Activity Report of the Nuclear Data Group at Centro Atomico Bariloche, Argentina

José Ignacio Márquez Damián
Florencia Cantargi
Christian Helman
José Rolando Granada

Neutron Physics Department
Centro Atomico Bariloche
Argentina

WPEC SG-42 third meeting
May 16th-18th, 2017
OECD, Paris, France

CONICET

Instituto Balseiro

CNEA

Who we are: Thermal scattering nuclear data group at Centro Atomico Bariloche

Rolando Granada

Scattering theory and advanced neutron sources

Florencia Cantargi

Cold moderator materials and neutron filters

Christian Helman

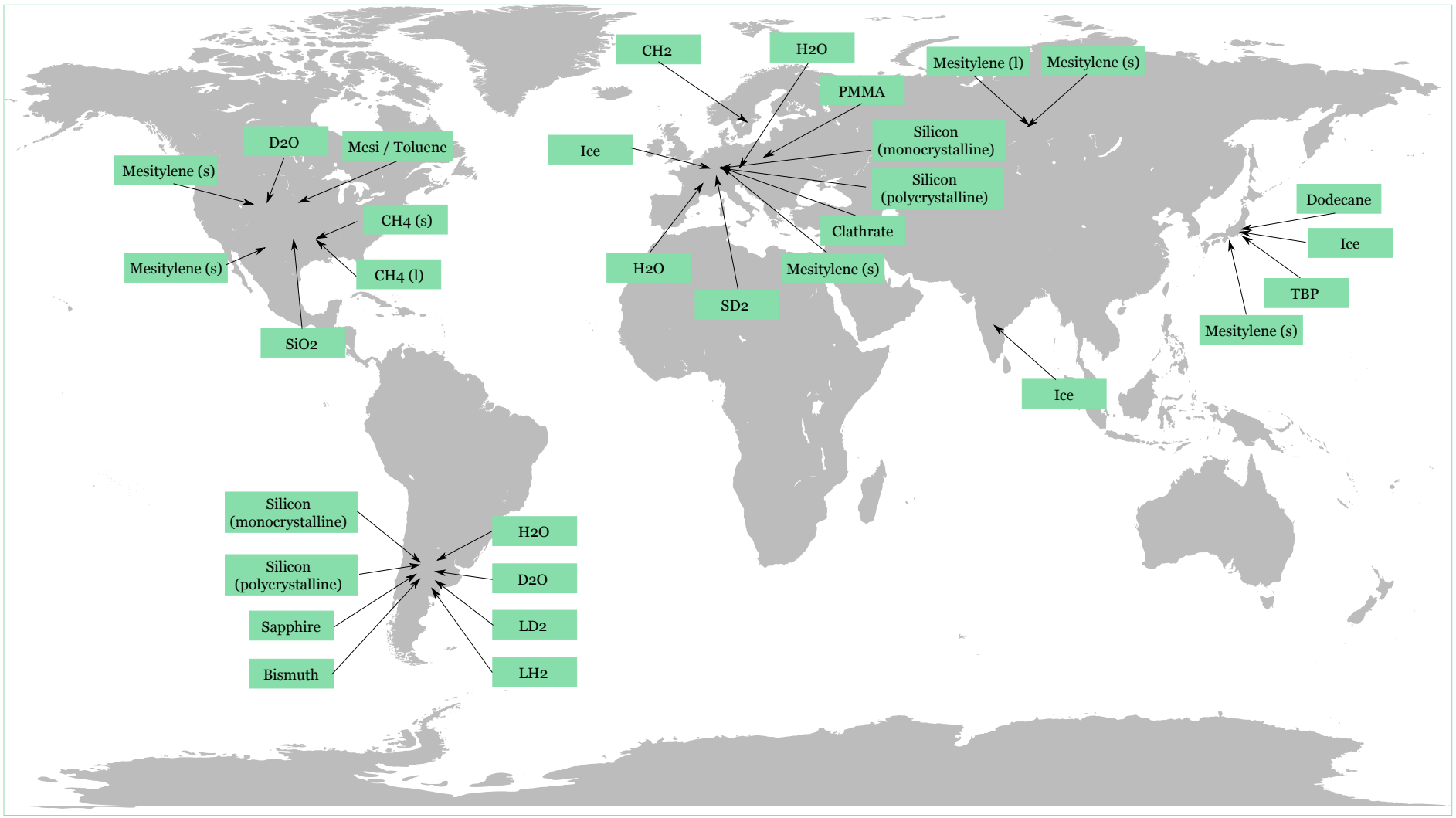
Solid state physics and ab initio methods

Ignacio Marquez

Nuclear reactor applications and benchmarking

Past members: Monica Sbaffoni (currently at IAEA), Victor Gillette (currently at University of Sharjah, U.A.E).

What we do


CH2
H2O
Mesitylene (l)
Mesitylene (s)
PMMA
Silicon (monocrystalline)
Ice
Silicon (polycrystalline)
Clathrate
Dodecane
Ice
TBP
Mesitylene (s)
H2O
Mesitylene (s)
SD2
Ice
D2O
Mesi / Toluene
Mesitylene (s)
CH4 (s)
Mesitylene (s)
CH4 (l)
SiO2
Silicon (monocrystalline)
H2O
Silicon (polycrystalline)
D2O
Sapphire
LD2
Bismuth
LH2

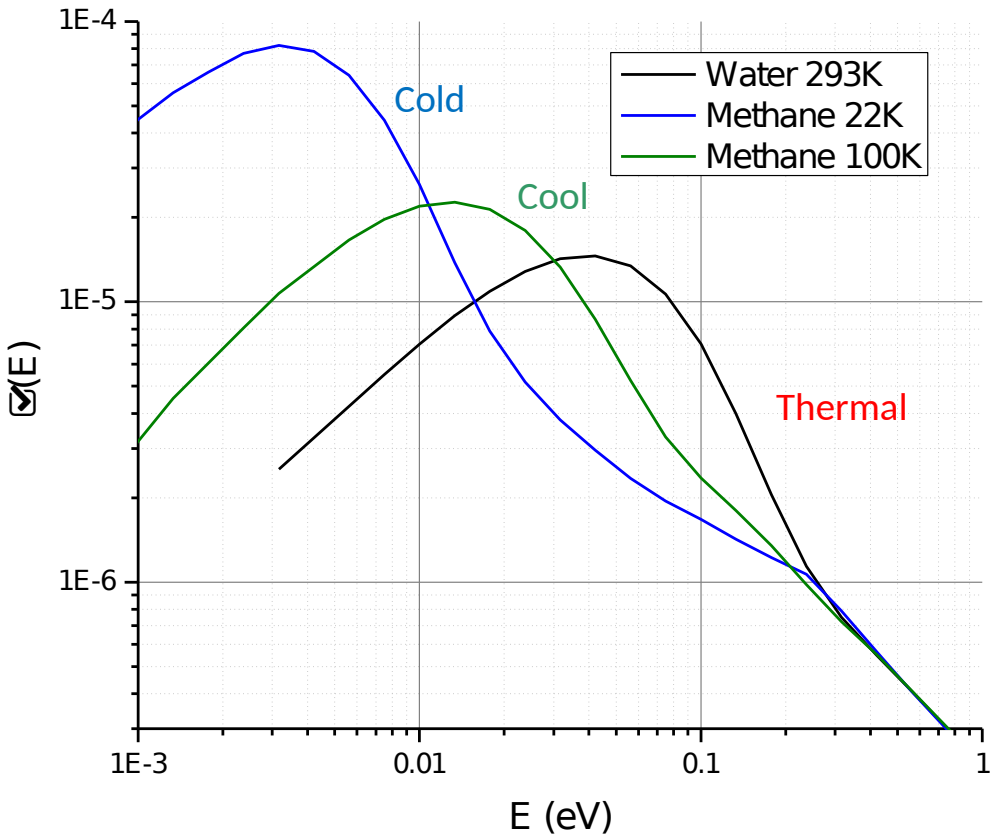
Activity report

1. Development of new scattering kernels.
2. Collaboration with NEA - JEFF.
3. Collaboration with CSEWG - ENDF/B.
4. Activities in support of LAHN Project.
5. Other R&D activities and collaborations.

1A) Development of new scattering kernels: liquid ethane

- Liquid ethane has been proposed by Dr. Granada as an interesting replacement for liquid methane as an intermediate energy "cool" neutron moderator:
  - Wide temperature range as a liquid (90 - 184 K).
  - Important protonic density (higher than liquid methane).
  - Presence of low energy CH_3 rotational modes.
- Development continues this year with transmission measurements at Vesubio (ISIS - UK).

1a) Development of new scattering kernels: liquid ethane



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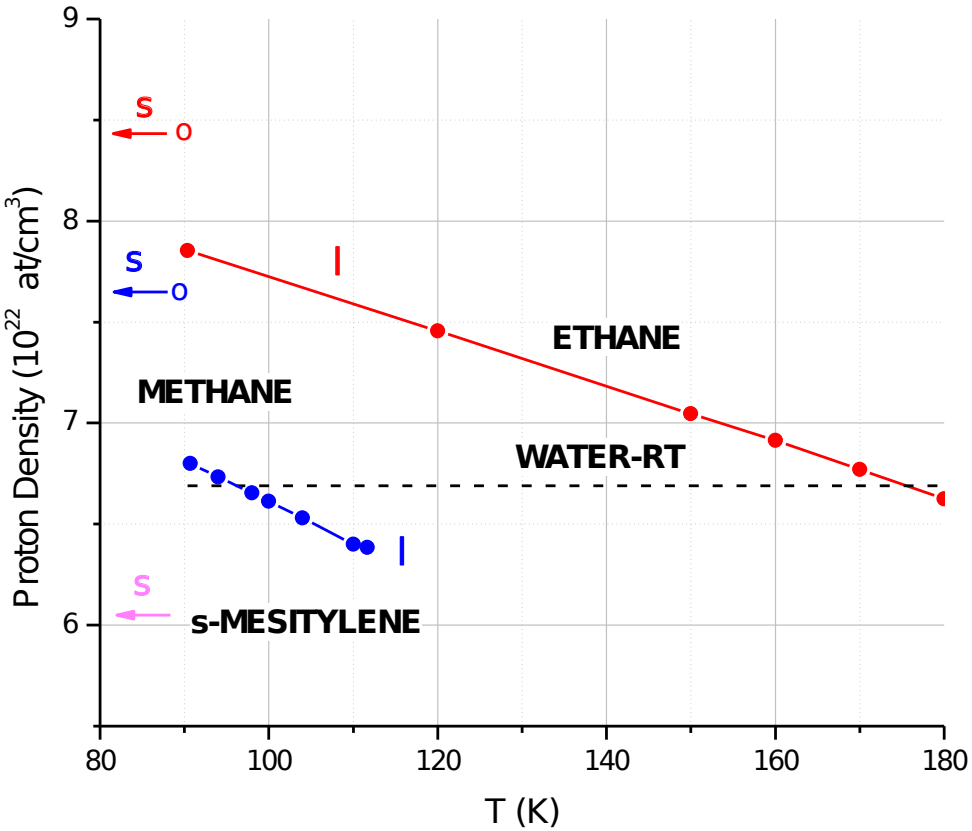

http://www.engineeringtoolbox.com/ethane-thermal-properties-d_1761.html

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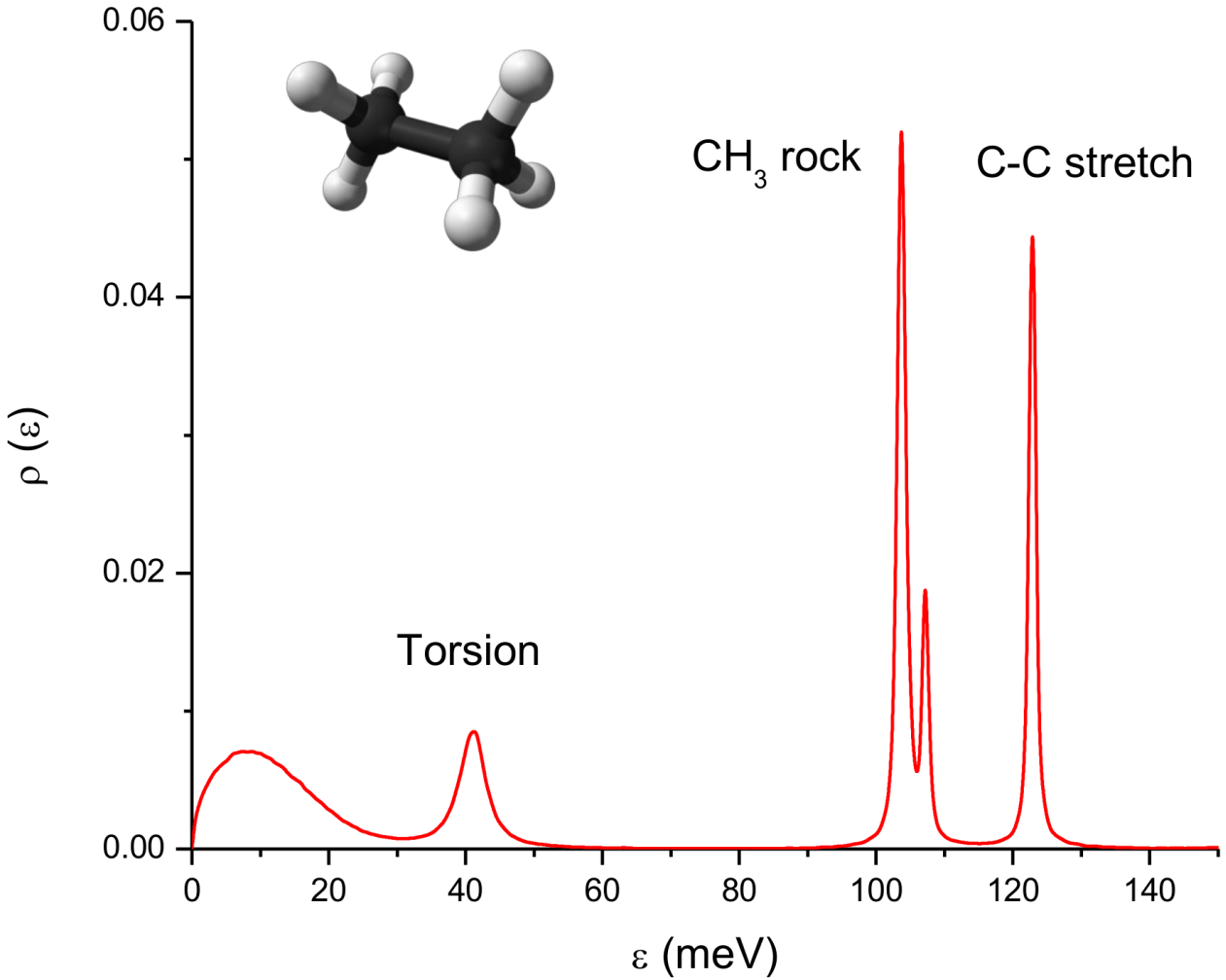

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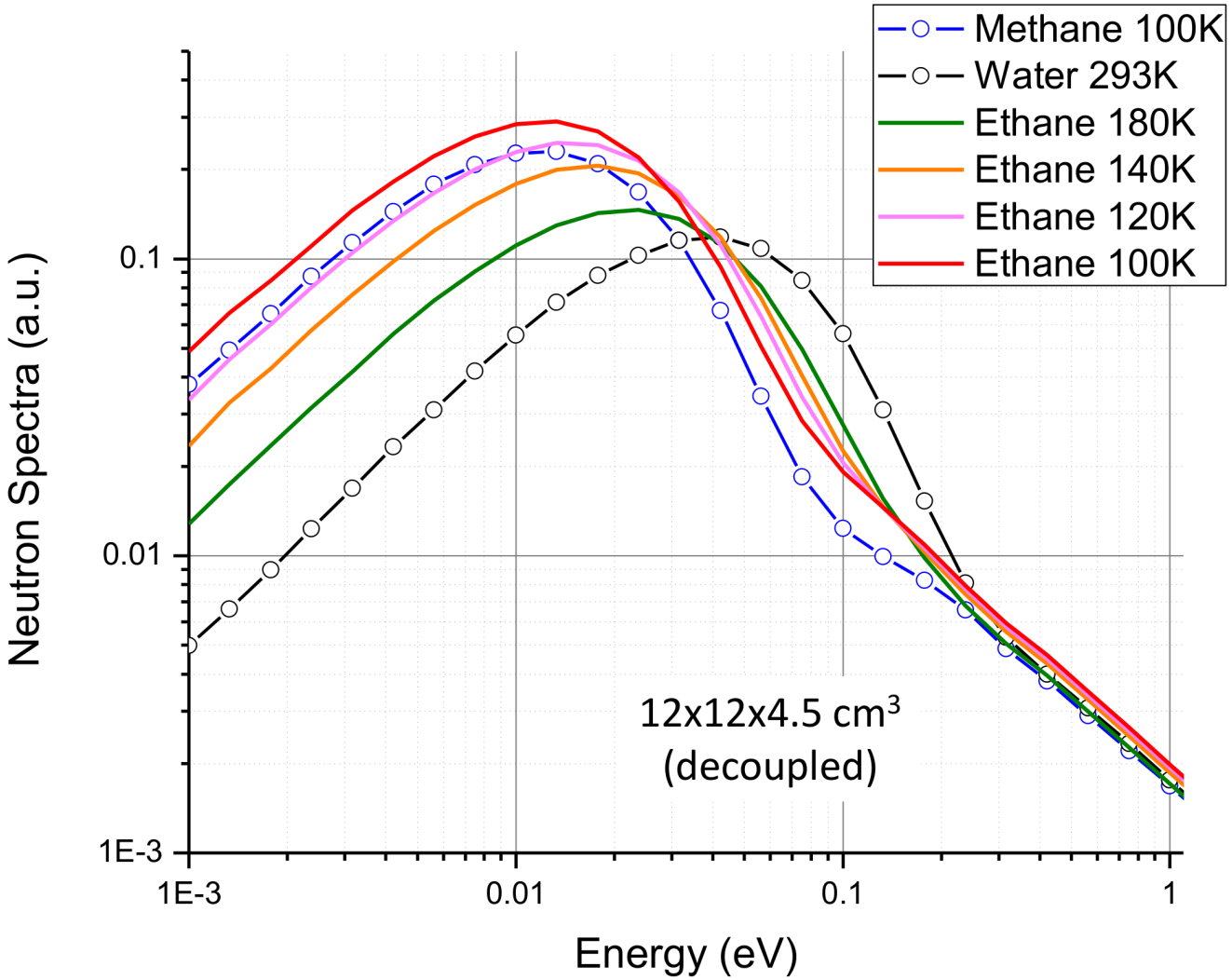
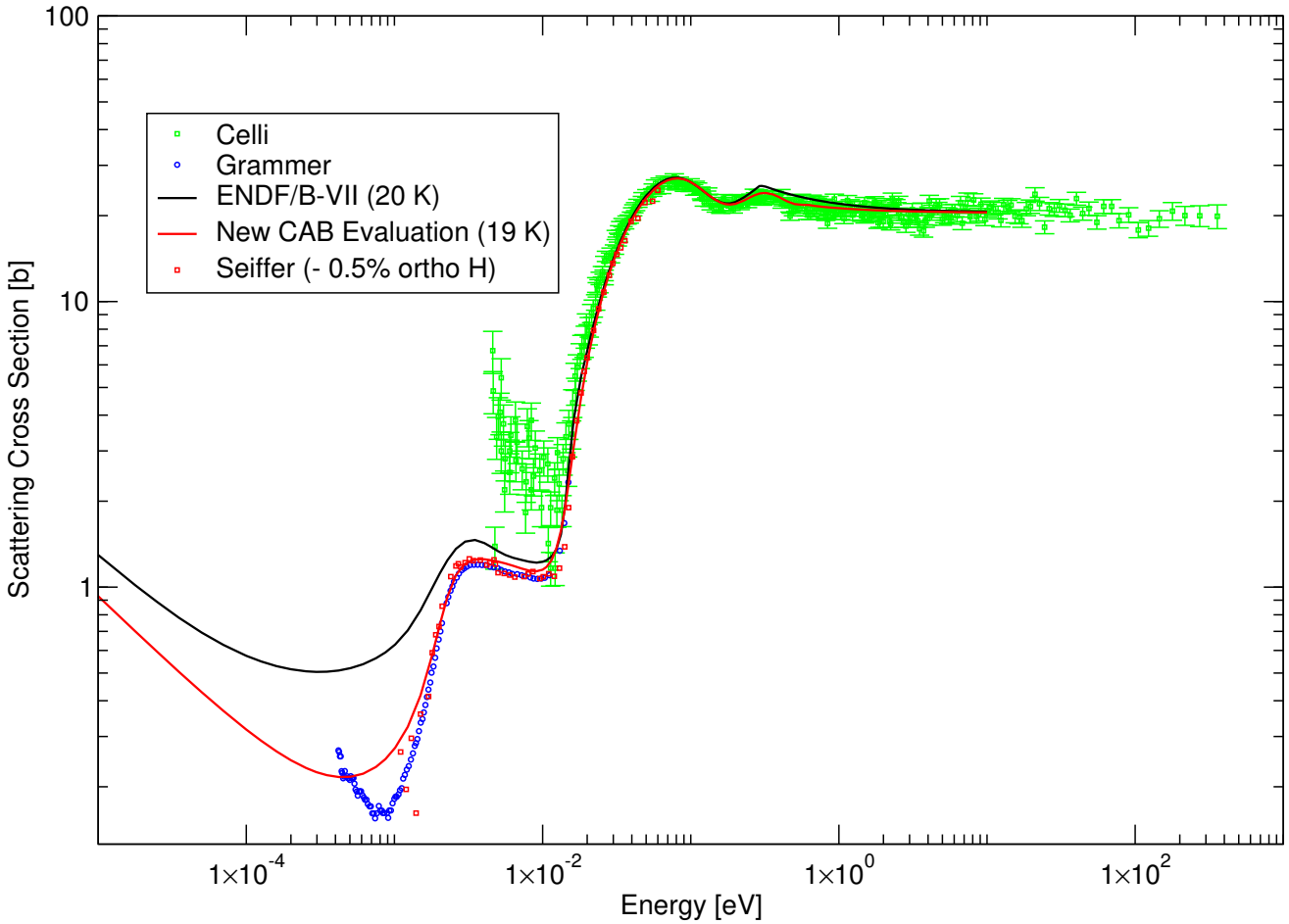


1b) Development of new scattering kernels: liquid hydrogen and deuterium

- The COLDH subroutine in LEAPR applies the Young-Koppel model for quantum rotators to hydrogen and deuterium.
- The subroutine applies a Vineyard correction to the translational motion of the molecule. This is incorrect, and was corrected by Granada and Gillette in 2004.
- The current model is an update of the model by Granada and Gillette, using the Sköld approximation for the coherent correction and updating the frequency spectra and structure factors.
- New evaluations available for 14 -20 K (ortho/para H_2) and 19-23 K (ortho/para D_2).

1b) Development of new scattering kernels: liquid hydrogen and deuterium



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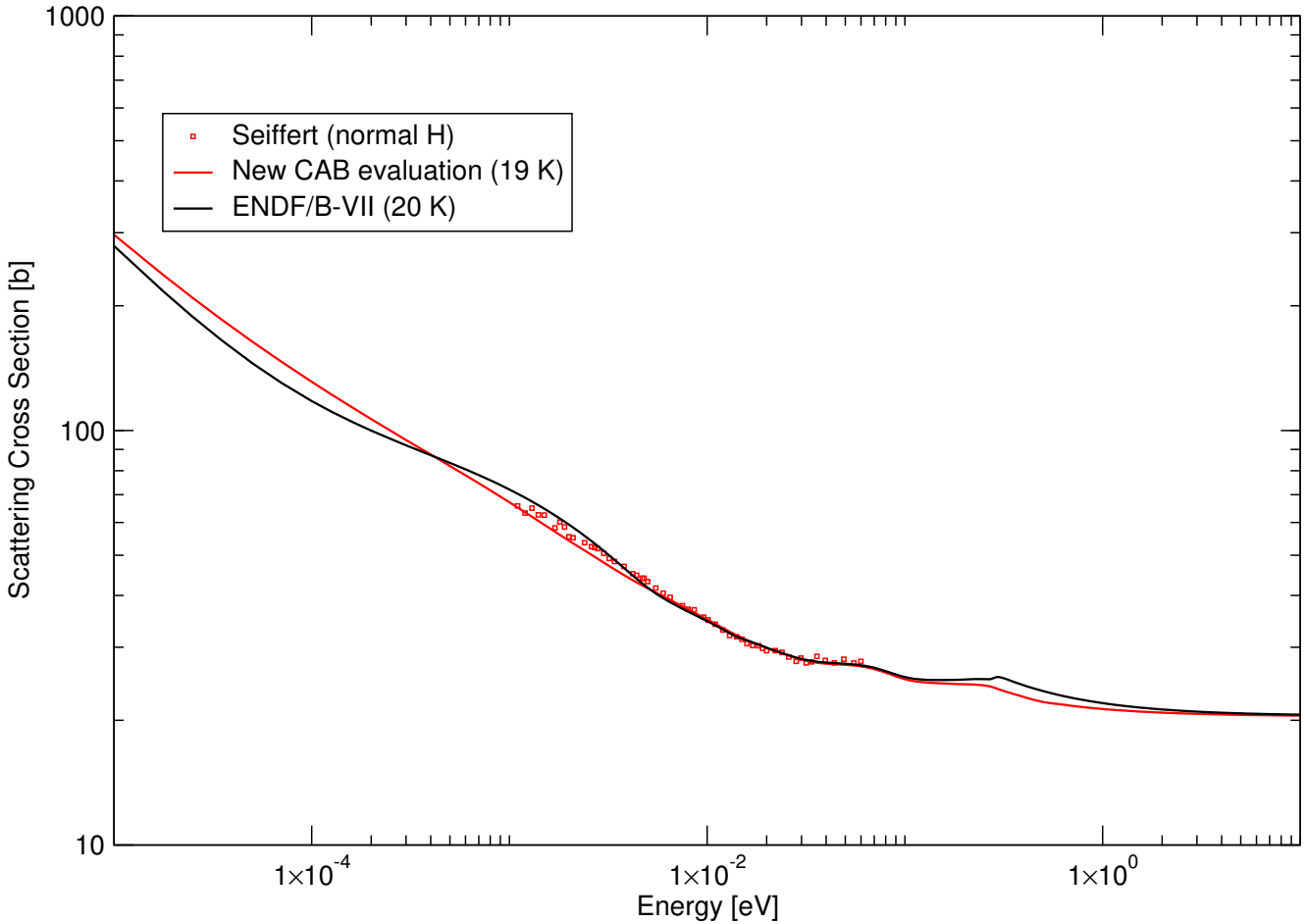

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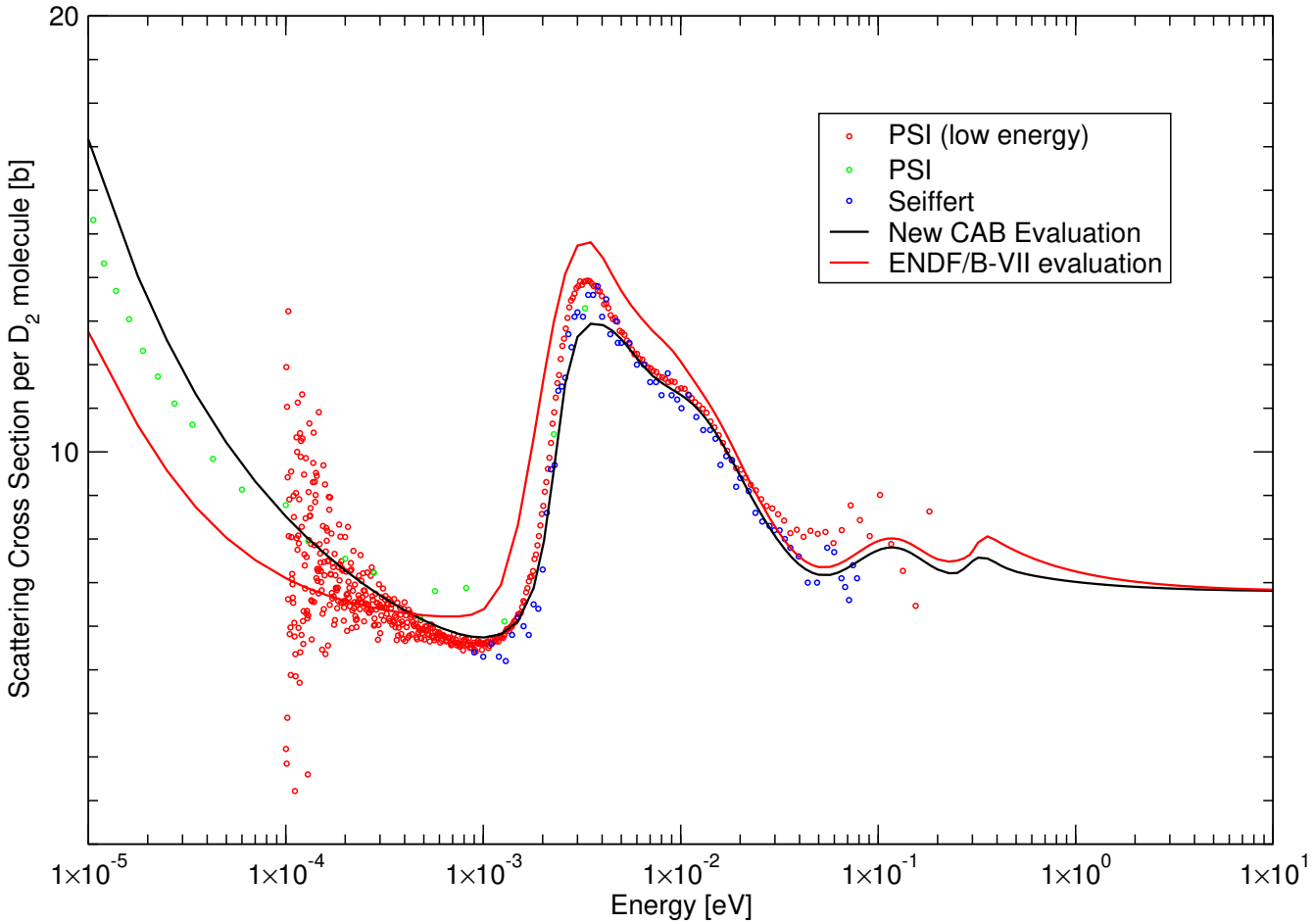


1b) Development of new scattering kernels: liquid hydrogen and deuterium

Code is available as a development branch of NJOY
in our repository at Github:

`https://github.com/marquezj/NJOY2016/tree/H2D2`

- Combining the options `ncold` and `nsk`, different models can be used:

ncold	nsk	model
1/2/3/4	0	ENDF/B-VI models
1/2/3/4	1	Granada model (2004)
1/2/3/4	2	Granada model (2017)

- The code also allows to change `smin` as an input parameter.

2) Collaboration with NEA - JEFF

- Collaboration NEA to provide scattering kernels to JEFF:
  - Thermal moderators: light water, heavy water.
  - Cold moderators: light water ice, mesitylene, tolune, methane, liquid hydrogen, liquid deuterium.
  - Neutron filters: silicon, sapphire.
- Nuclear data users from the advanced neutron sources community (many in Europe) will be benefited.
- JEFF will become the most complete evaluated data library for neutron scattering applications

(see talk by Florencia Cantargi at 15:30)

3) Collaboration with CSEWG - ENDF/B

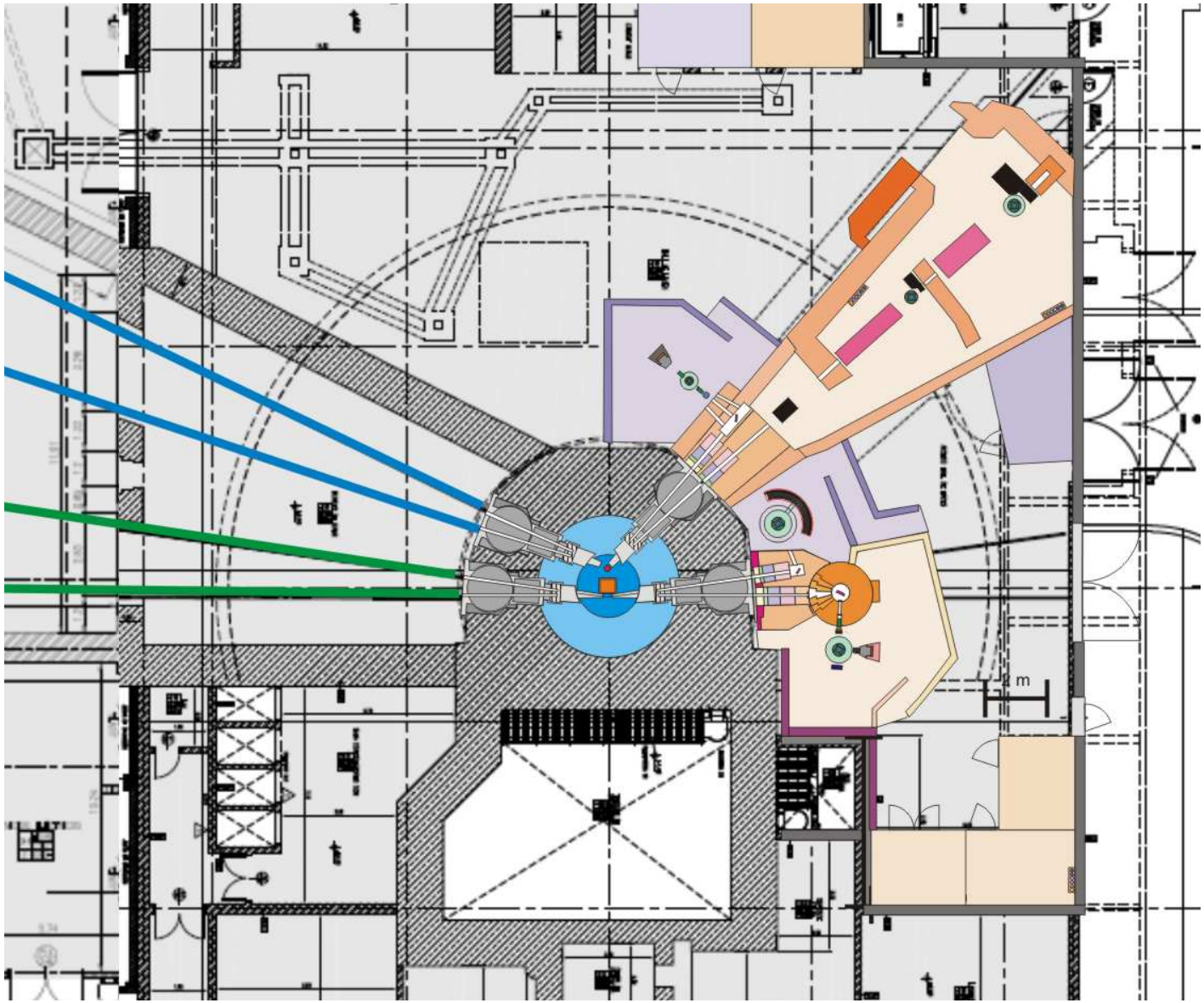
Participation in CSEWG in support of ENDF/B, in collaboration with Danila Roubtsov from Canadian Nuclear Laboratories:

- Continued support for light and heavy water libraries: extrapolation to 650 and 800 K (light water) and 650 K (heavy water).
- Coordination of TSL section in the ”big paper”.
- Collaboration with BNL on QA of TSL libraries: standarization of basic TSL checks.

4) Activities in support of LAHN Project.

- LAHN (Laboratorio Argentino de Haces de Neutrones) is a project for the scientific utilization of neutron beams at the future RA-10 reactor.
- RA-10 is a 30 MW experimental reactor being built at Centro Atómico Ezeiza, Argentina.
- First concrete poured on May 6th, expected to become critical in 2019.
- The Nuclear Data Group is supporting this project by providing shielding and beam shielding calculations, and helping with education and training.

4) Activities in support of LAHN Project.

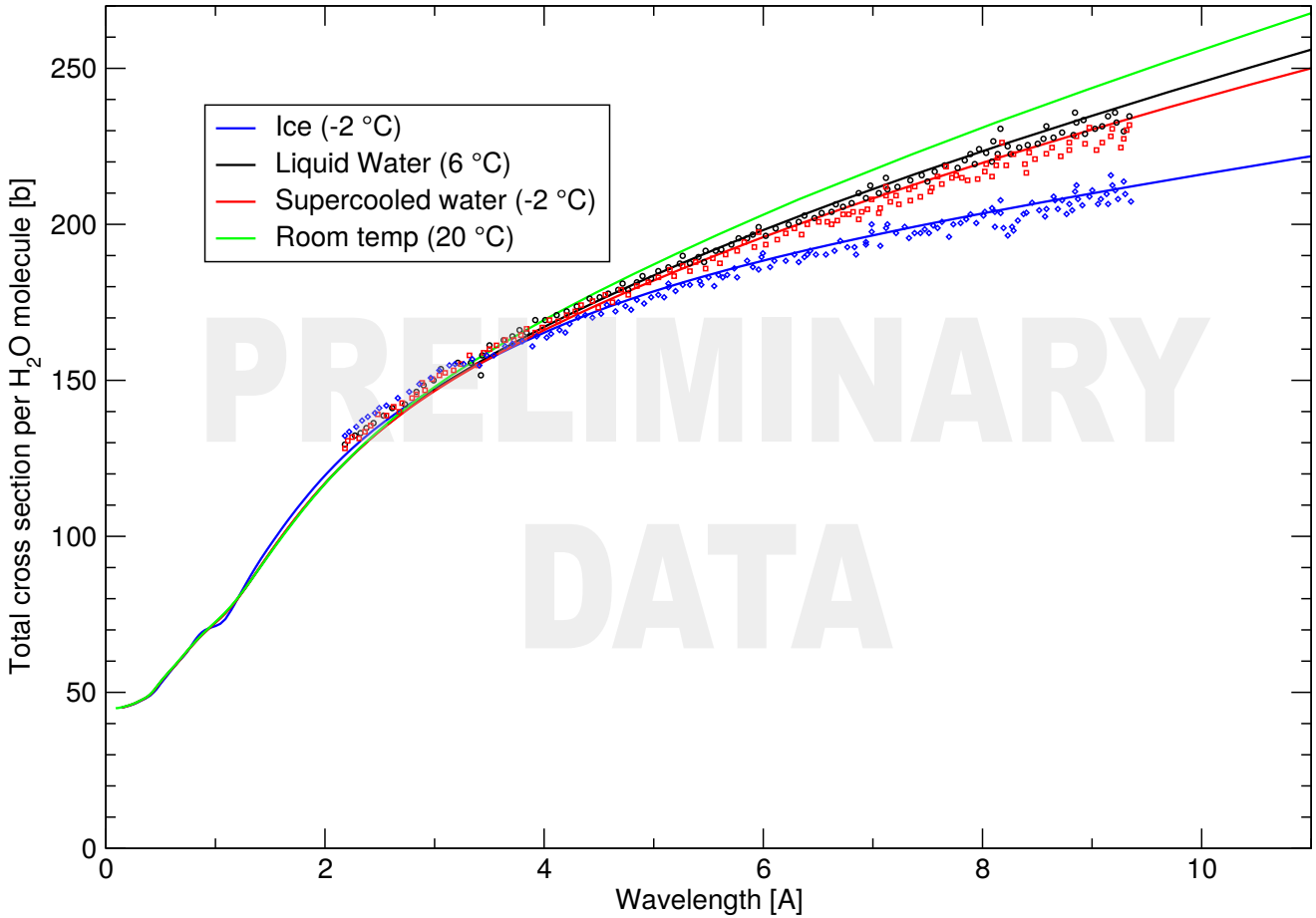


4) Activities in support of LAHN Project.

5) Other R&D activities and collaborations

- Ab initio calculations: beryllium and uranium dioxide.
- Development of LEAPR/NJOY: contributions will be made available online.
- Collaboration with CCHEN (Chile): calculation of delayed neutron fraction and effective delayed neutron fraction.
- Collaboration with PSI (Switzerland): transmission experiments in cold water / ice.
- Participation in UCANS / ICANS.
- IAEA CRP on Advanced Moderators for Intense Cold Neutron Beams in Materials Research.

5) Collaboration with PSI.



Comparison of preliminary ice and water transmission data with TSL models. Data was measured by Pierre Boilat and Muriel Siegwart from PSI at the test beamline of BER II reactor.


Thanks for your time.
Questions?
Patagonia, Argentina