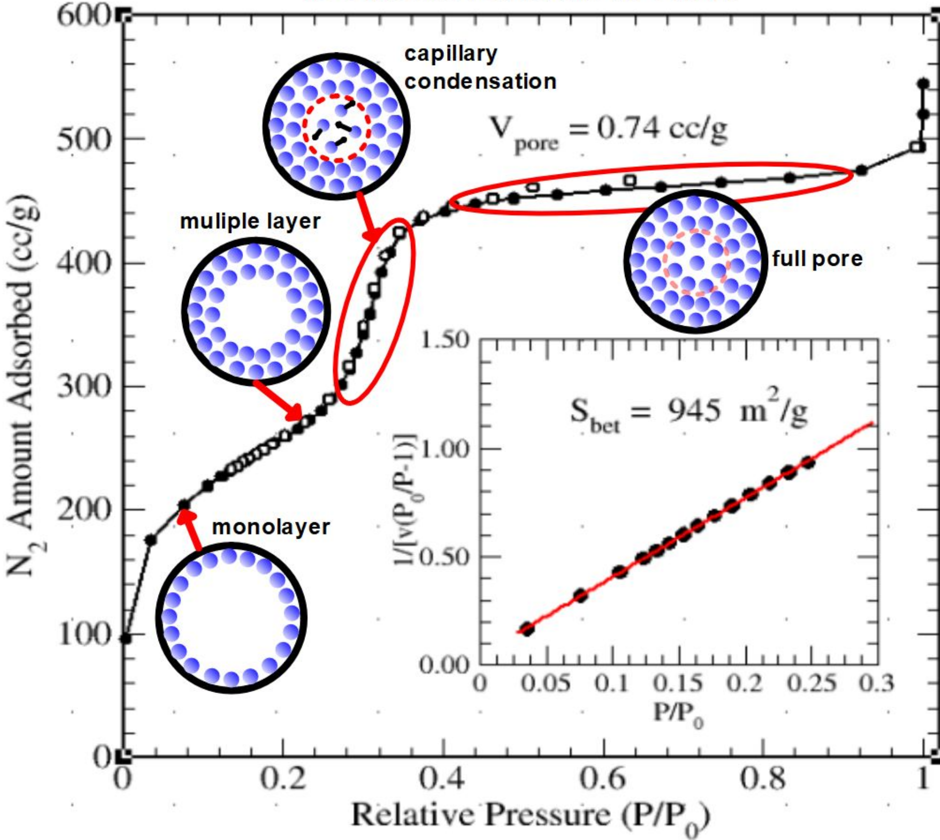
Our interest is in the full pore phase





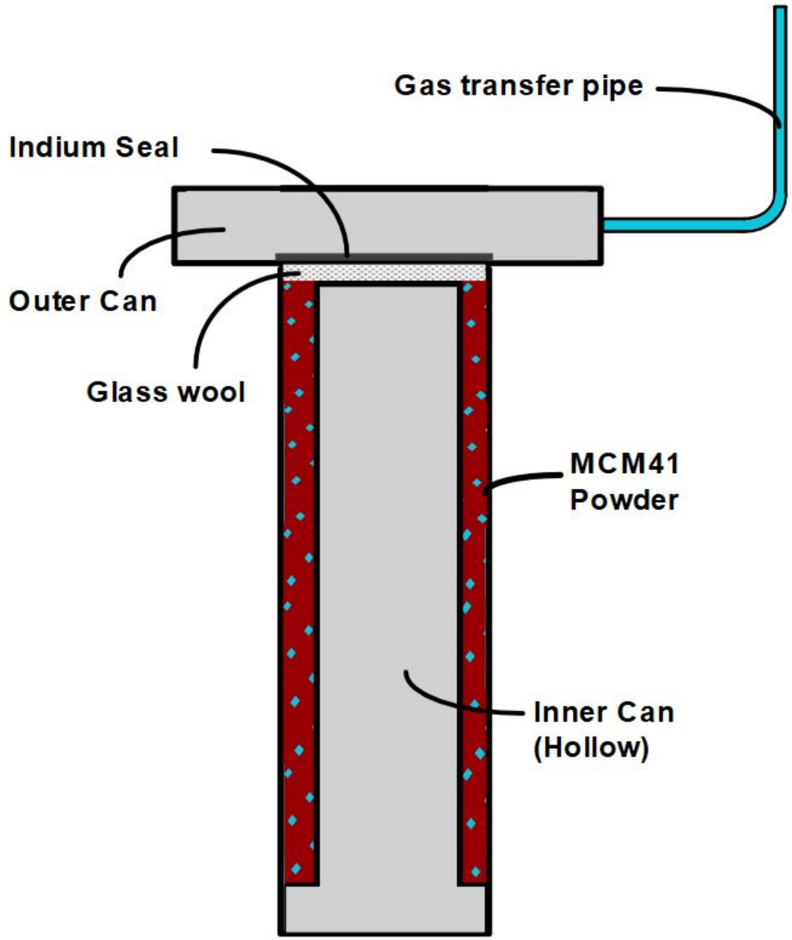
Fodor et.al., Microporous and Mesoporous Materials **56**, 101-109 (2002)

Isotherm for N_2 in MCM41

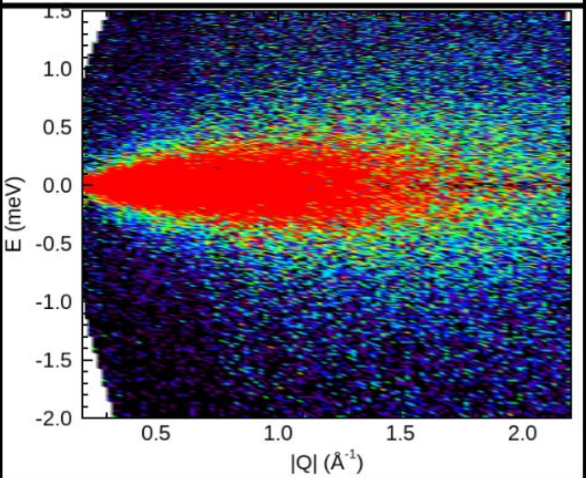
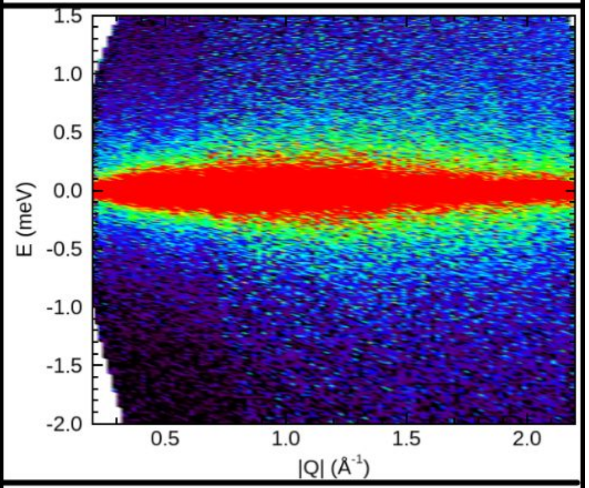
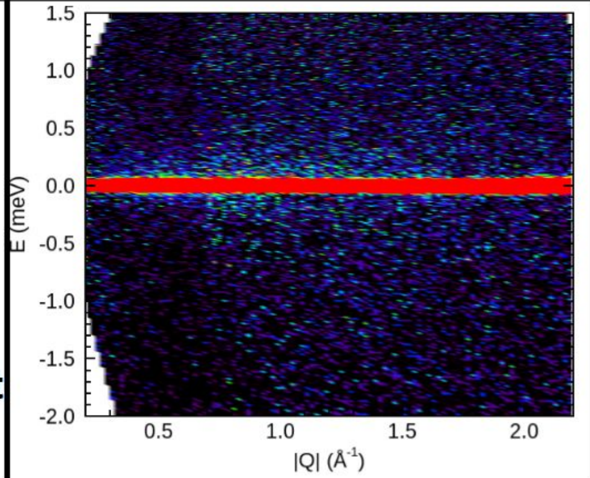
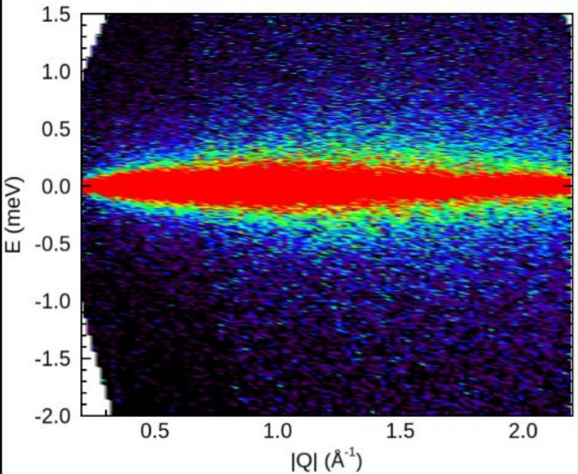


Experiment Details

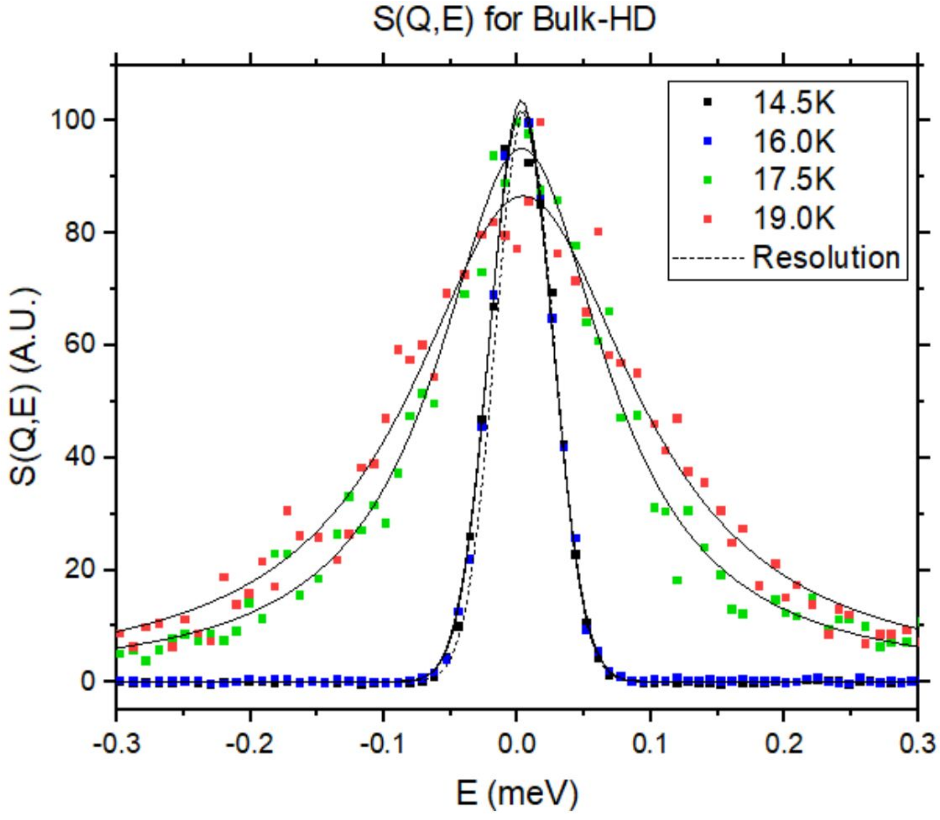
- Preparation of MCM-41
- Sample Can
  - ~1mm annular radius for 10% scattering.
- DCS settings
  - Medium resolution, λ = 4.8 Å
- Measured confined HD at five different temperatures:
  - 14.5K to 20.5K which consist of temperatures below and above the triple point of HD (16.6K).
- Measured bulk HD at the same DCS settings but in the 0.1 mm annular can.

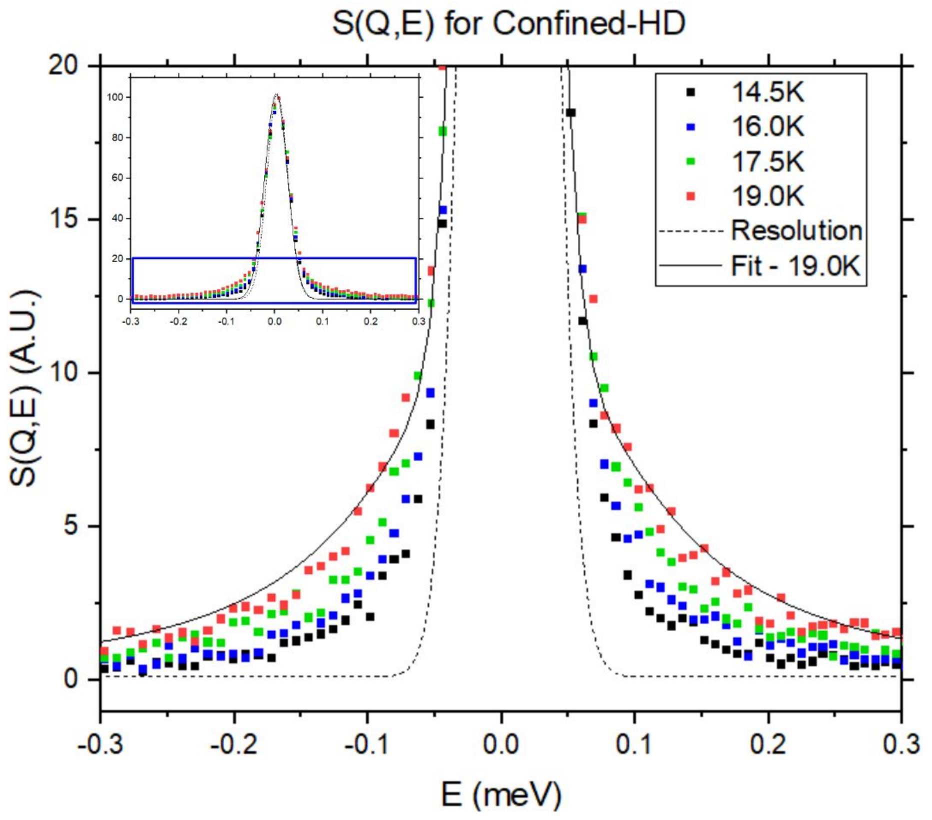


S(Q,E) for Bulk and Confined HD

	Bulk HD	Confined HD
17.4K Above triple point (16.6K)		
16.0K Below triple point		

Bulk and Confined HD: Cut at Q=0.56 Å^-1





Further Analysis

- Determine a diffusive model of liquid HD in confinement.

$$D = \frac{k_B T}{6\pi \eta r}$$

***η* is the dynamic viscosity**

Future Study

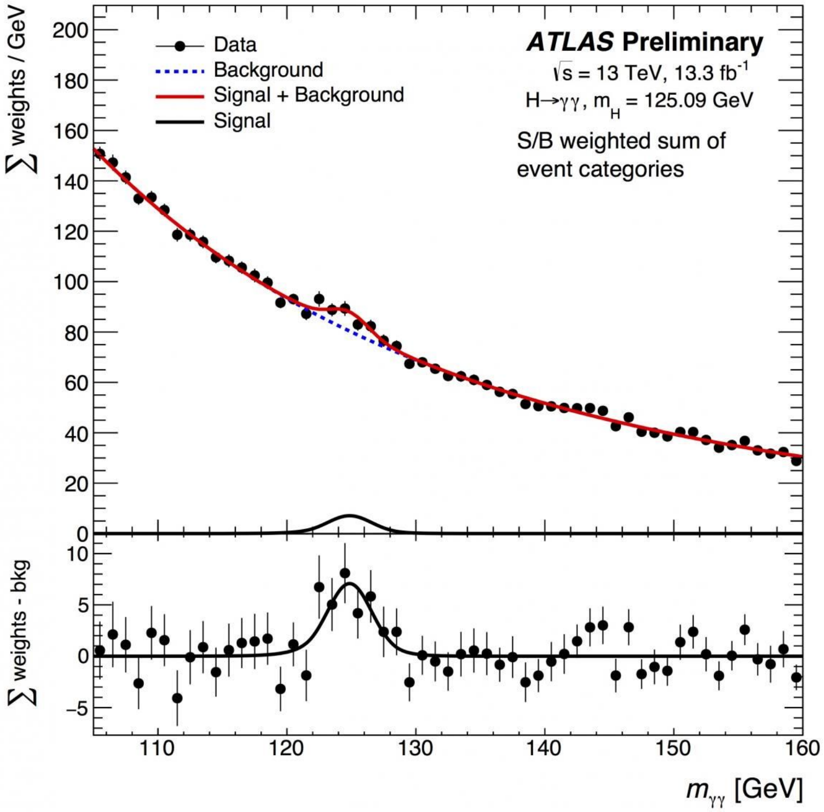
- At what lowest temperature do we continue to see quasi-elastic broadening?

- Perform the experiment for p-H2. Theoretical models suggests p-H2 superfluidity at ~6K [1].

- Quantify pore-size influence on the suppression of freezing temperature.

What did I learn and experience?

- Continuing work on an ongoing project
- Taking part in the summer school
- Science is hard work
- Constant reassessment and refinement.



Atlas Collaboration, “Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC”

Last year: Inquiry based experimentation

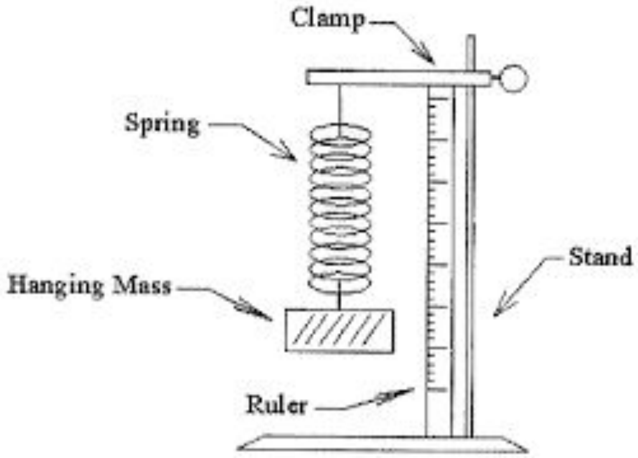
Pose an inquiry question with a selection of hypothetical theoretical explanations.

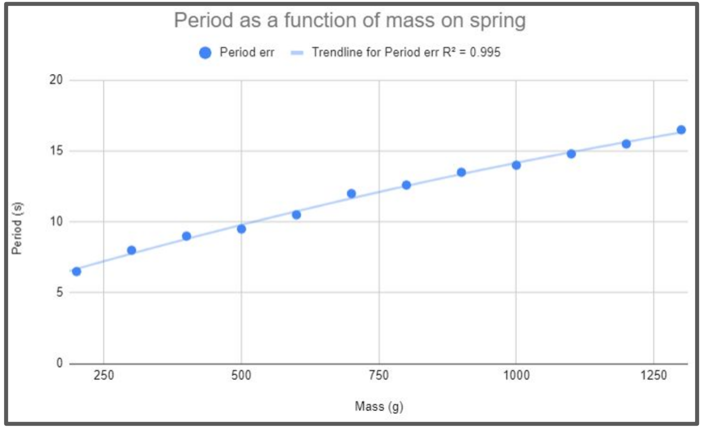
Students formulate their own experimental methodology

- Choose independent variable and controls
- Choose materials and measuring devices

Experimental uncertainties

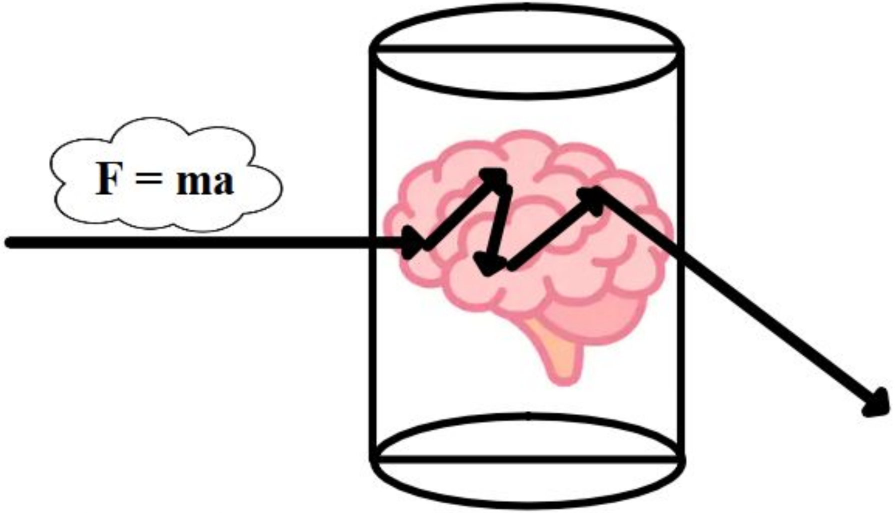
Presentation of results and inferences.





Results from implementation

- Managed to convert 5 major labs
- Students dove right in.
- “But my R^2 value is close to 1”
- Common issues in student reports:
  - Lack of detail on sources of error, environmental factors.
  - Lack of referencing results in formulation of conclusion.
- Assessing reports was a lot of work on my part.



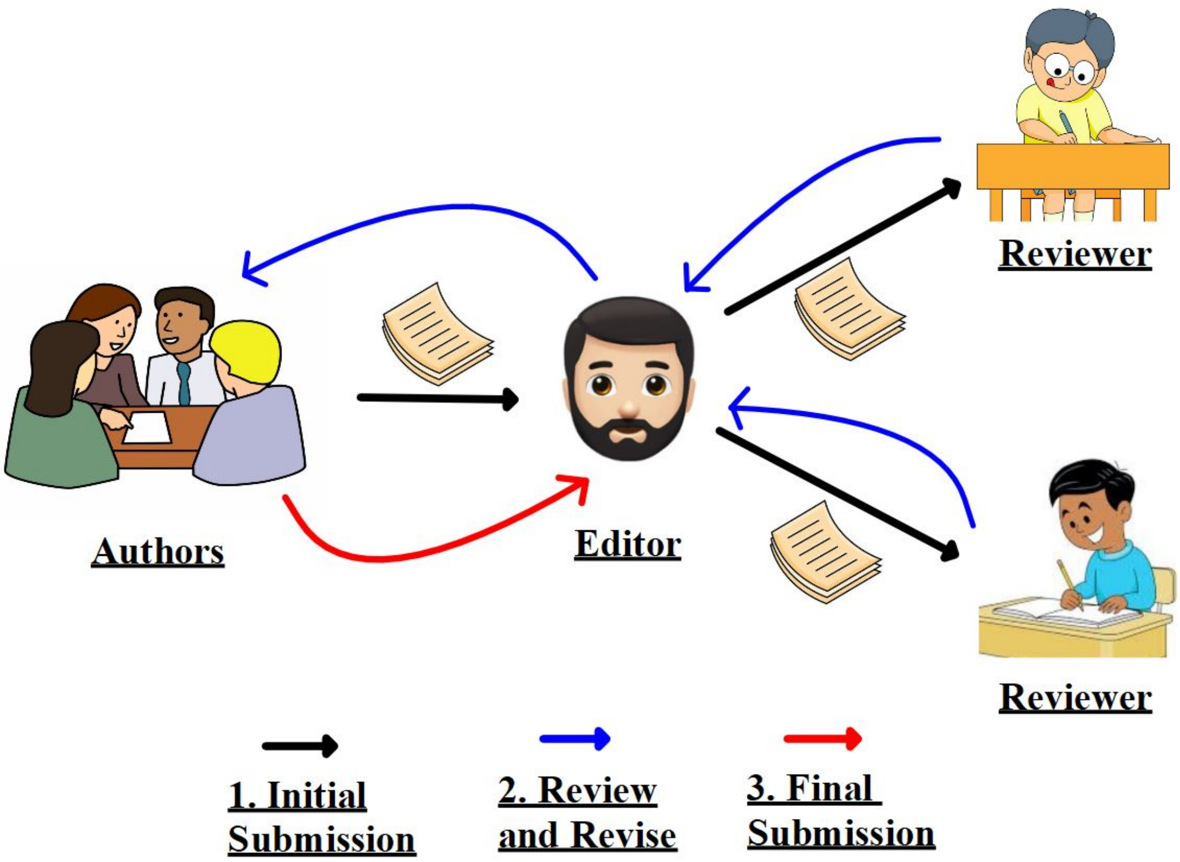
Variable cross-section and high rate of multiscattering!

Expanding on inquiry based research

Who is the arbiter of validity?

Q: How can we make the process of writing and getting feedback on a research paper more realistic and at the same time give students experience interpreting research papers?

A: Implement a peer review process.



Research Review Criteria

Soundness of Design:

- Is the work technically correct?
- Is the data reliable? What environmental factors did they fail to account for?
- Does the data support their conclusion? Is there a logical flow to their reasoning?

Quality of writing:

- Can you follow the experimental design?
- Are the figures clear and do they support their findings?
- Are the calculations clear and correct?

Thank You!

Experiment Supervisors: Timothy Prisk and Richard Azuah

Yamali Hernandez, Dan Neumann, Rob Dimeo

Antonio Faraone, Michihiro Nagao, Elizabeth Kelley, Madhu Tyagi

Juscelino Leao, Yegor Vekhov, Tanya Dax, Yiming Qiu, Taner Yildirim

Nick Butch, Wei Zhou, Craig Brown

Questions?