Recent Studies on Materials of Interest for Very Cold and Ultra Cold Neutron Sources

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OVERVIEW

Development of Scattering Kernels:

"Tradicional" cold moderator materials:

Liquid Hydrogen & Deuterium

Materials for VCN/UCN sources

Solid Deuterium

Methane Phase II

Ethane Phase III

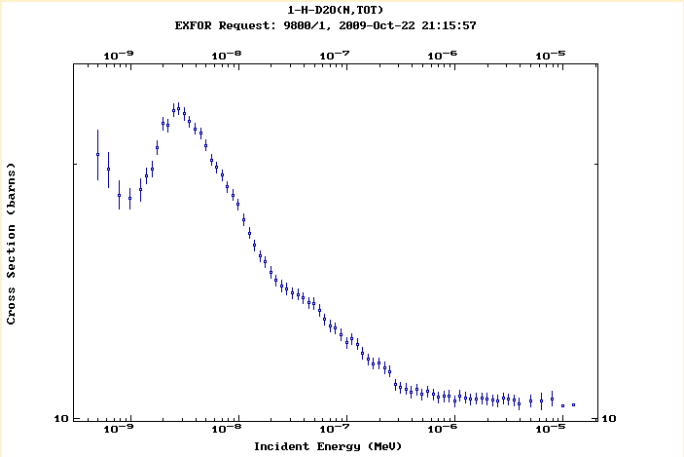
^{4}He superfluid

Old stuff revisited:

Methane Clathrate

Bi, Pb

Final comments



AUTHOR (F.Kropff,J.R.Latorre,J.R.Granada,C.Castro MAdero)
TITLE Total neutron cross-section of D2O at 20 degrees-C between 0.0005 and 10 eV.
EXP-YEAR (1973)
FACILITY (LINAC) Pulsed 25 MeV Linac.
Nuclear Data Section, IAEA, EXFOR 30283 (1974)
Neutron Moderator: Paraffin at 77 K.

LIQUID HYDROGEN

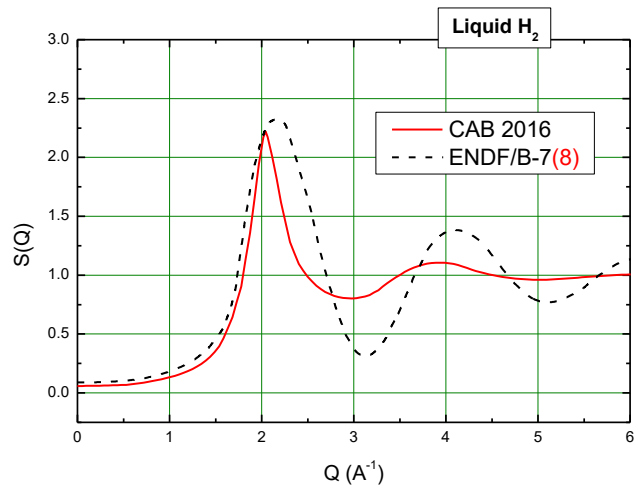
International Collaboration on Advanced Neutron Sources (ICANS XXII)

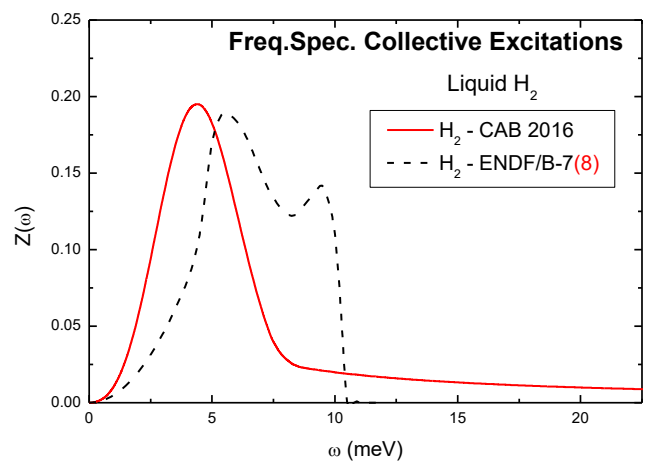
ICANS XXII Oxford 2017

27–31 March 2017, Saïd Business School, University of Oxford, UK

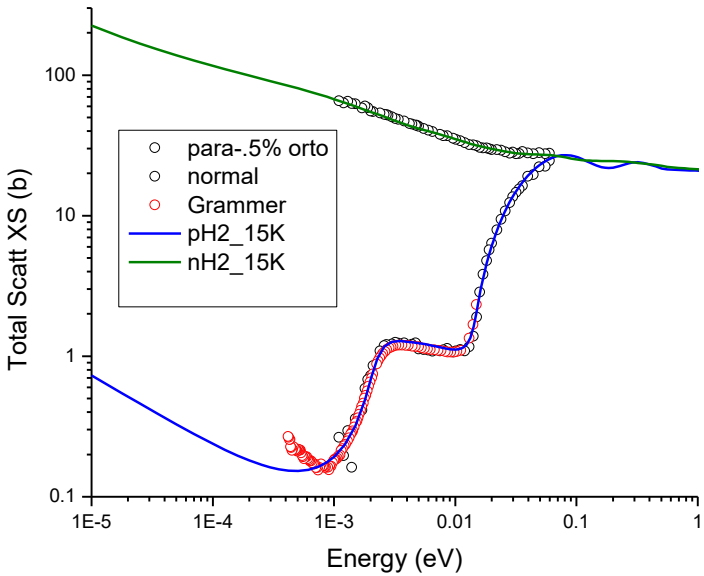
New Neutron Scattering Kernels for Liquid Hydrogen and Deuterium

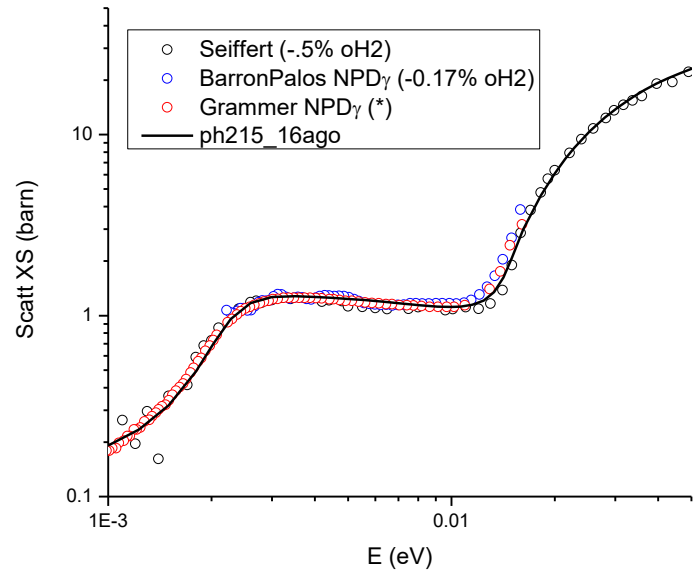
J.R. Granada[1], J.I. Márquez Damián[1,2] and F. Cantargi[1]

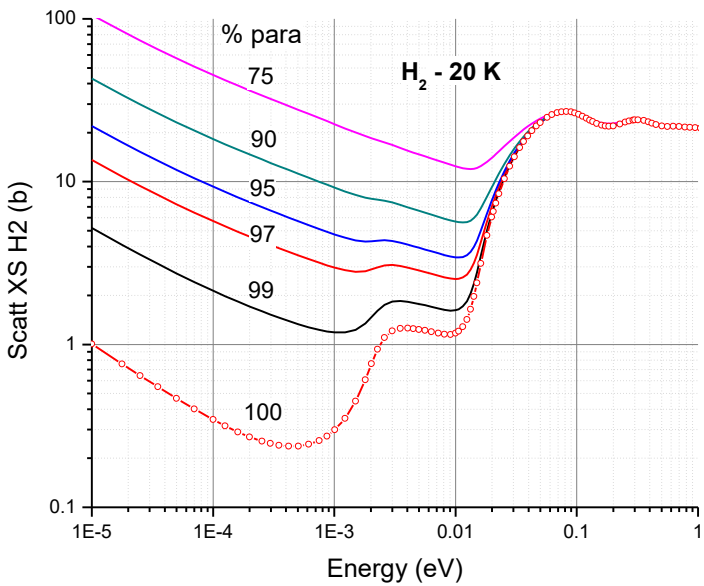


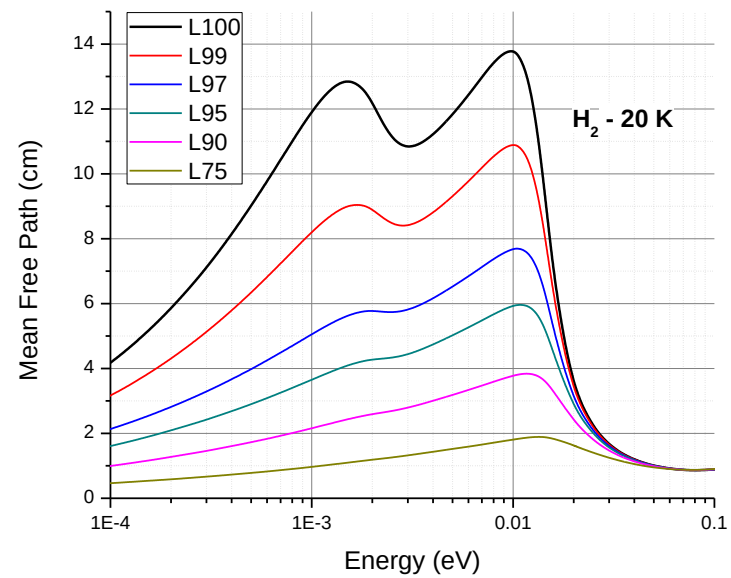


(H in) LIQUID HYDROGEN

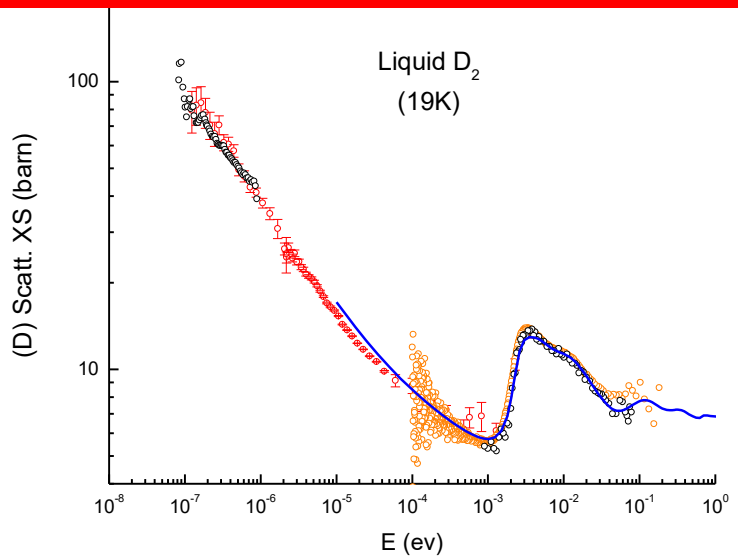


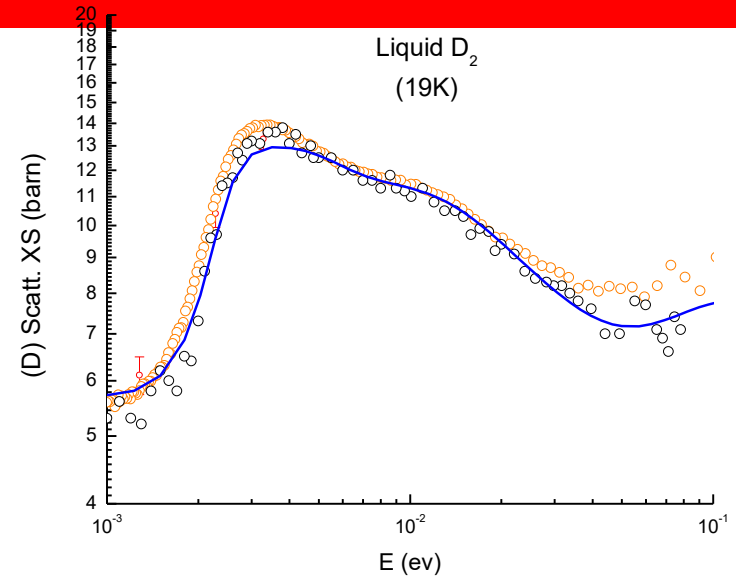


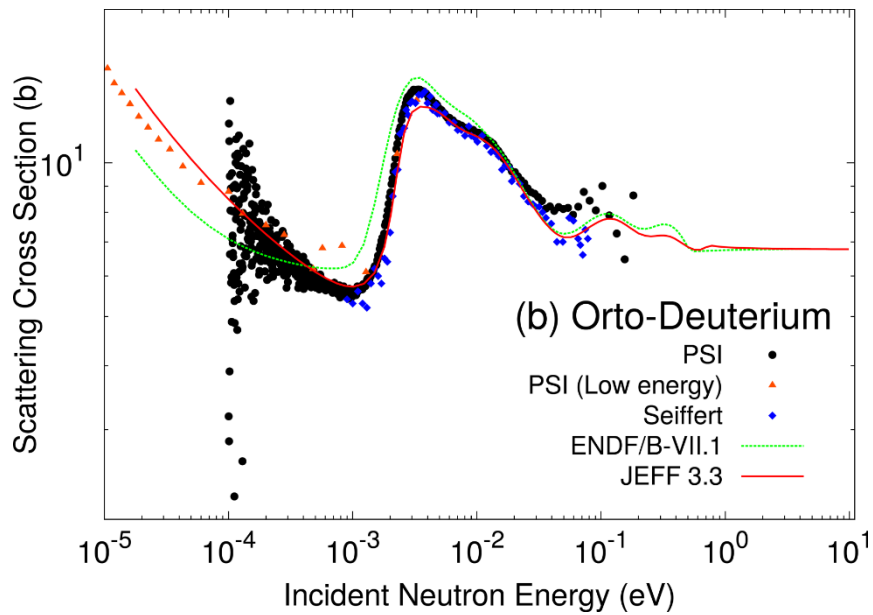




LIQUID DEUTERIUM







SOLID DEUTERIUM

- A new scattering kernel to describe the interaction of slow neutrons with solid Deuterium has been developed.

- The main characteristics of this molecular solid are contained in the formalism, including dynamical aspects related to:
    - the lattice's density of states,
    - the Young-Koppel quantum treatment of the rotational motion,
    - the internal molecular vibration.
- The elastic processes involving coherent and incoherent contributions are also fully described, as well as the spin-correlation effects caused by the coupling of intrinsic and rotational angular momenta.
- The one-phonon coherent term in the upscattering cross section is considered outside the incoherent approximation.

A Letters Journal Exploring the Frontiers of Physics

June 2009

EPL, **86** (2009) 66007
doi: 10.1209/0295-5075/86/66007

www.epljournal.org

Neutron scattering kernel for solid deuterium

J. R. Granada[(a)]

NEW MODEL

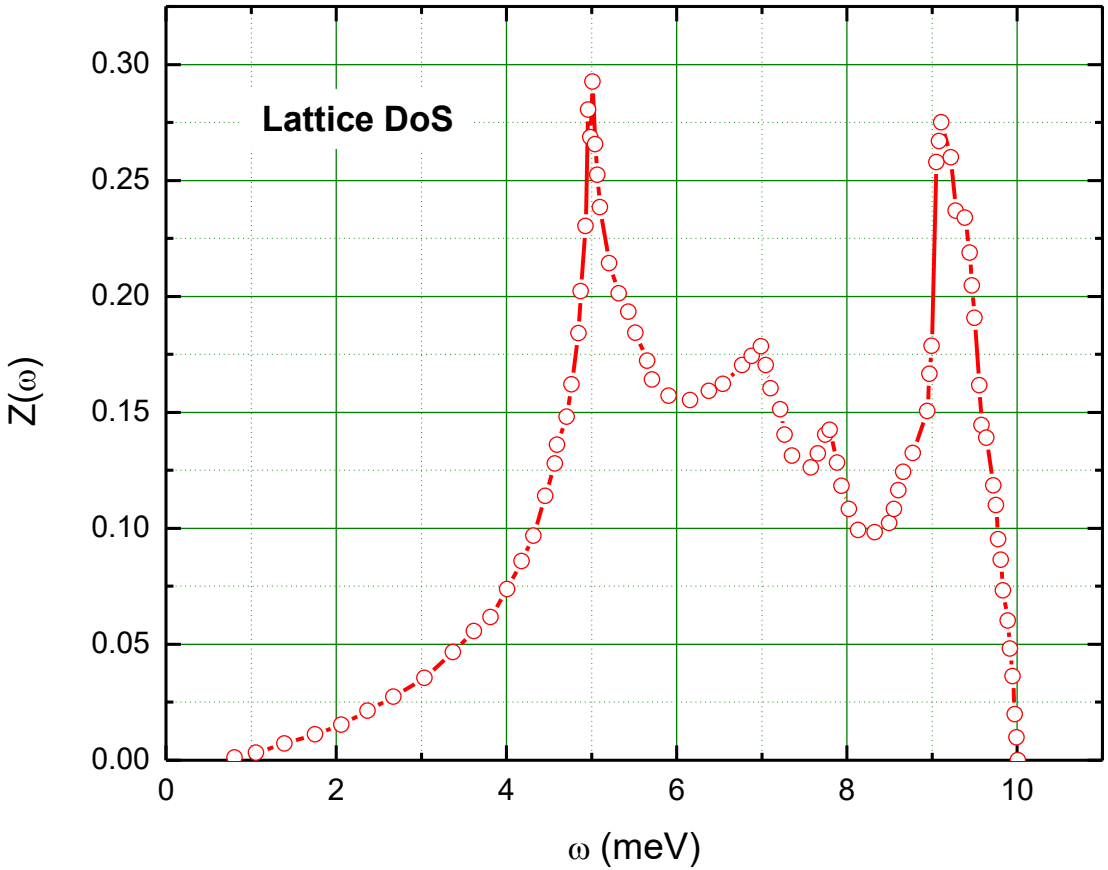
$$S^{el}(\mathbf{Q},0) = [4\, b_c^2\, j_0^2\,(Qd/2)\, |F(\mathbf{Q})|^2 + 2\, b_i^2 +$$

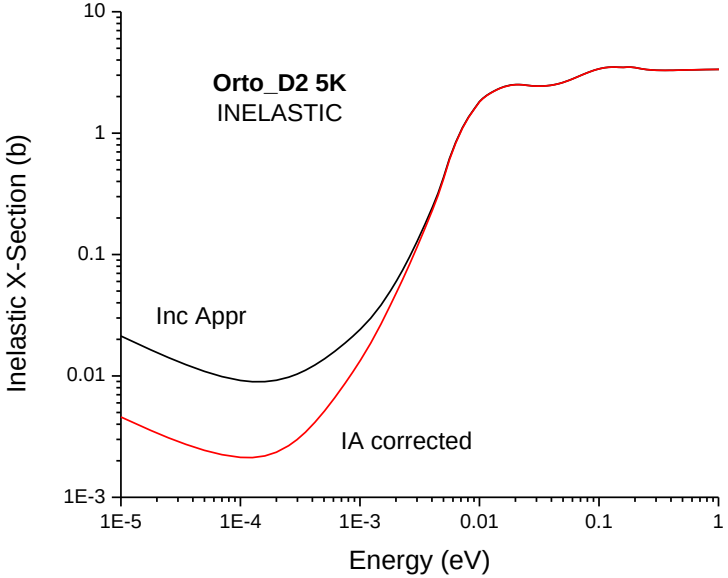
$$+ 2\, b_i^2\, \alpha\, j_0\,(Qd) + 2\, b_c^2\, \{1 + j_0\,(Qd) - 2\, j_0^2\,(Qd/2)\}]\, e^{-2W}$$

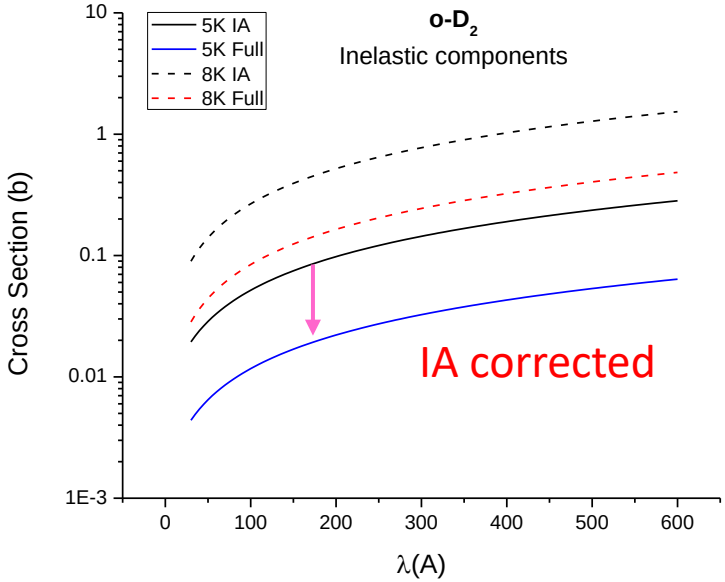
$$S^{inel}(\mathbf{Q},\omega) = [4\, b_c^2\, j_0^2\,(Qd/2)\, \{S^{1ph}(\mathbf{Q},\omega) - S_s^{\,1ph}(\mathbf{Q},\omega)\} + V_o^{rot}(\mathbf{Q},\omega) \otimes S_s(\mathbf{Q},\omega)\,]\, e^{-2W}$$

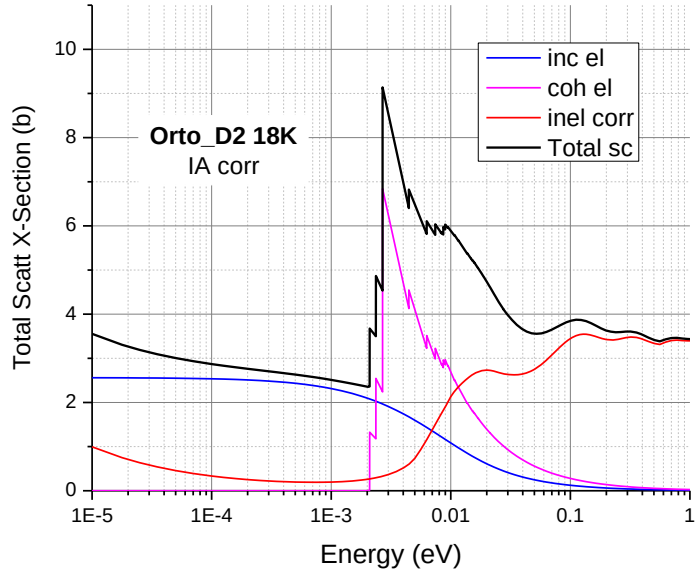
Marked terms: not included in the conventional NJOY´s algorithm.

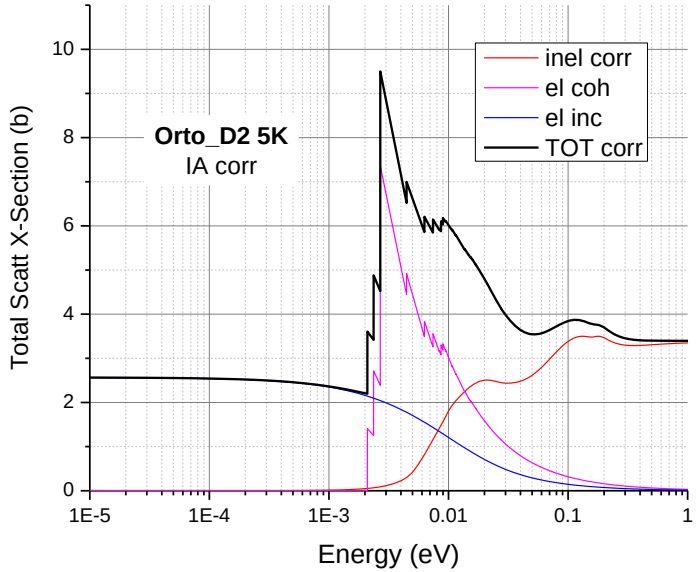
J.W.Schmidt *et al.*, Phys.Rev.**B 30**, 6308 (1984)

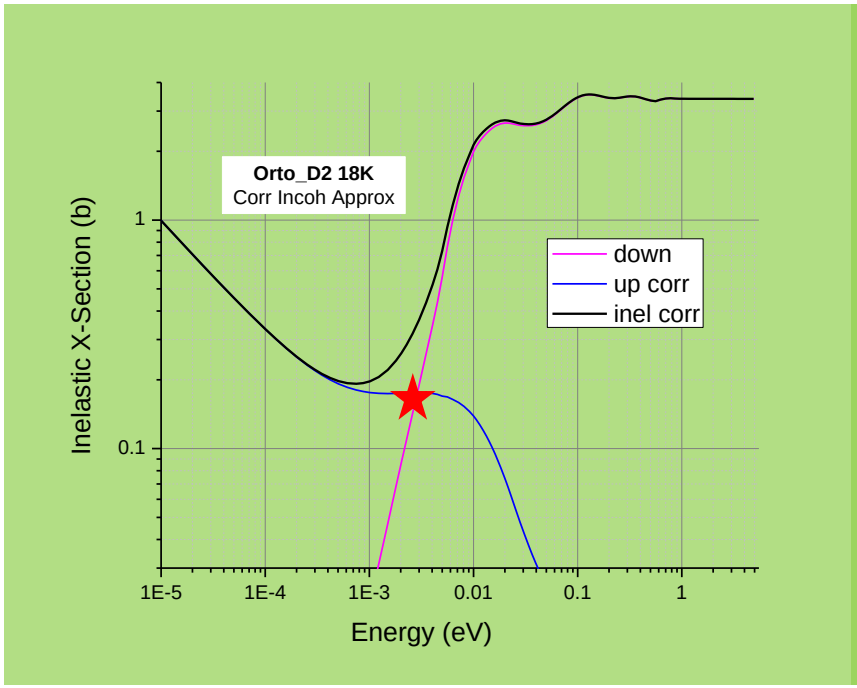


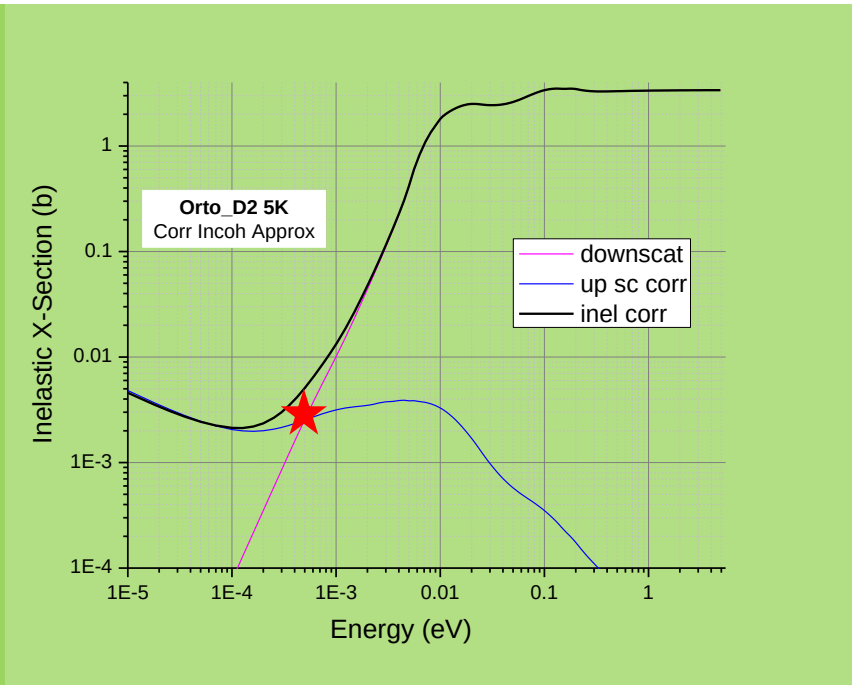

Orto_D2 5K
INELASTIC
Inc Appr
IA corrected
Inelastic X-Section (b)
Energy (eV)
10
1
0.1
0.01
1E-3
1E-5
1E-4
1E-3
0.01
0.1
1


5K IA
5K Full
8K IA
8K Full
o-D2
Inelastic components
IA corrected
Cross Section (b)
λ(A)
10
1
0.1
0.01
1E-3
0
100
200
300
400
500
600

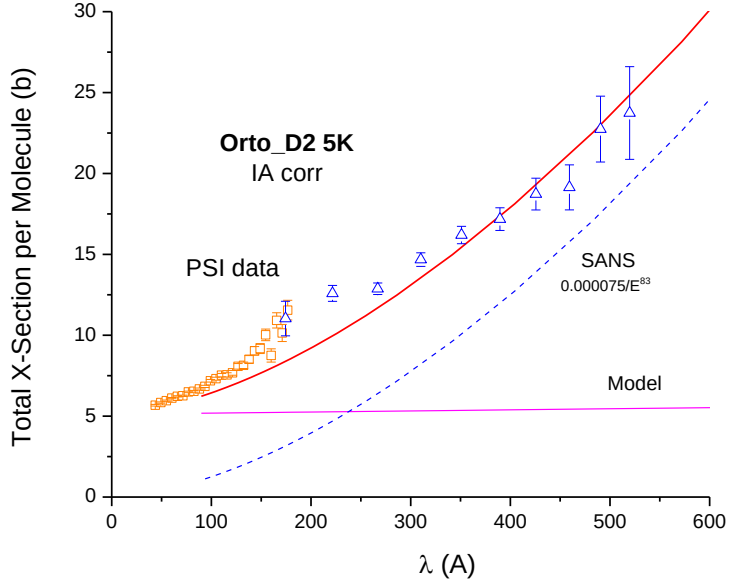

Orto_D2 18K
IA corr
inc el
coh el
inel corr
Total sc
Total Scatt X-Section (b)
Energy (eV)
0
2
4
6
8
10
1E-5
1E-4
1E-3
0.01
0.1
1

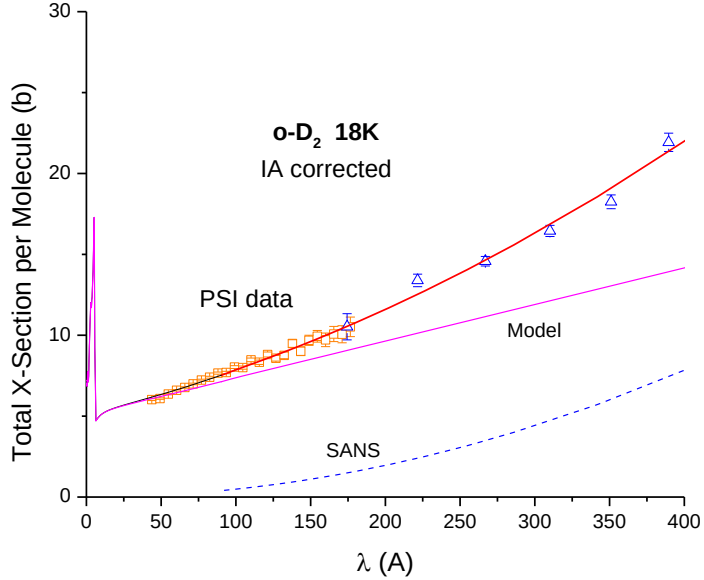

Orto_D2 5K
IA corr
inel corr
el coh
el inc
TOT corr
Total Scatt X-Section (b)
Energy (eV)
0
2
4
6
8
10
1E-5
1E-4
1E-3
0.01
0.1
1

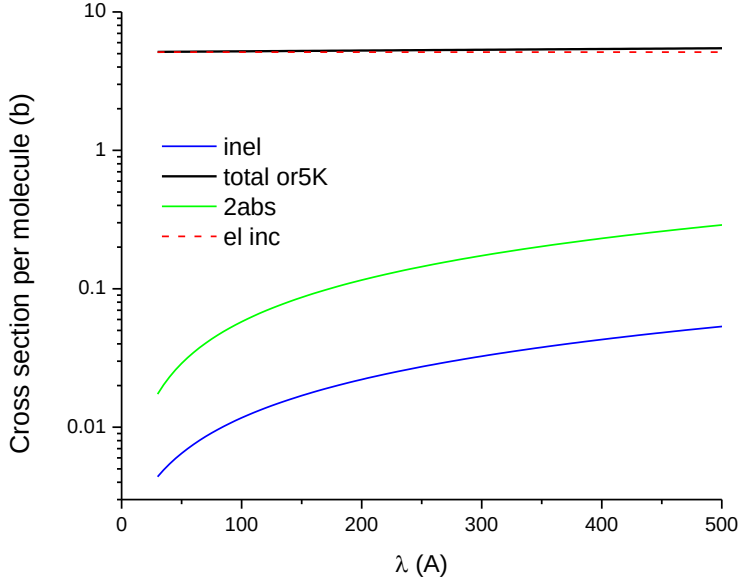

Orto_D2 18K
Corr Incoh Approx
down
up corr
inel corr
Inelastic X-Section (b)
Energy (eV)
0.1
1
1E-5
1E-4
1E-3
0.01
0.1
1

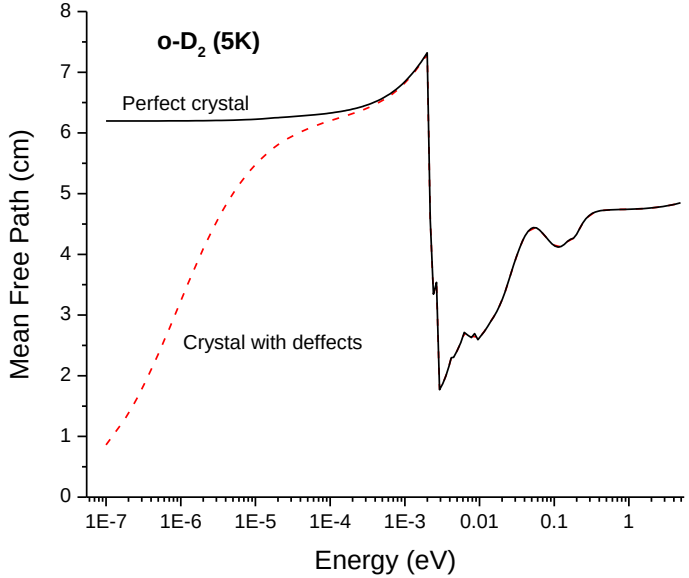

Orto_D2 5K
Corr Incoh Approx
downscat
up sc corr
inel corr
Inelastic X-Section (b)
Energy (eV)
1E-4
1E-3
0.01
0.1
1
1E-5
1E-4
1E-3
0.01
0.1
1

Experimental data from PSI

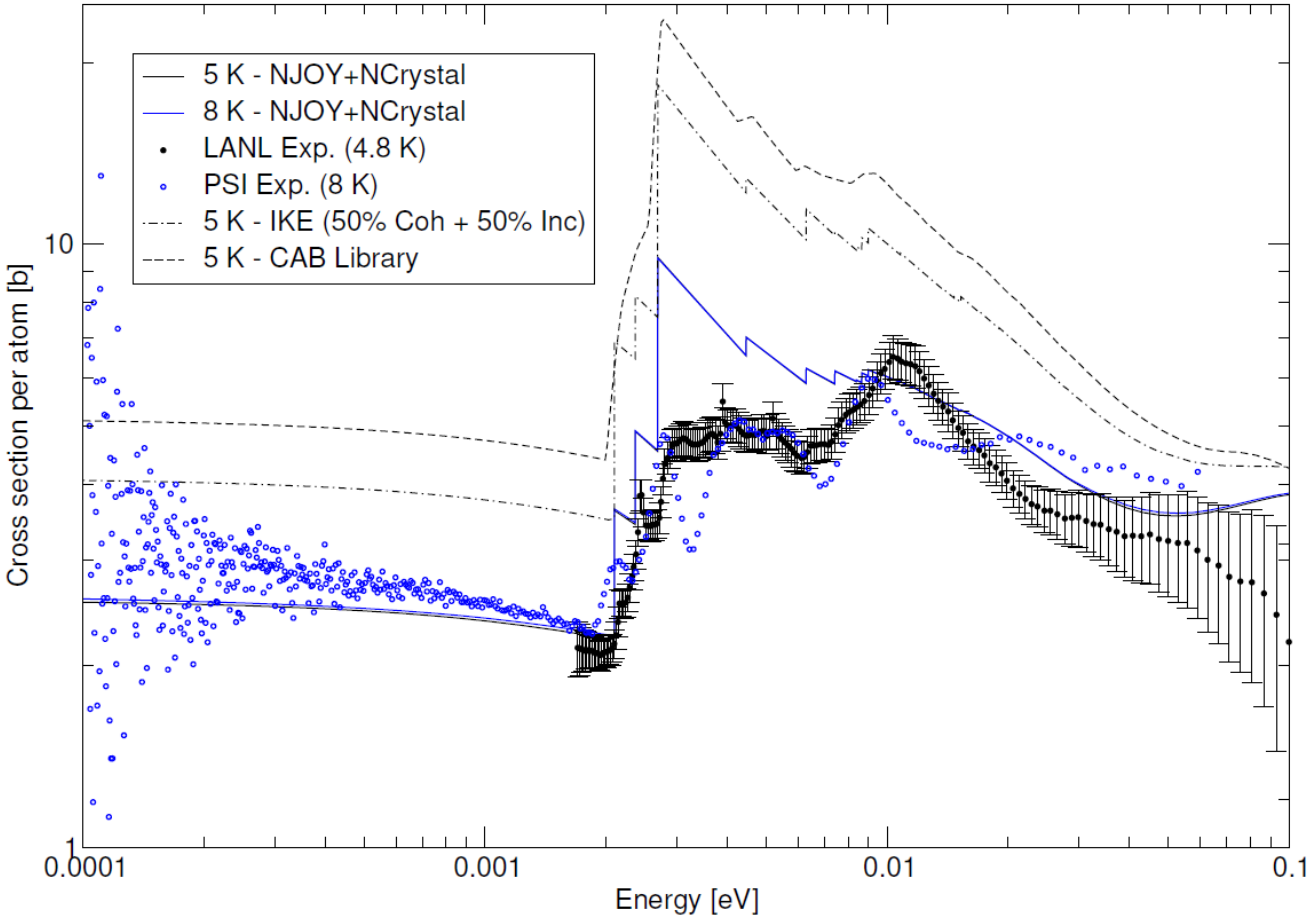




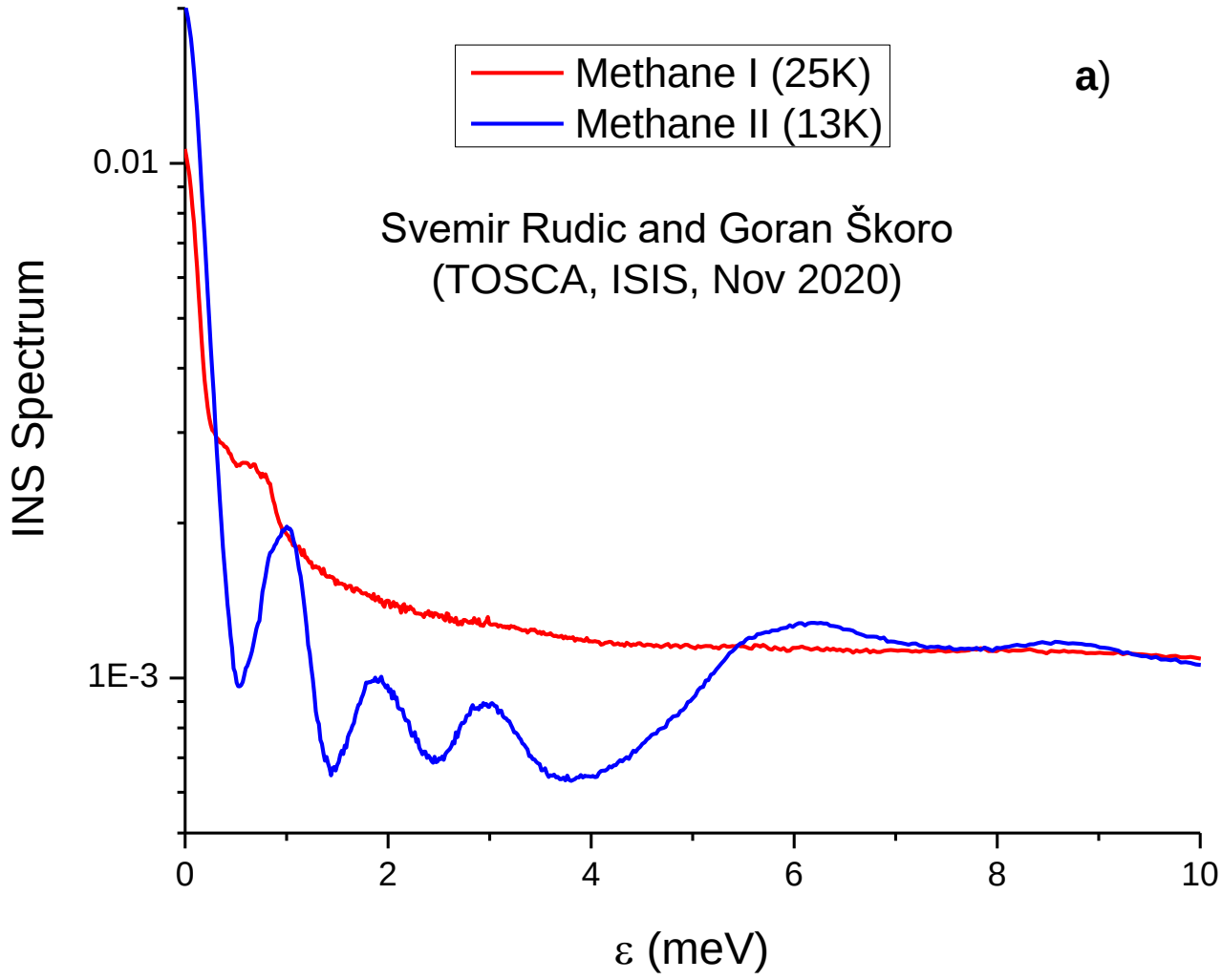


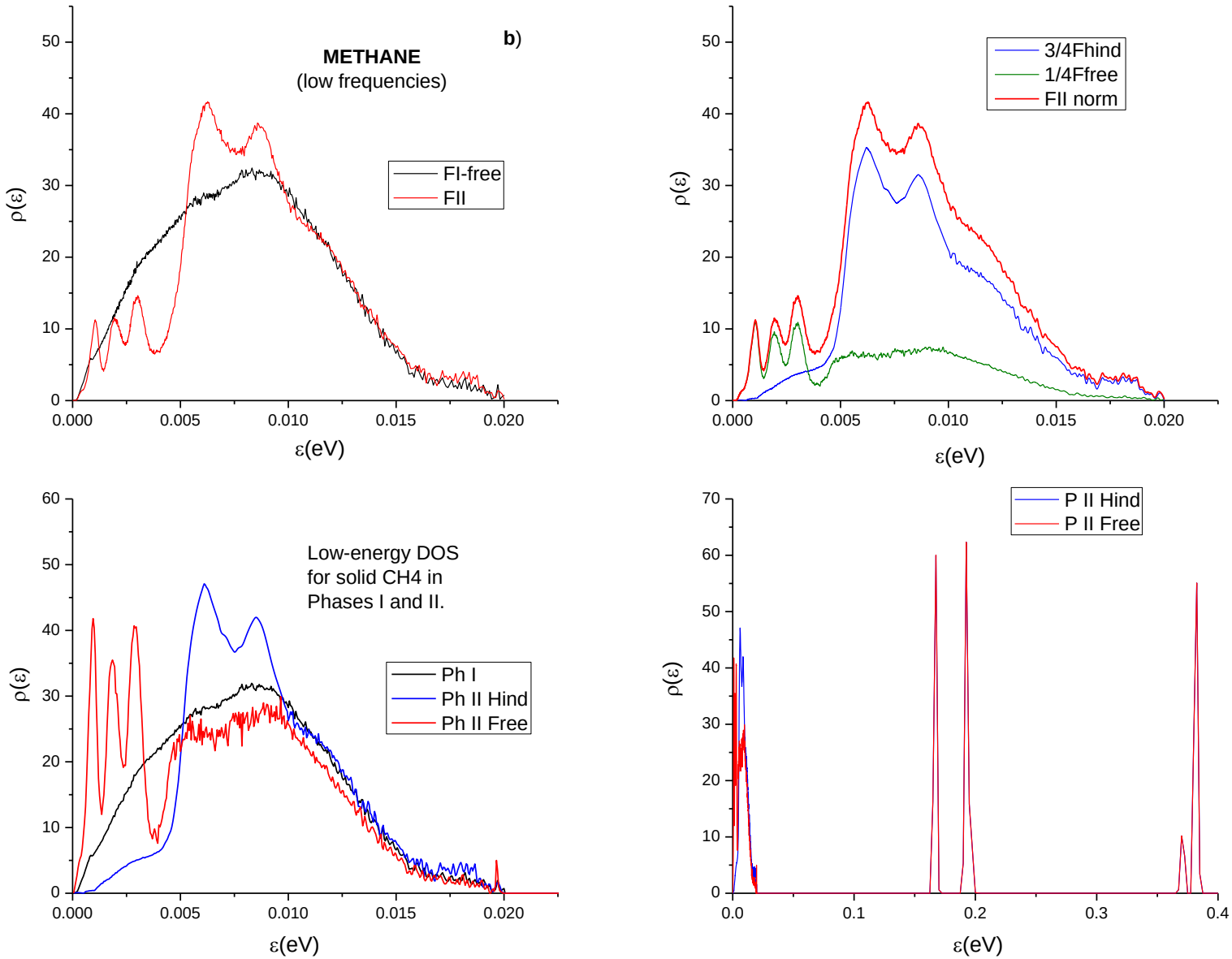


Thermal neutron scattering nuclear data work at ESS



METHANE I & II


Methane I (25K)
Methane II (13K)
a)
Svemir Rudic and Goran Škoro
(TOSCA, ISIS, Nov 2020)
INS Spectrum
0.01
1E-3
0
2
4
6
8
10
ε (meV)


b)
METHANE
(low frequencies)
FI-free
FII
3/4Fhind
1/4Ffree
FII norm
Low-energy DOS
for solid CH4 in
Phases I and II.
Ph I
Ph II Hind
Ph II Free
P II Hind
P II Free
ρ(ε)
ε(eV)

METHANE II

$$\chi^{\text{inter}}(\mathbf{Q},t) = \left(b_c^C\right)^2 \langle\ f'_{C,C}\ \rangle + 4\left(b_c^C b_c^H\right) \langle\ f'_{C,H}\ \rangle + 16\left(b_c^H\right)^2 \langle\ f'_{H,H}\ \rangle$$

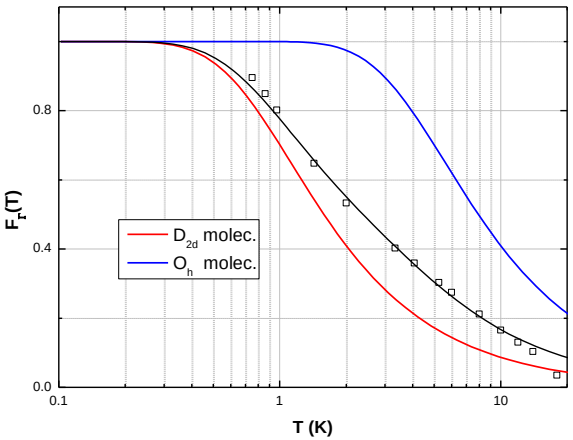
$$\chi^{\text{intra}}(\mathbf{Q},t) \cong \left(b_c^C\right)^2 \langle f_{CC} \rangle + \sum_{\Gamma} g_\Gamma \left[4\left\{ \left(b_c^H\right)^2 + \left(b_i^H\right)^2 \right\} \langle f_{HH}^{\Gamma}(\mathbf{Q},t) \rangle + \right.$$

$$\left. +3 \left\langle \left\{ \left(b_c^H\right)^2 + \left(b_i^H\right)^2 \frac{(\mathbf{S}_H.\mathbf{S}_H)}{S(S+1)} \right\} \left[f_{HH'}^{\Gamma}(\mathbf{Q},0) - 1 \right] \right\rangle \right]$$

$$S_H(\mathbf{Q},\omega) \cong 4 \sum_{\Gamma} g_\Gamma \left[\left\{ \left(b_c^H\right)^2 + \left(b_i^H\right)^2 \right\} S^{\Gamma}(\mathbf{Q},\omega) + \right.$$

$$\left. + \left\{ \tfrac{3}{4} \left(b_c^H\right)^2 + \left(b_i^H\right)^2 F_\Gamma(T) \right\} j_0(Qr_{HH}) e^{-\gamma_\Gamma Q^2} \delta(\hbar\omega) \right]$$

NEW $F_d(T)$ CALCULATION



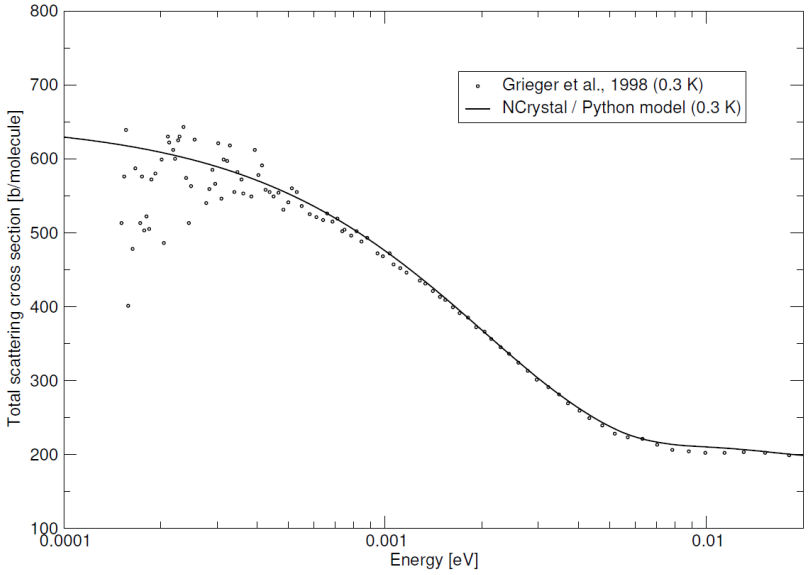
Book 6 columnas B y C

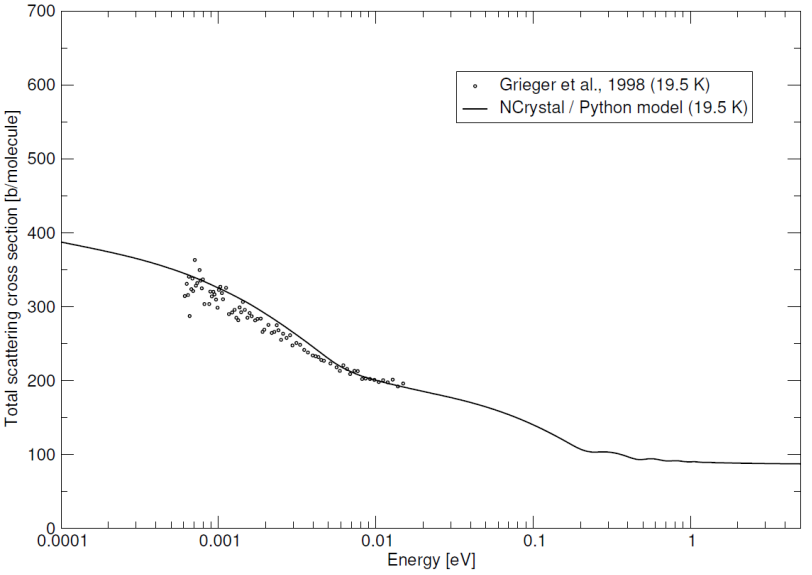
1. The $F_d(T)$ corresponding to "hindered" molecules (D_{2d}) is the theoretical result of Yamamoto et al. (J.Chem.Phys. **66**, 2701 (1977) (Fig.26).
2. The $F_d(T)$ corresponding to "free" molecules (O_h) is given by tanh(ε /2/kT), with ε = 0.00075 eV.
3. The value of ε used in 2., allows a good fit to the total spin correlation dependence with T, as quoted by Lushington & Morrison (Can.J.Phys., **55**, 1580 (1977) (Table 1).
4. It is argued in the literature that the theoretical free-molecule spin correlation <I(I+1)> (as calculated by Yamamoto et al.) might not be an accurate description of the actual O_h molecules in CH_4 Phase II, as they may suffer some hindering effect from the actual molecular lattice.

Thermal neutron scattering nuclear data work at ESS

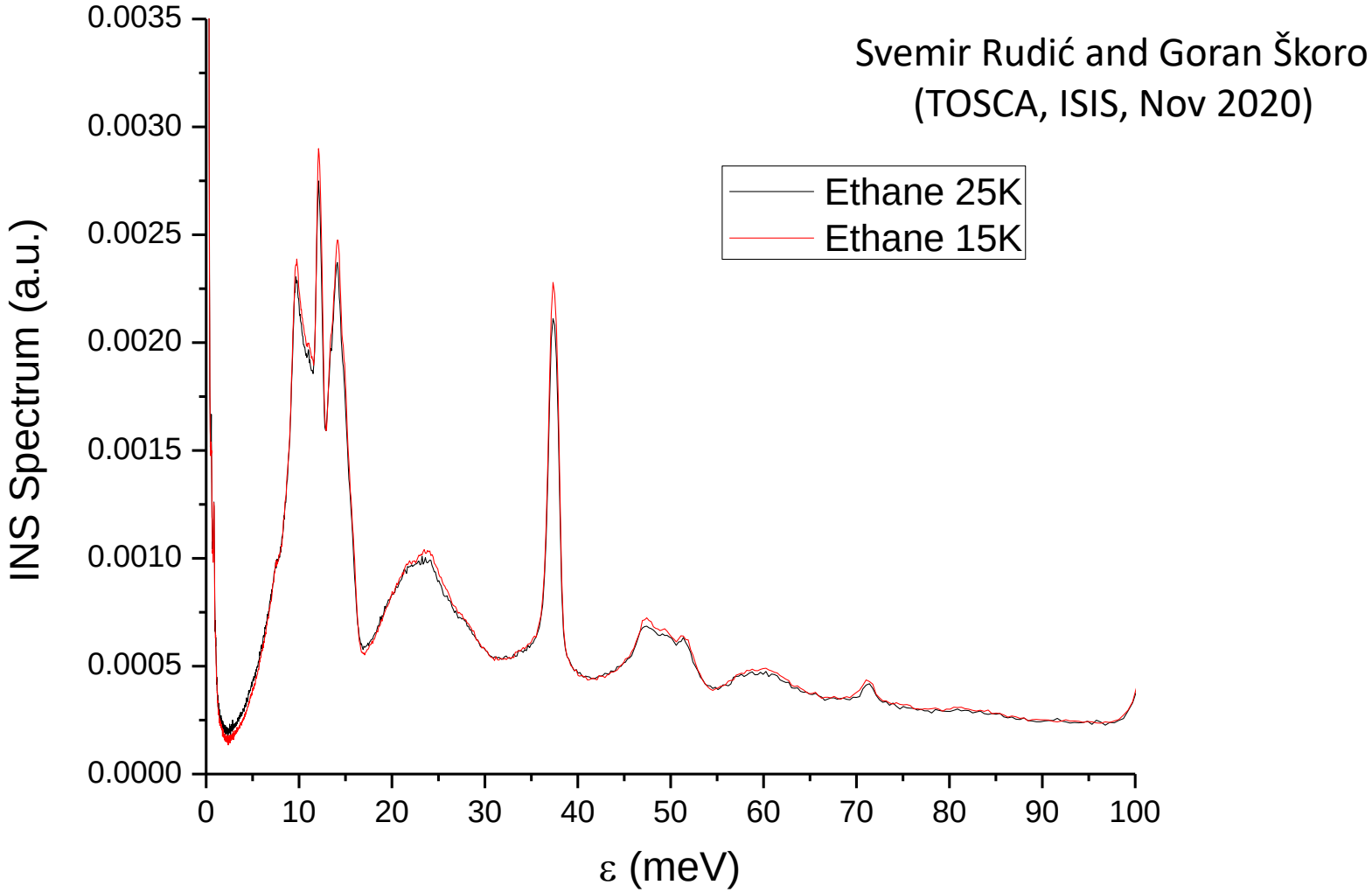
Methane in phase II

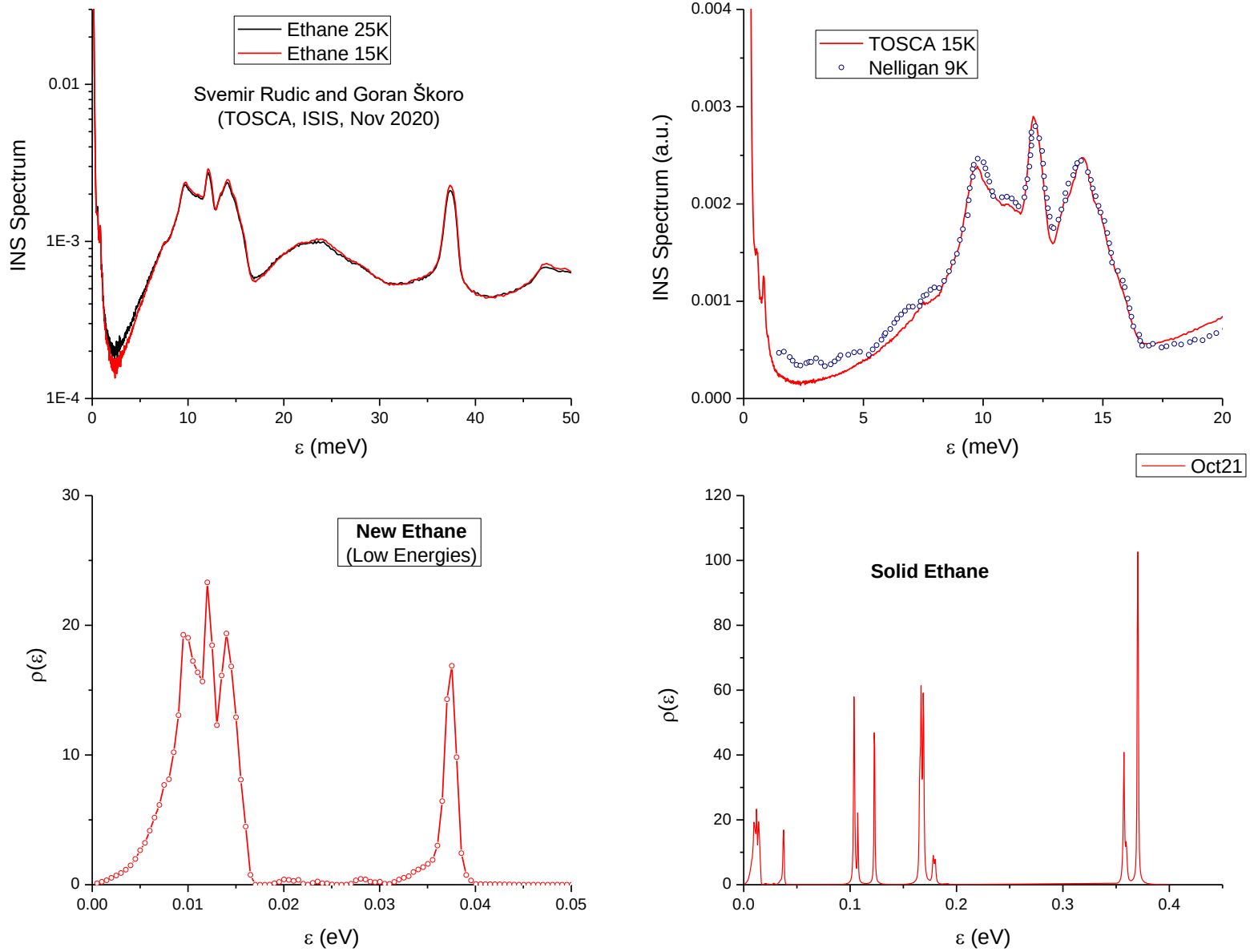
- Preliminary model in Python and NCrystal, based on the models by Granada.

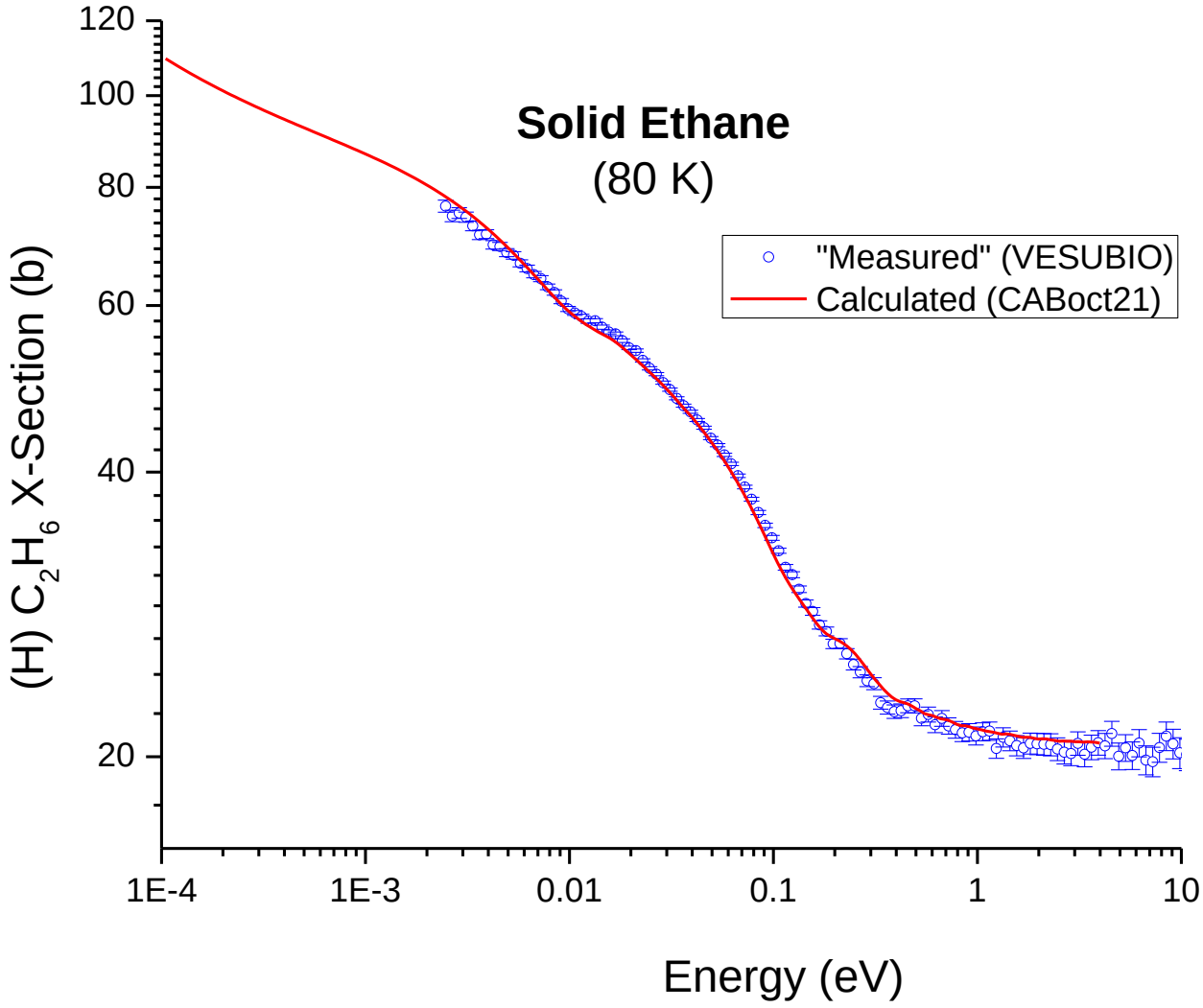


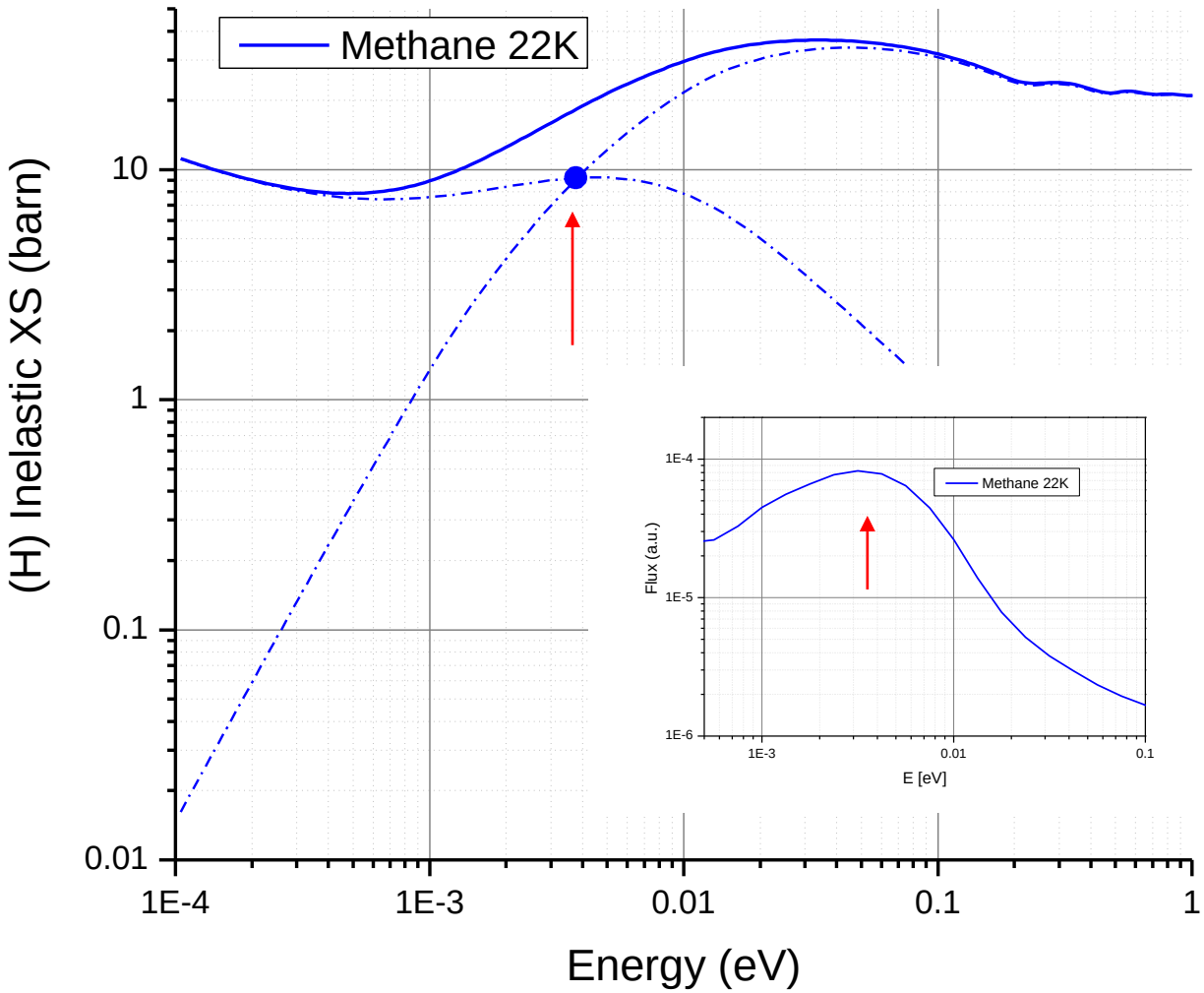


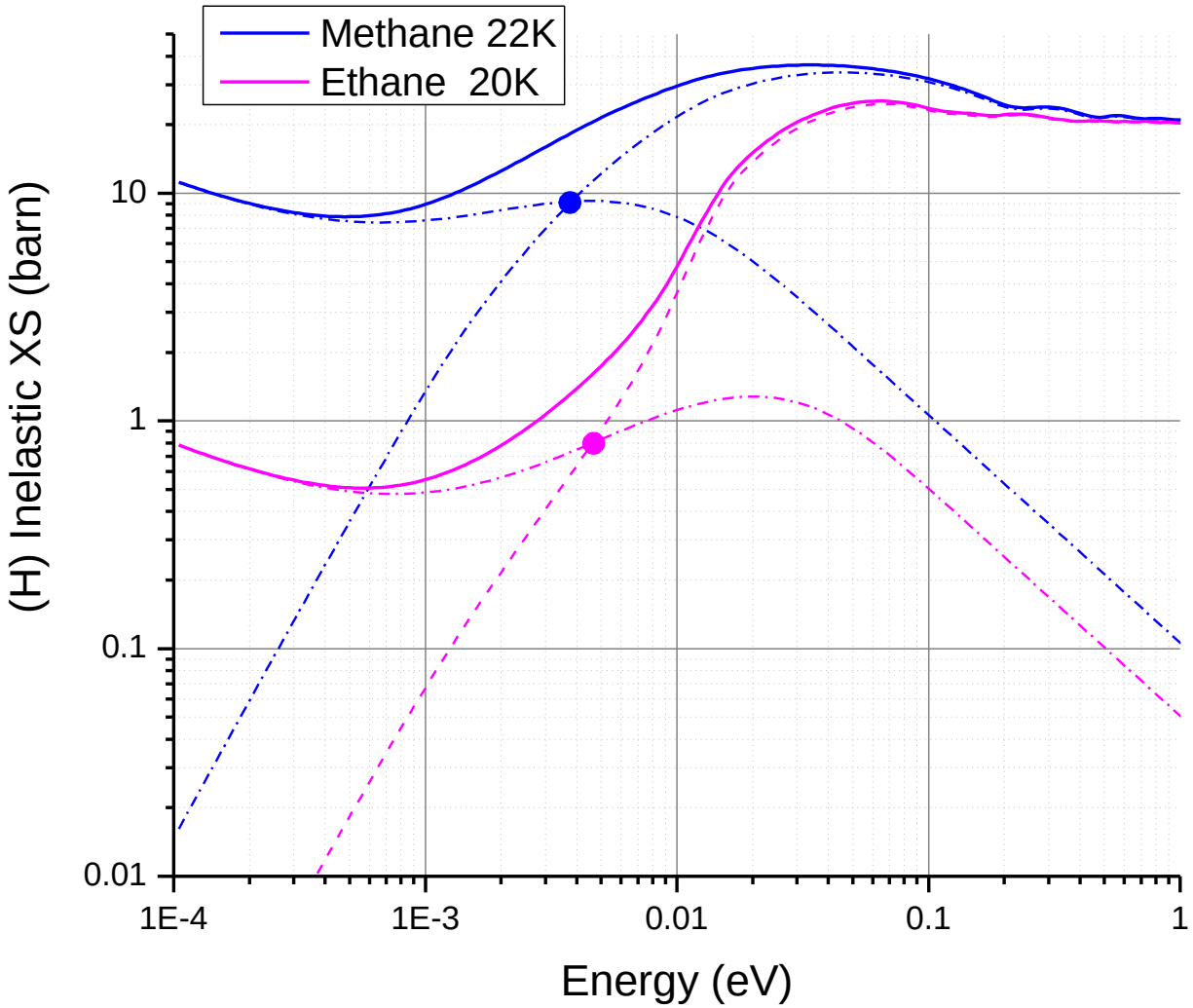
ETHANE III

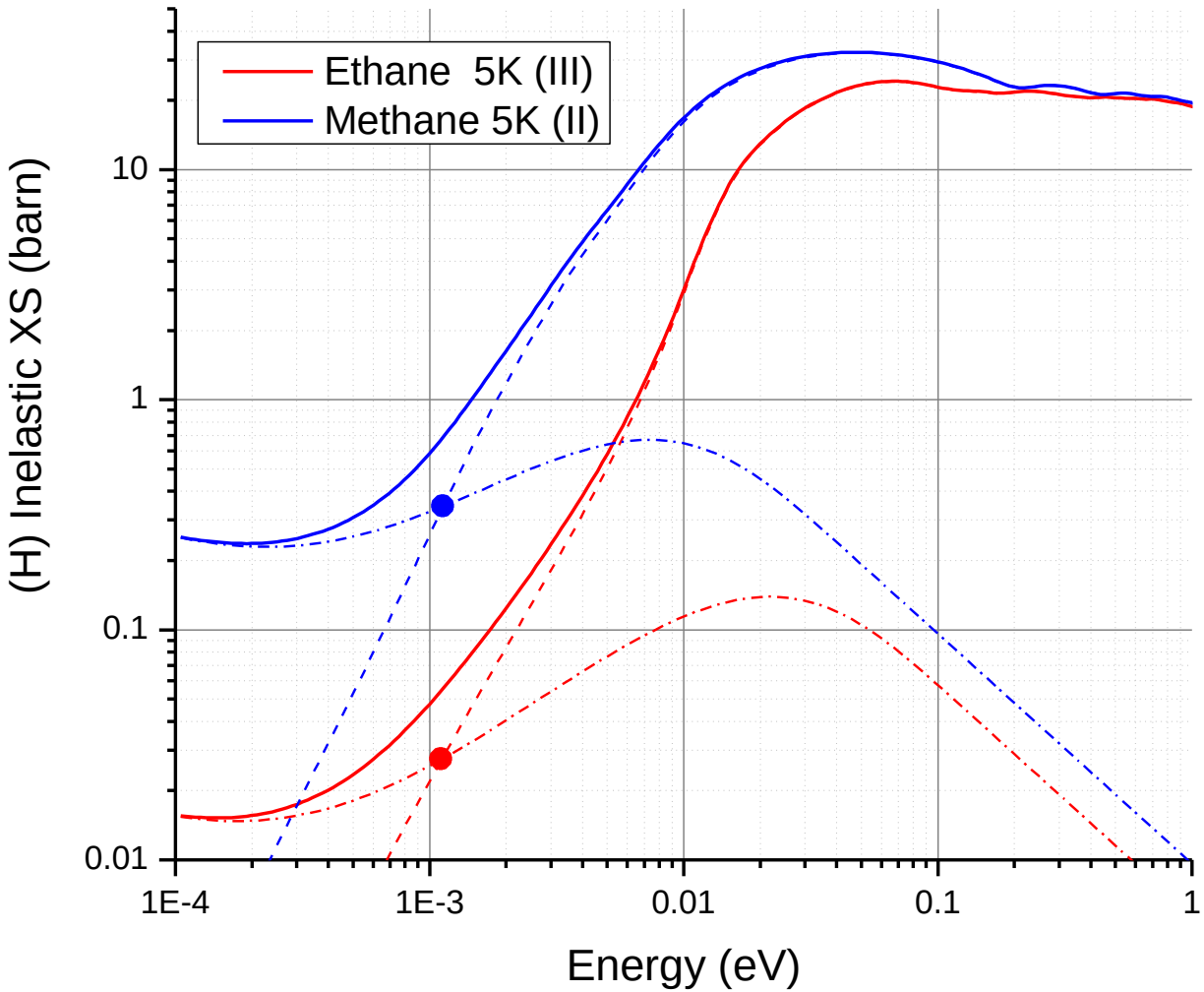

Svemir Rudić and Goran Škoro
(TOSCA, ISIS, Nov 2020)
Ethane 25K
Ethane 15K
INS Spectrum (a.u.)
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
0
10
20
30
40
50
60
70
80
90
100
ε (meV)


Ethane 25K
Ethane 15K
Svemir Rudic and Goran Škoro
(TOSCA, ISIS, Nov 2020)
INS Spectrum
0.01
1E-3
1E-4
0
10
20
30
40
50
ε (meV)
TOSCA 15K
Nelligan 9K
INS Spectrum (a.u.)
0.004
0.003
0.002
0.001
0.000
0
5
10
15
20
ε (meV)
New Ethane
(Low Energies)
ρ(ε)
30
20
10
0
0.00
0.01
0.02
0.03
0.04
0.05
ε (eV)
Oct21
Solid Ethane
ρ(ε)
120
100
80
60
40
20
0
0.0
0.1
0.2
0.3
0.4
ε (eV)


Solid Ethane
(80 K)
"Measured" (VESUBIO)
Calculated (CABoct21)
(H) C_2H_6 X-Section (b)
120
100
80
60
40
20
1E-4
1E-3
0.01
0.1
1
10
Energy (eV)


Methane 22K
(H) Inelastic XS (barn)
10
1
0.1
0.01
1E-4
1E-3
0.01
0.1
1
Energy (eV)
Methane 22K
Flux (a.u.)
1E-4
1E-5
1E-6
1E-3
0.01
0.1
E [eV]

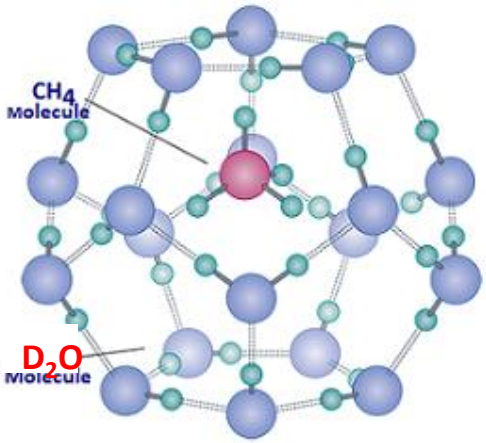

Methane 22K
Ethane 20K
(H) Inelastic XS (barn)
10
1
0.1
0.01
1E-4
1E-3
0.01
0.1
1
Energy (eV)

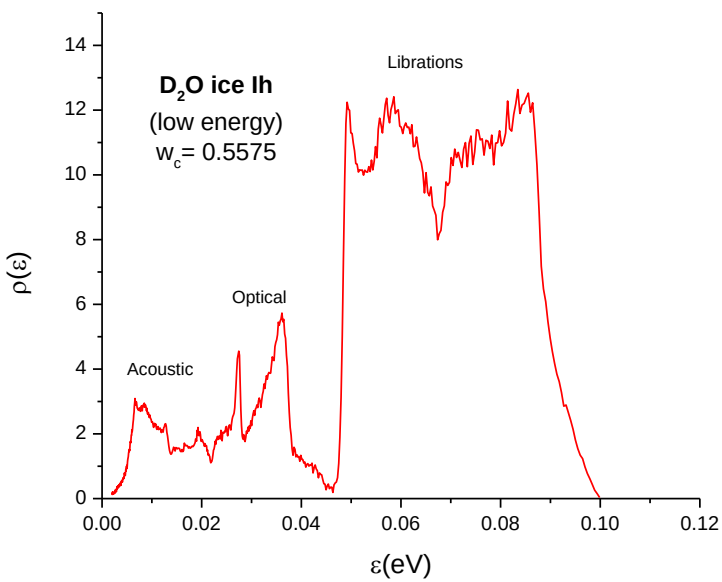

Ethane 5K (III)
Methane 5K (II)
(H) Inelastic XS (barn)
10
1
0.1
0.01
1E-4
1E-3
0.01
0.1
1
Energy (eV)

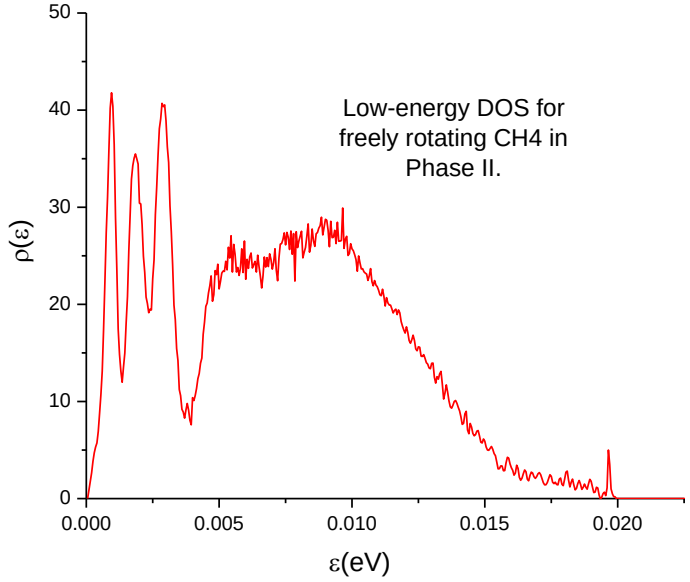
CLATHRATES

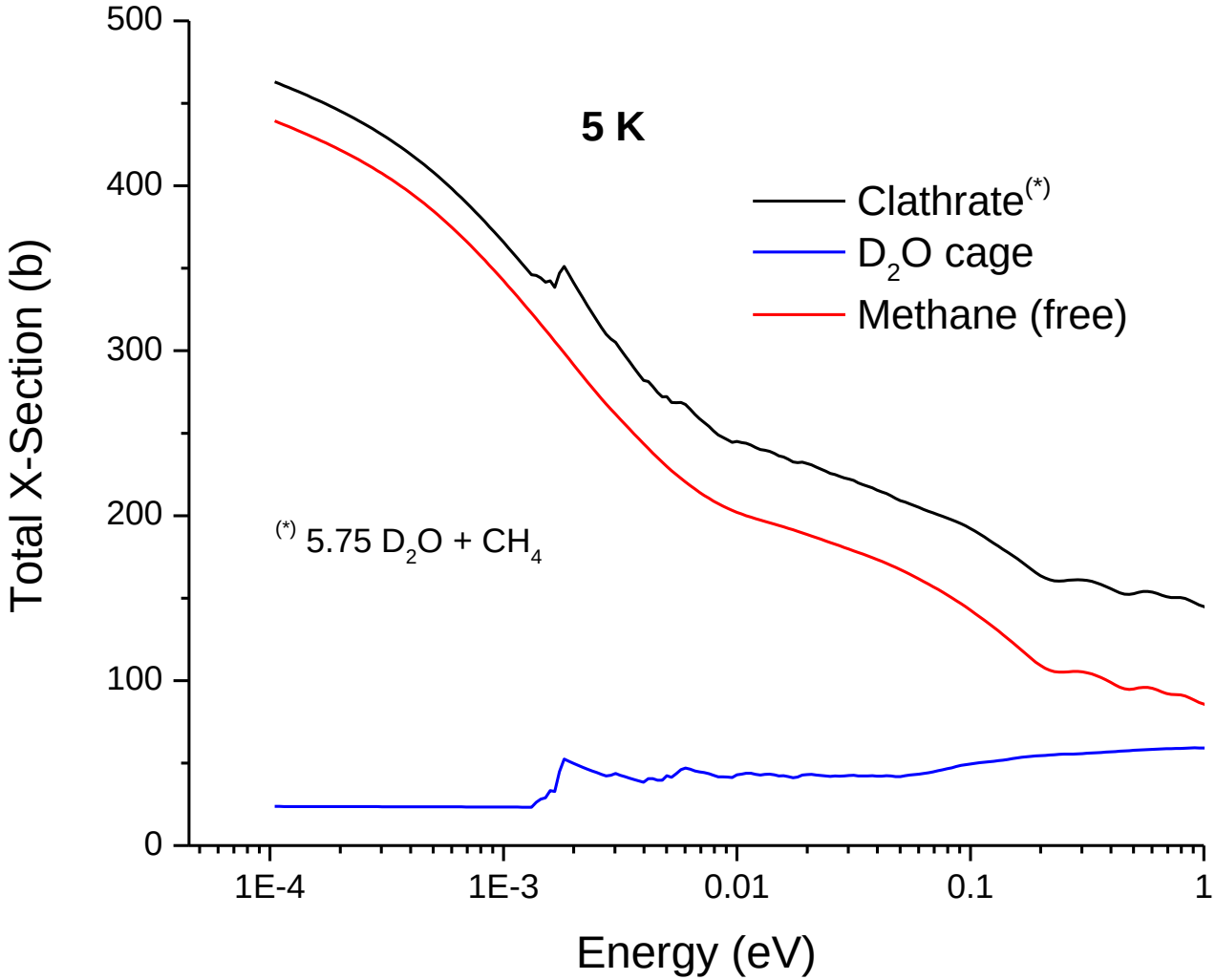
Host: **D_2O ice**

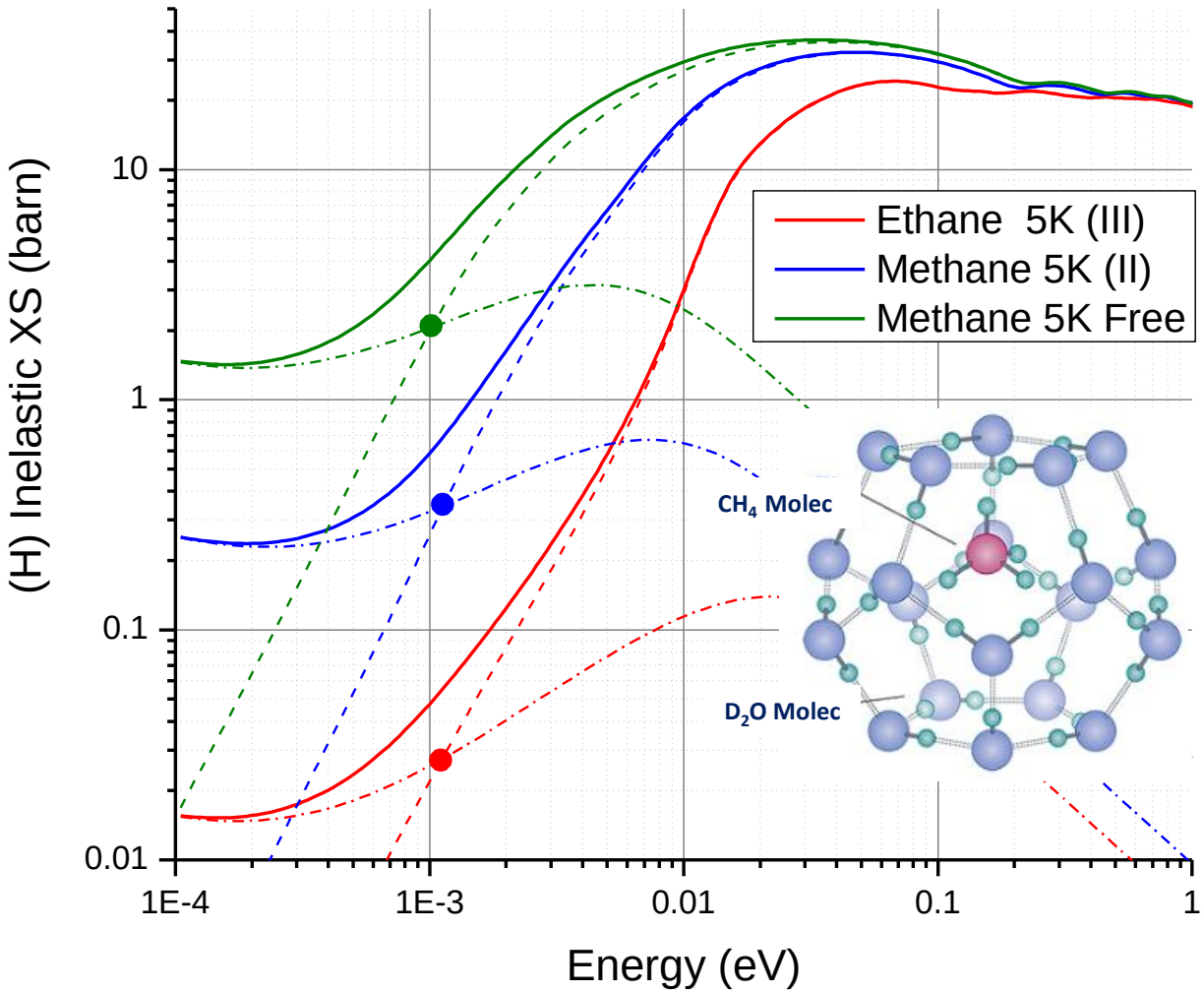
Guest: **CH_4**

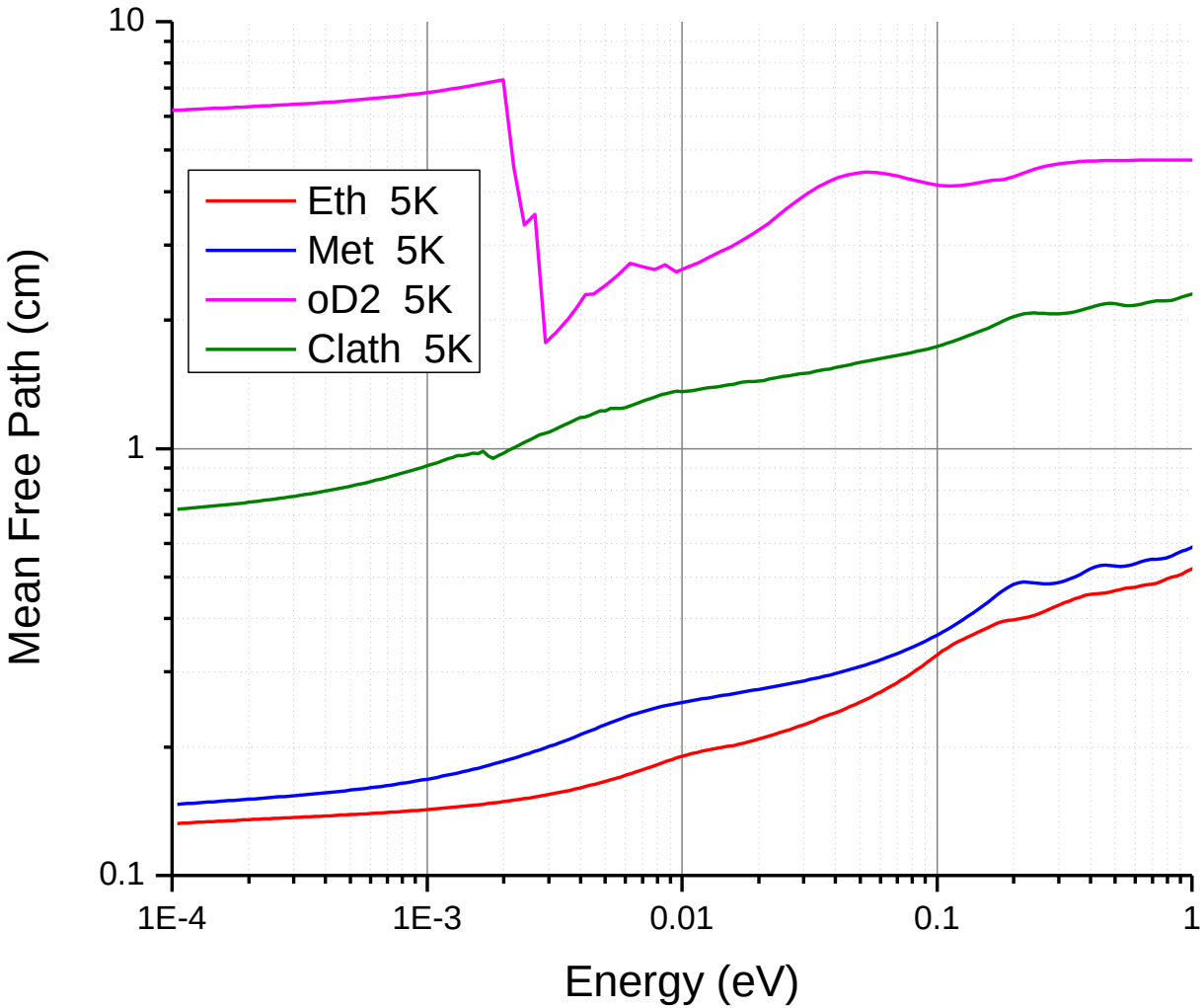


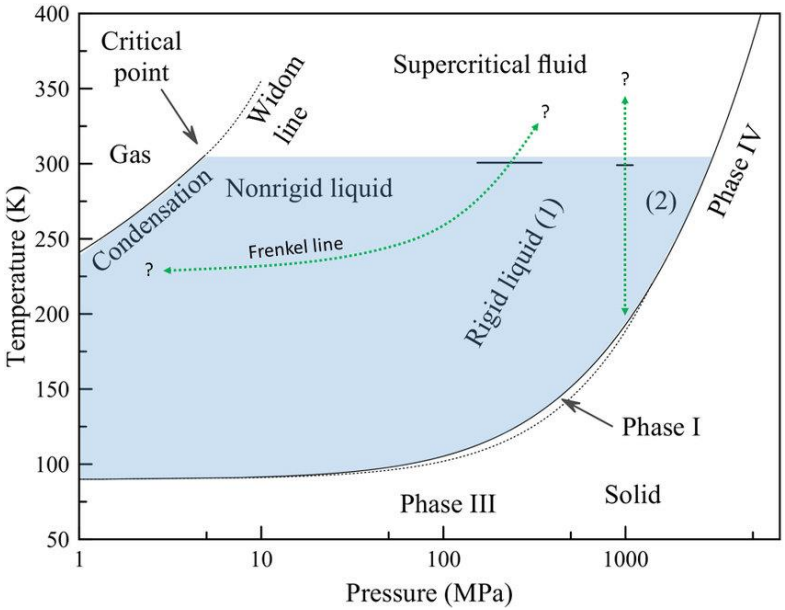


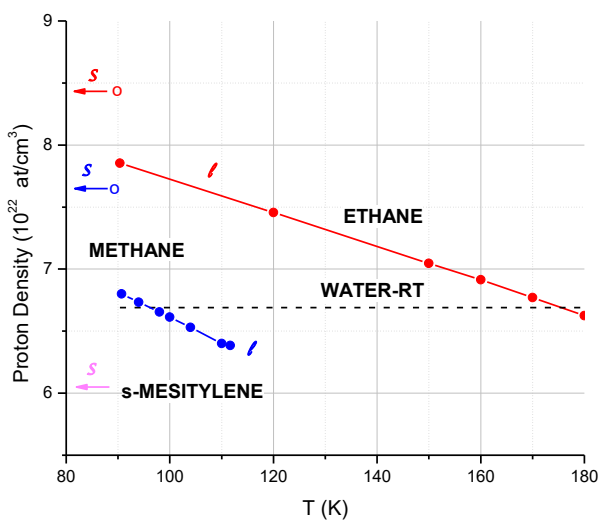



5 K
Clathrate(*)
D2O cage
Methane (free)
(*) 5.75 D2O + CH4
Total X-Section (b)
Energy (eV)
500
400
300
200
100
0
1E-4
1E-3
0.01
0.1
1


(H) Inelastic XS (barn)
10
1
0.1
0.01
1E-4
1E-3
0.01
0.1
1
Energy (eV)
Ethane 5K (III)
Methane 5K (II)
Methane 5K Free
CH4 Molec
D2O Molec


10
1
0.1
1E-4
1E-3
0.01
0.1
1
Mean Free Path (cm)
Energy (eV)
Eth 5K
Met 5K
oD2 5K
Clath 5K



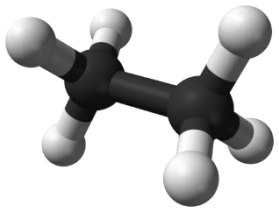


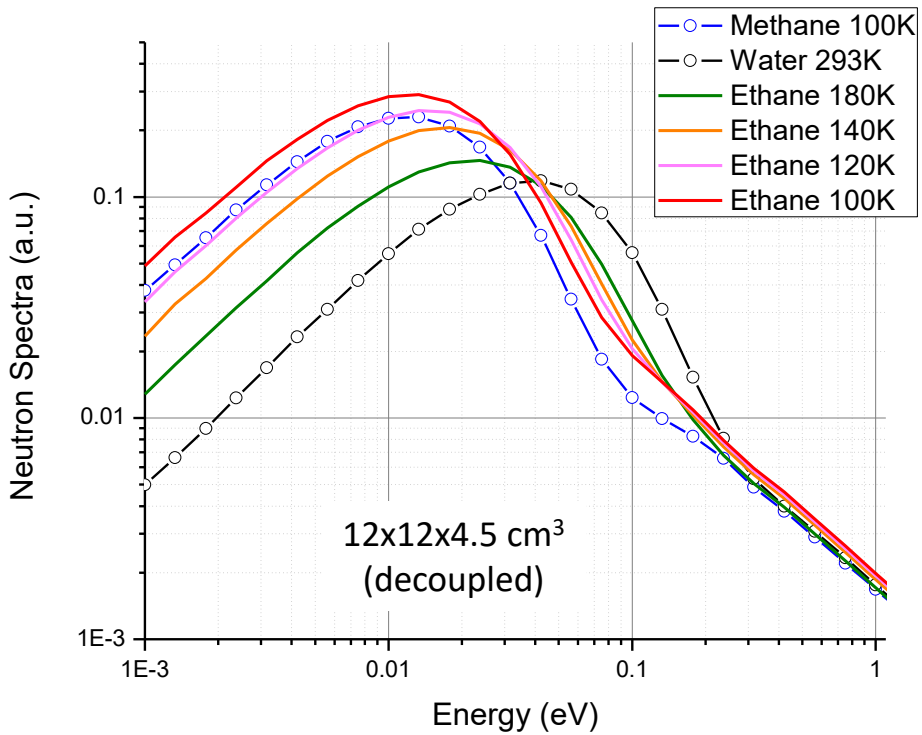
http://www.engineeringtoolbox.com/ethane-thermal-properties-d_1761.html

AN INTERESTING "COOL" MODERATOR:

ETHANE

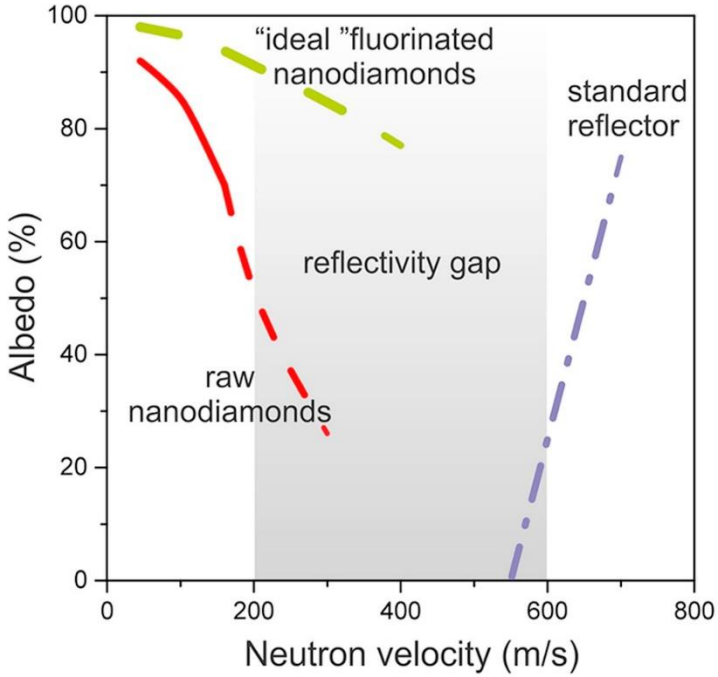
C_2H_6





NEUTRON REFLECTORS

Valery Nesvizhevsky *et al.*, Carbon 130 (2018) 799e805



Journal of Neutron Research 23 (2021) 167–177 167
DOI 10.3233/JNR-210013
IOS Press

Development of neutron scattering kernels for cold neutron reflector materials

José Rolando Granada [a,*], José Ignacio Márquez Damián [b], Javier Dawidowski [a,c], José Ignacio Robledo [c], Christian Helman [a], Giovanni Romanelli [d] and Goran Škoro [d]

INGREDIENTS FOR A COLD NEUTRON REFLECTOR

LARGE SCATTERING CROSS SECTION

LARGE ELASTIC CROSS SECTIONS

HIGHLY ISOTROPIC ANGULAR CROSS SECTION

LARGE [ELASTIC/INELASTIC] CROSS SECTIONS RATIO

SMALL ABSORPTION CROSS SECTION

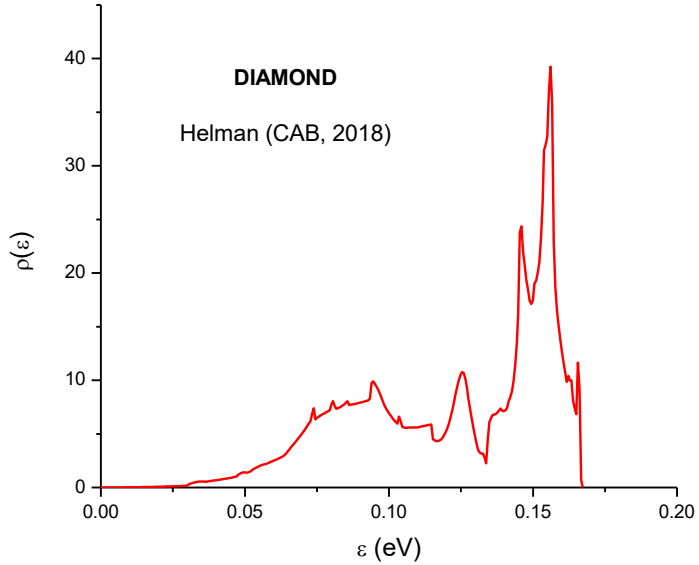
HYDROGEN (σ_s = 82.02 b)

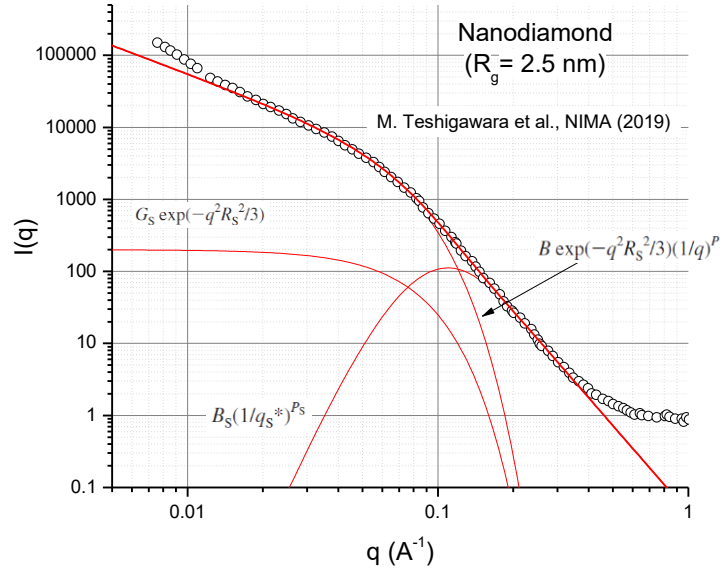
SOLID

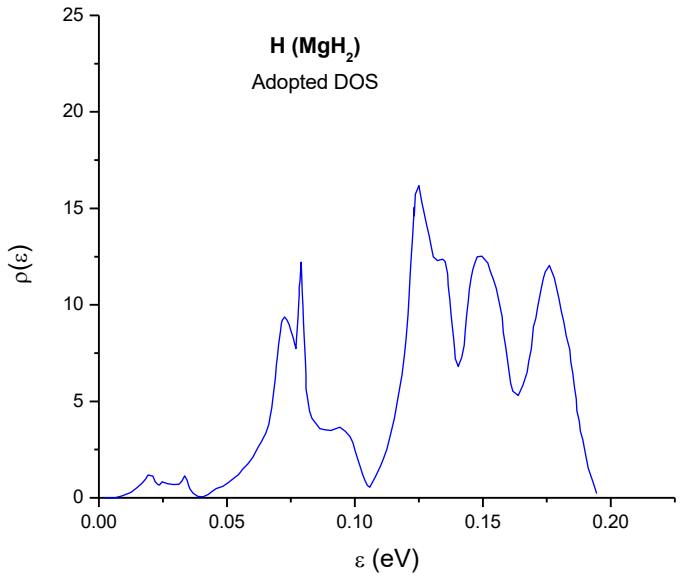
LARGE EFFECTIVE MASS

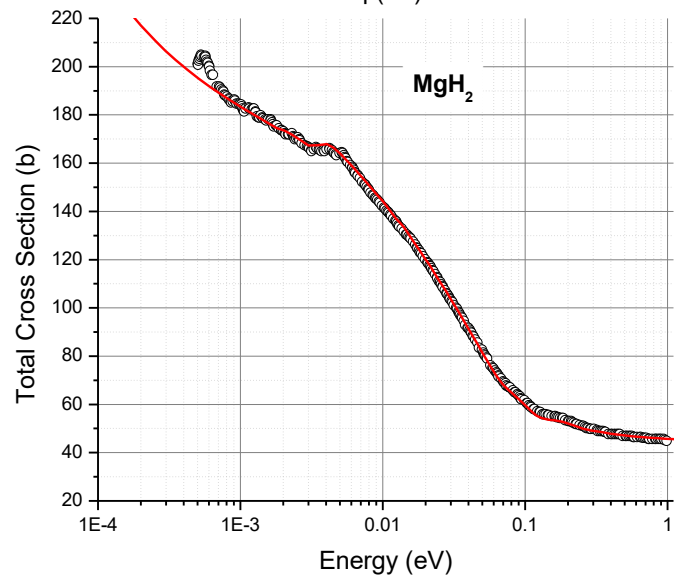
NO LOW-FREQUENCY MODES

OUR SCATTERING MODEL FOR ND AND MgH_2



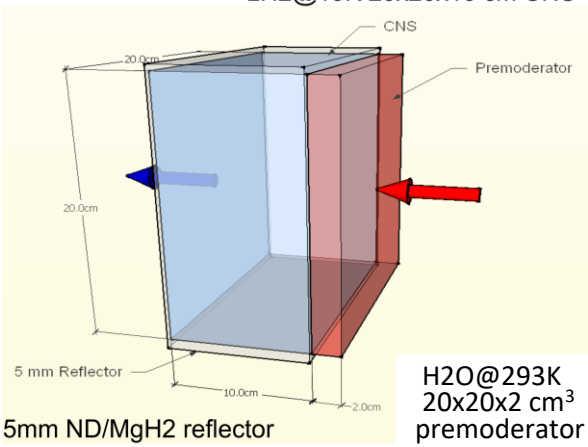






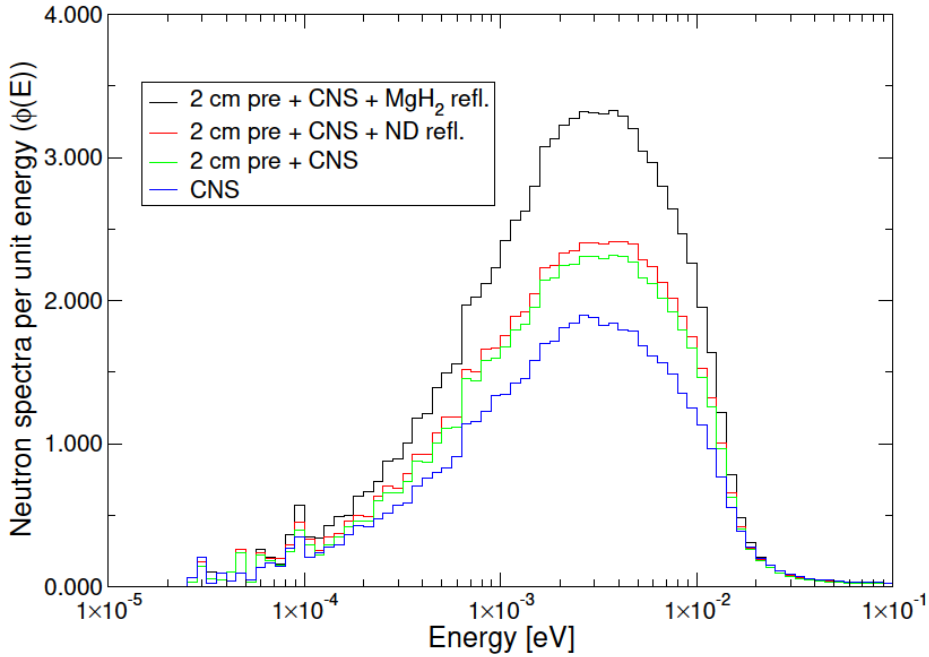
CNS CALCULATIONS

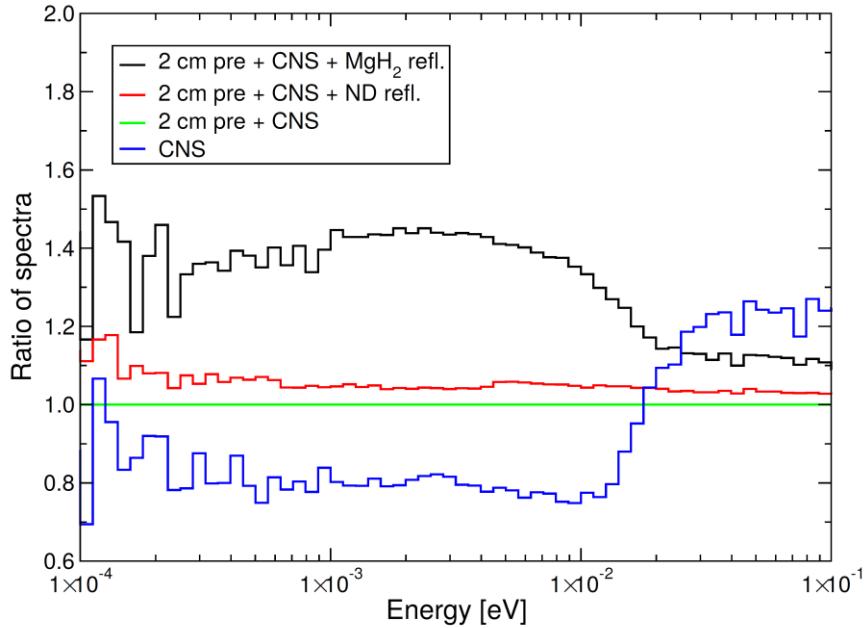
LH2@19K 20x20x10 cm CNS

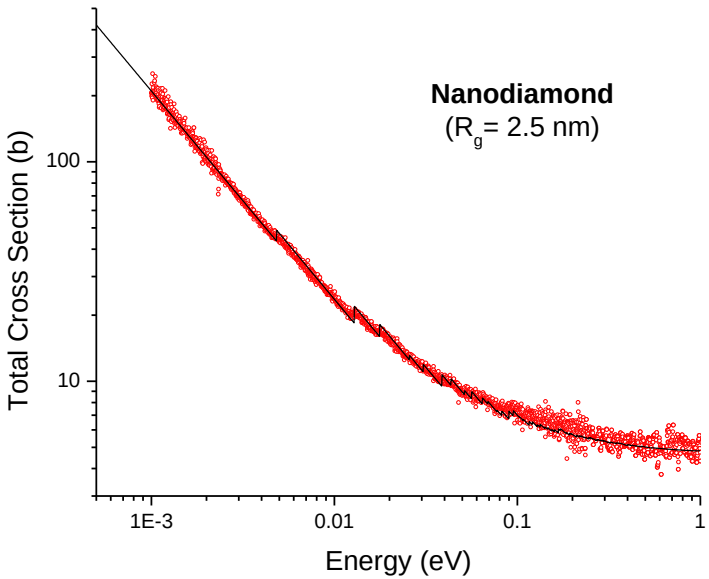


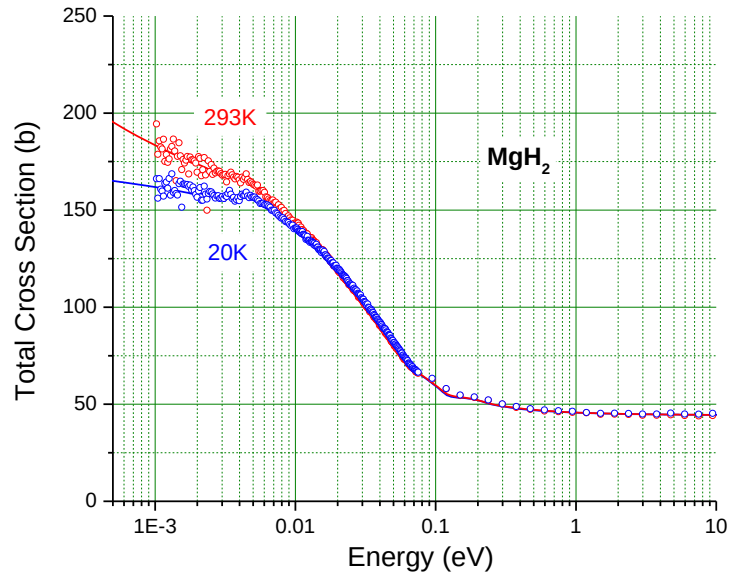
5mm ND/MgH2 reflector

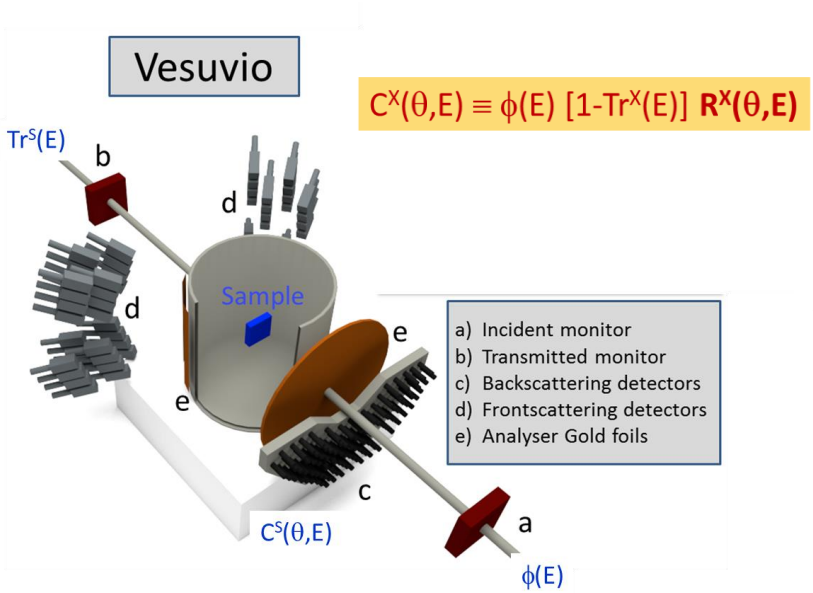
H2O@293K
20x20x2 cm^3
premoderator

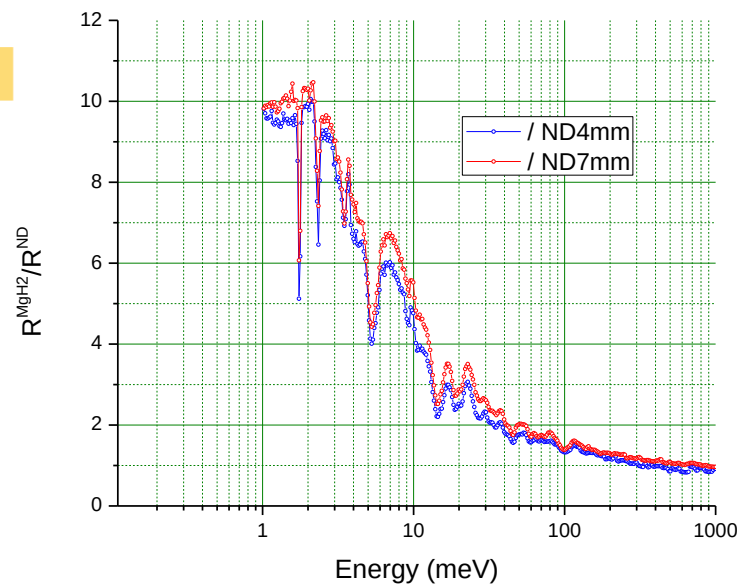





Nanodiamond
(R_g= 2.5 nm)
Total Cross Section (b)
100
10
1E-3
0.01
0.1
1
Energy (eV)

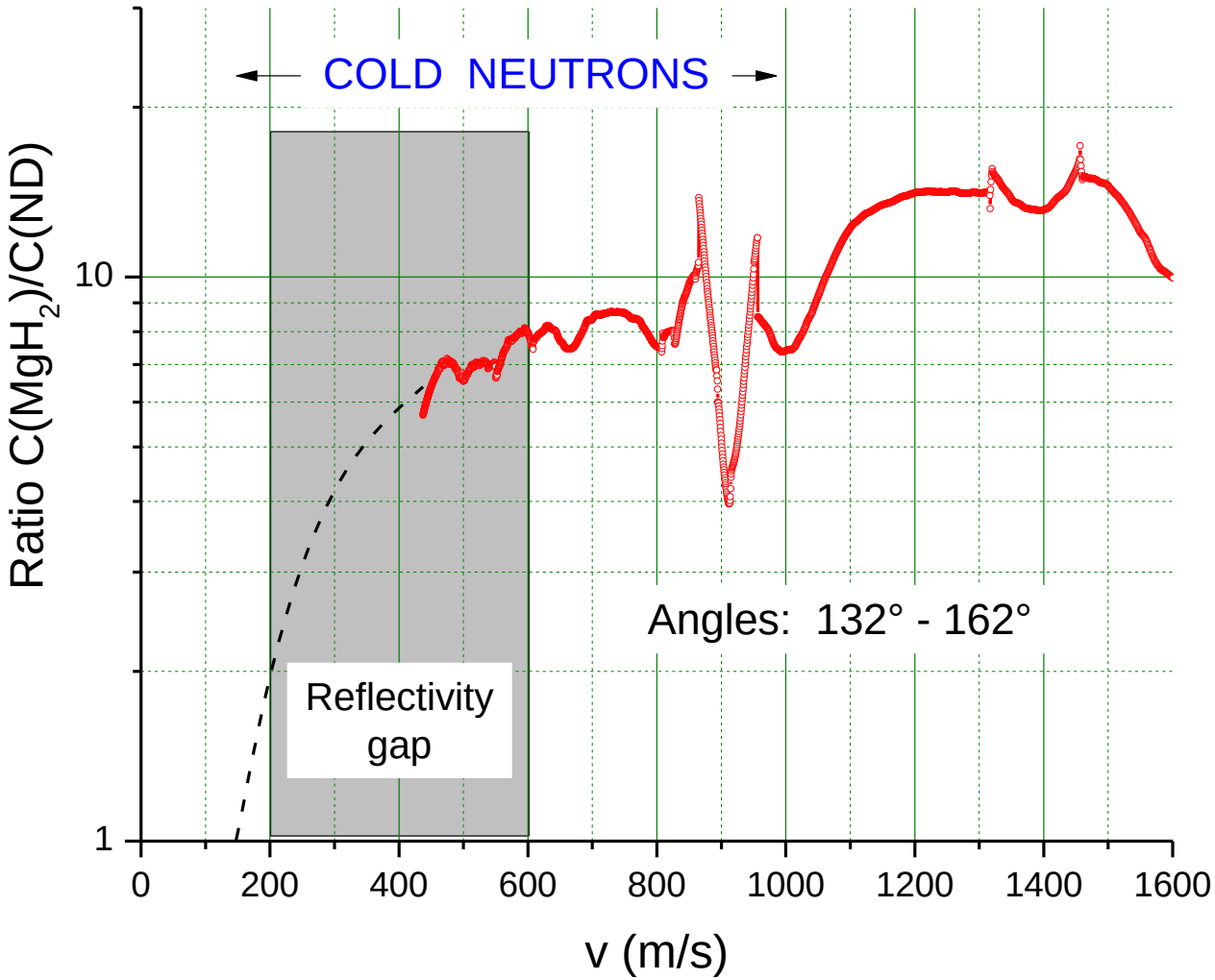

293K
20K
MgH_2
Total Cross Section (b)
250
200
150
100
50
0
1E-3
0.01
0.1
1
10
Energy (eV)


Vesuvio
$C^X(\theta,E) \equiv \phi(E)\ [1-Tr^X(E)]\ \mathbf{R^X(\theta,E)}$
$Tr^S(E)$
b
d
d
Sample
e
e
c
a
$C^S(\theta,E)$
$\phi(E)$
a) Incident monitor
b) Transmitted monitor
c) Backscattering detectors
d) Frontscattering detectors
e) Analyser Gold foils


/ ND4mm
/ ND7mm
R^{MgH2}/R^{ND}
12
10
8
6
4
2
0
1
10
100
1000
Energy (meV)

RATIO from BACKWARD ANGLE DETECTORS

Preliminary Results



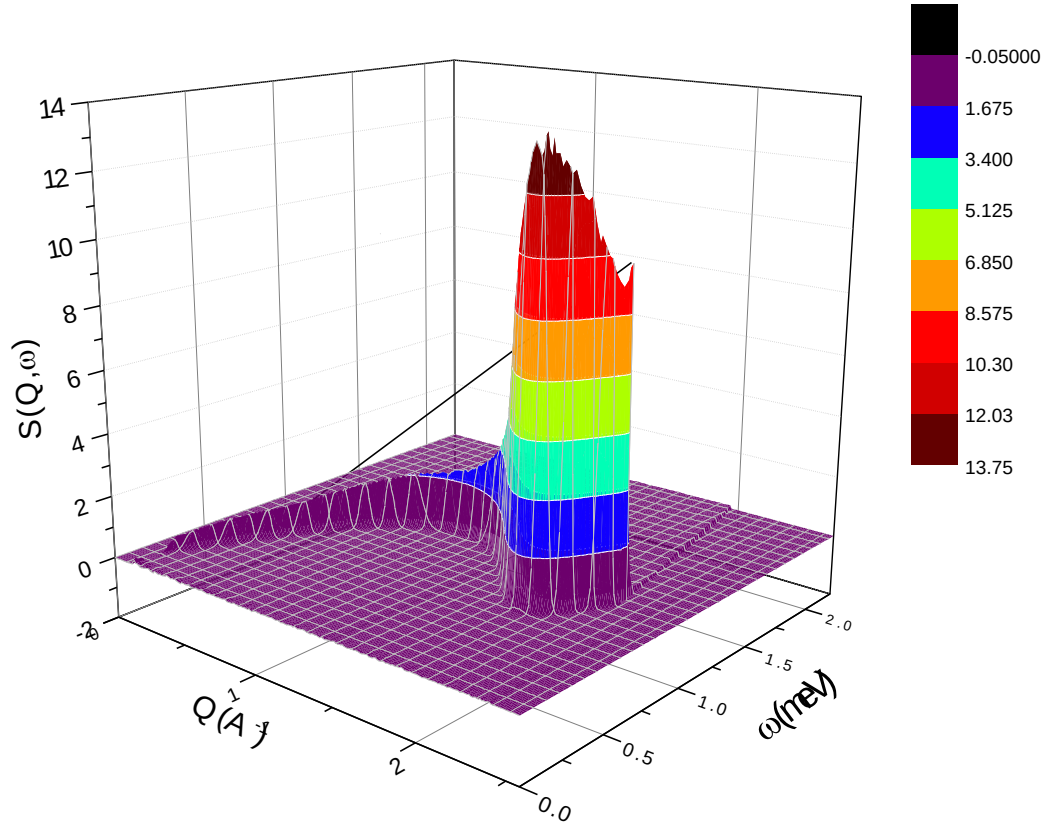
^{4}He SUPERFLUID

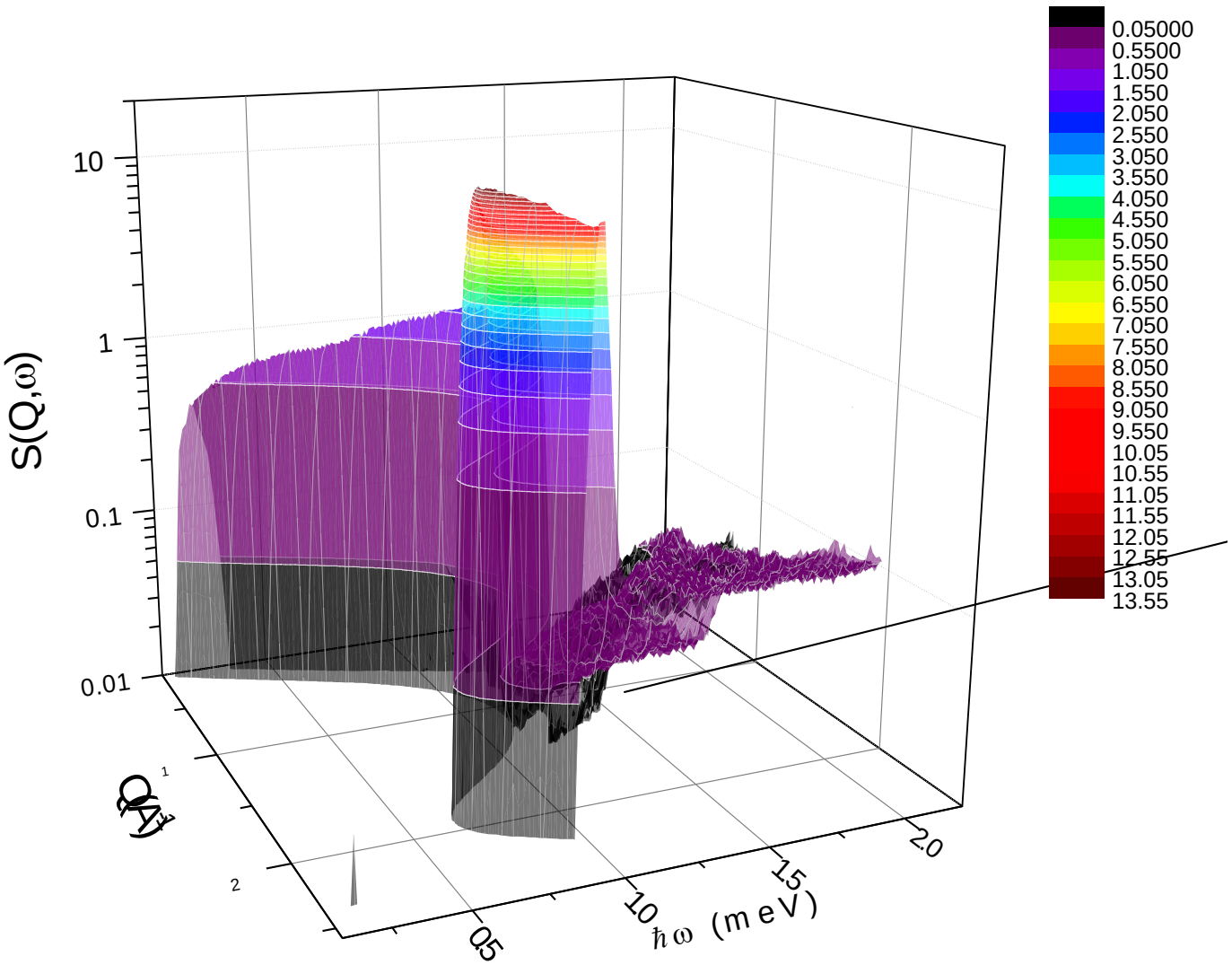
PHYSICAL REVIEW B **103**, 104516 (2021)

Editors' Suggestion Featured in Physics

Dispersion relation of Landau elementary excitations and thermodynamic properties of superfluid ^{4}He

H. Godfrin,[1,*] K. Beauvois,[1,2] A. Sultan,[1,2] E. Krotscheck,[3,4] J. Dawidowski,[5] B. Fåk,[2] and J. Ollivier[2]




S(Q,ω)
10
1
0.1
0.01
Q (Å⁻¹)
1
2
0.5
1.0
1.5
2.0
ħω (meV)
0.05000
0.5500
1.050
1.550
2.050
2.550
3.050
3.550
4.050
4.550
5.050
5.550
6.050
6.550
7.050
7.550
8.050
8.550
9.050
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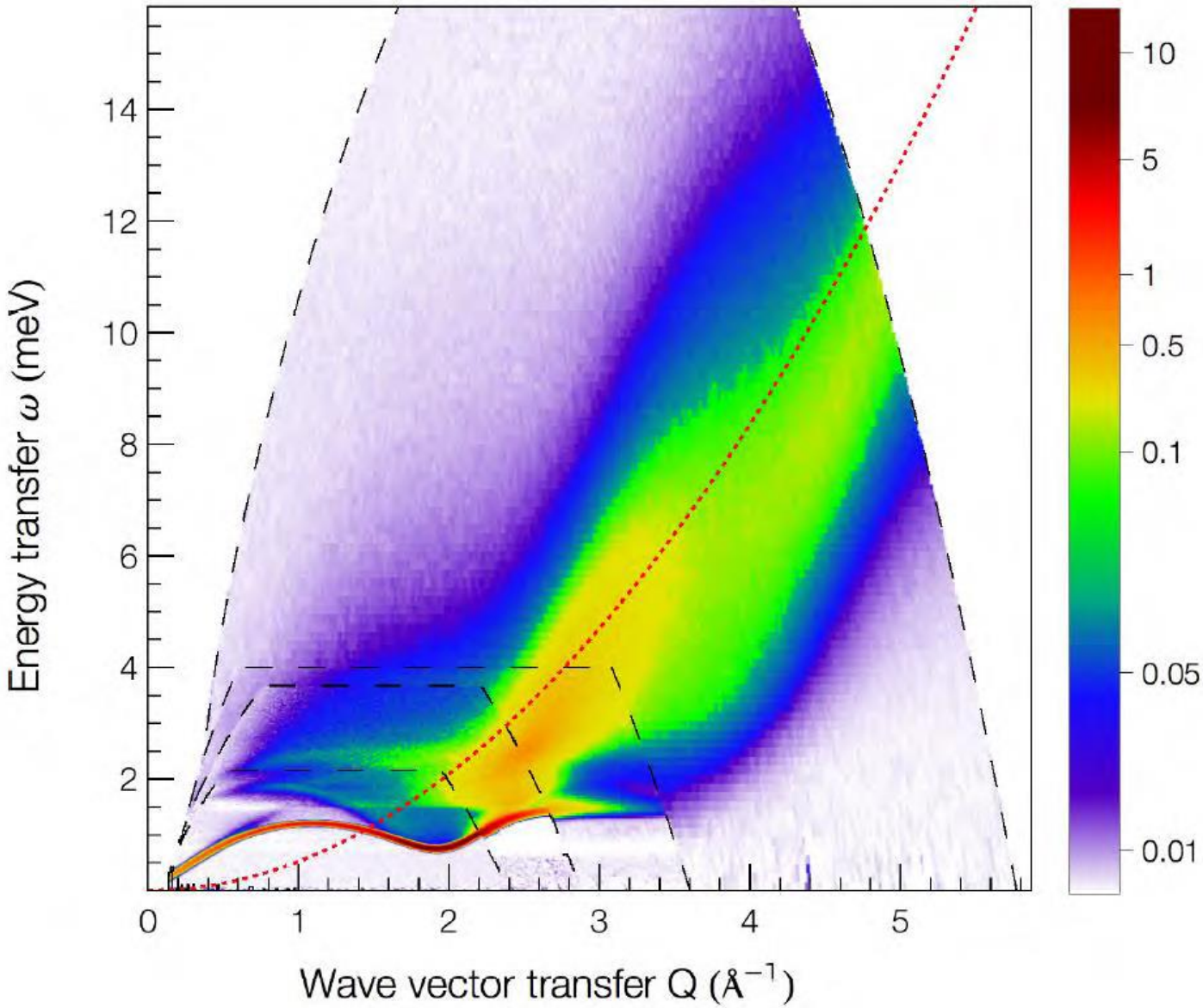
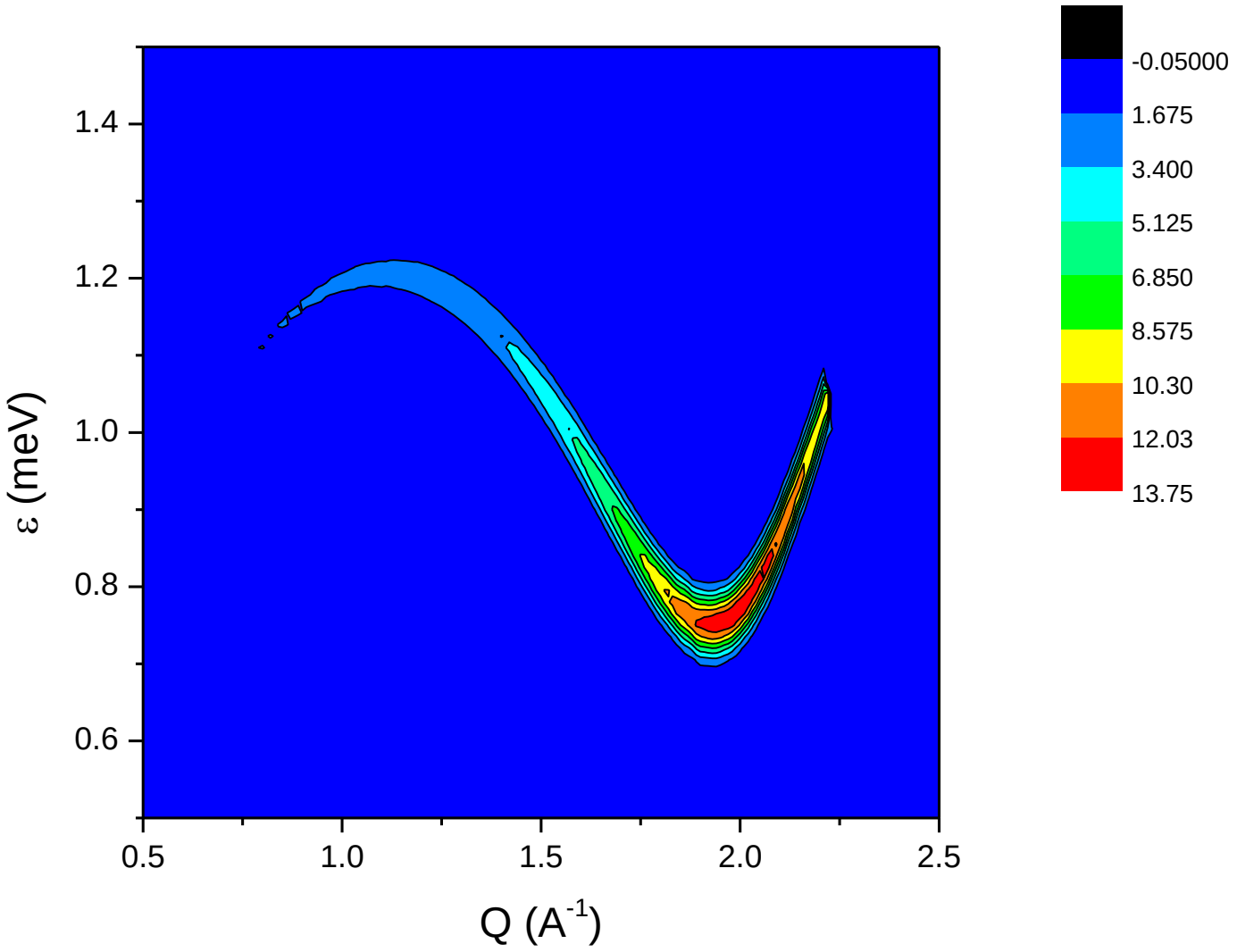
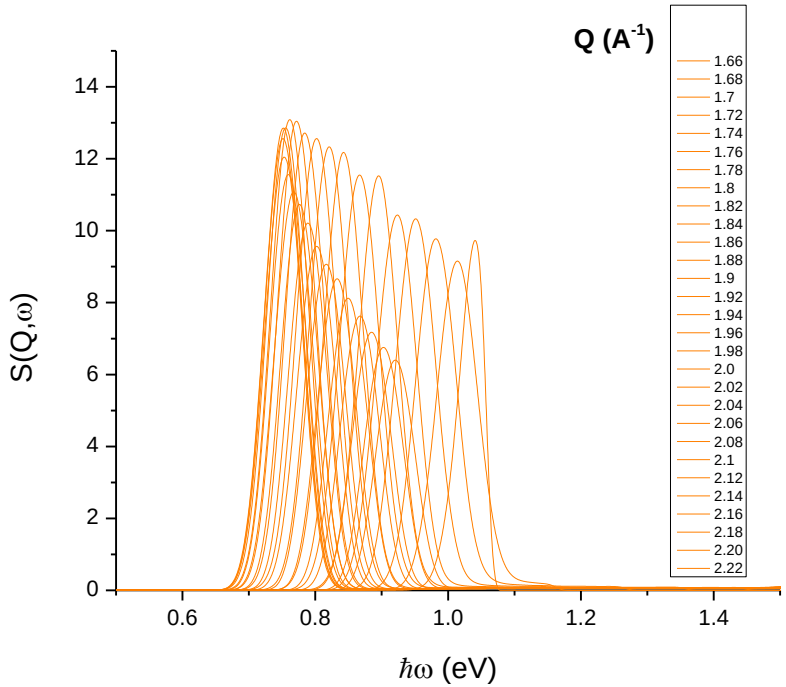
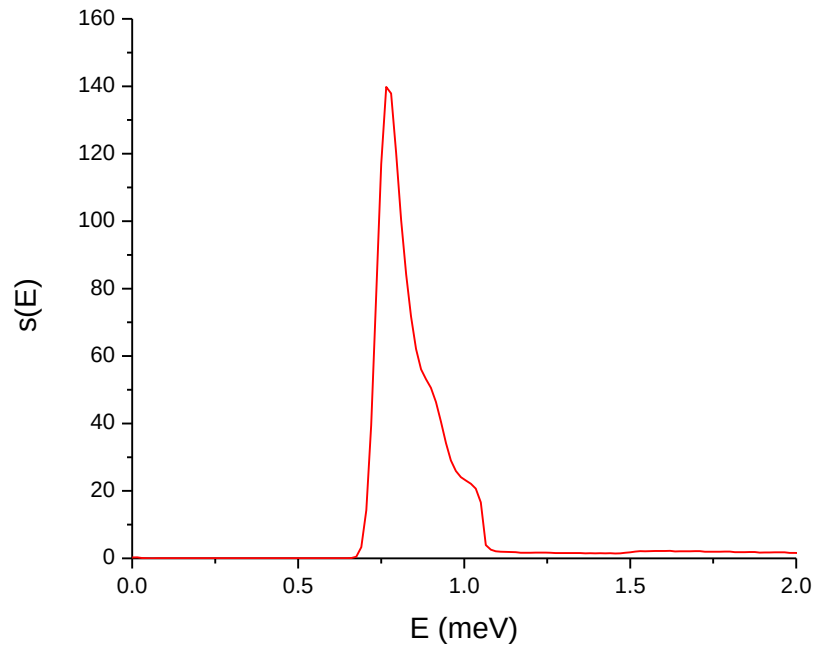
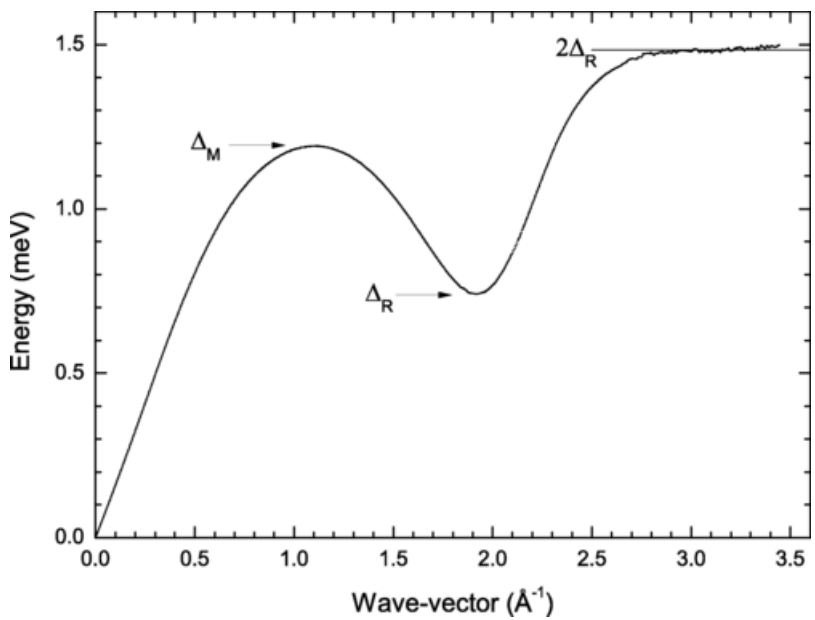
11.05
11.55
12.05
12.55
13.05
13.55

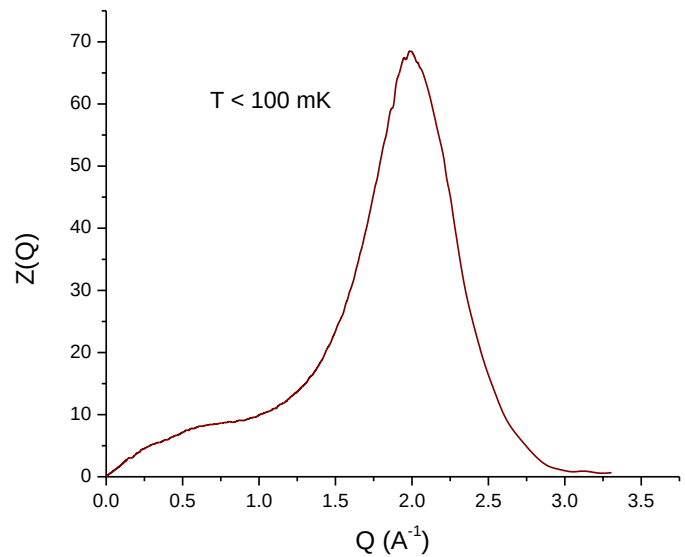

Energy transfer ω (meV)
14
12
10
8
6
4
2
0
1
2
3
4
5
Wave vector transfer Q (Å^{-1})
10
5
1
0.5
0.1
0.05
0.01


1.4
1.2
1.0
0.8
0.6
ε (meV)
0.5
1.0
1.5
2.0
2.5
Q (A-1)
-0.05000
1.675
3.400
5.125
6.850
8.575
10.30
12.03
13.75


Q (A-1)
1.66
1.68
1.7
1.72
1.74
1.76
1.78
1.8
1.82
1.84
1.86
1.88
1.9
1.92
1.94
1.96
1.98
2.0
2.02
2.04
2.06
2.08
2.1
2.12
2.14
2.16
2.18
2.20
2.22
S(Q,ω)
ħω (eV)


s(E)
E (meV)

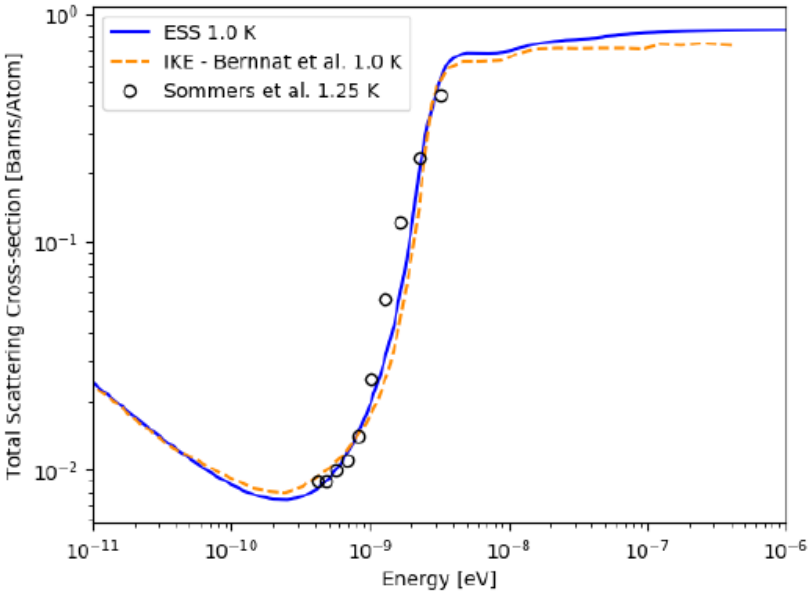

2ΔR
ΔM
ΔR
Energy (meV)
Wave-vector (Å-1)

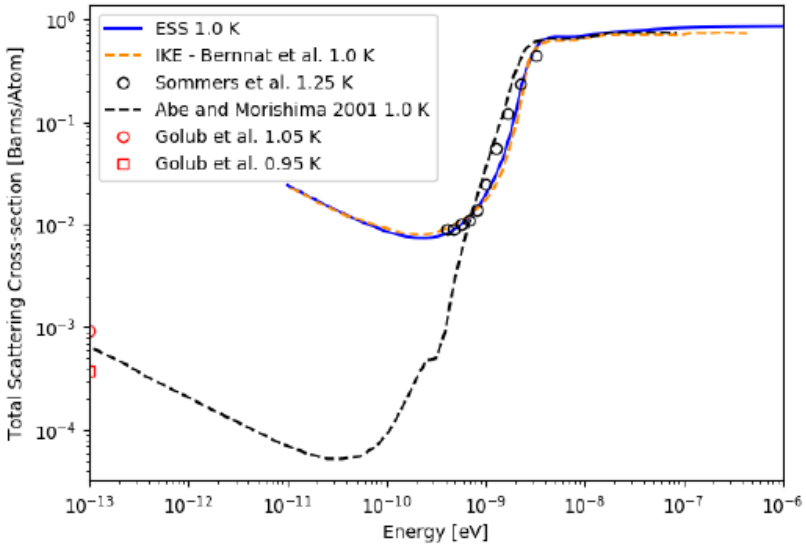

T < 100 mK
Z(Q)
Q (A-1)

Thermal neutron scattering nuclear data work at ESS

Liquid ^{4}He

- Initial work on development of a liquid ^{4}He kernel at 1.0 K.
- Differences in models found in literature and experimental data is sparse.

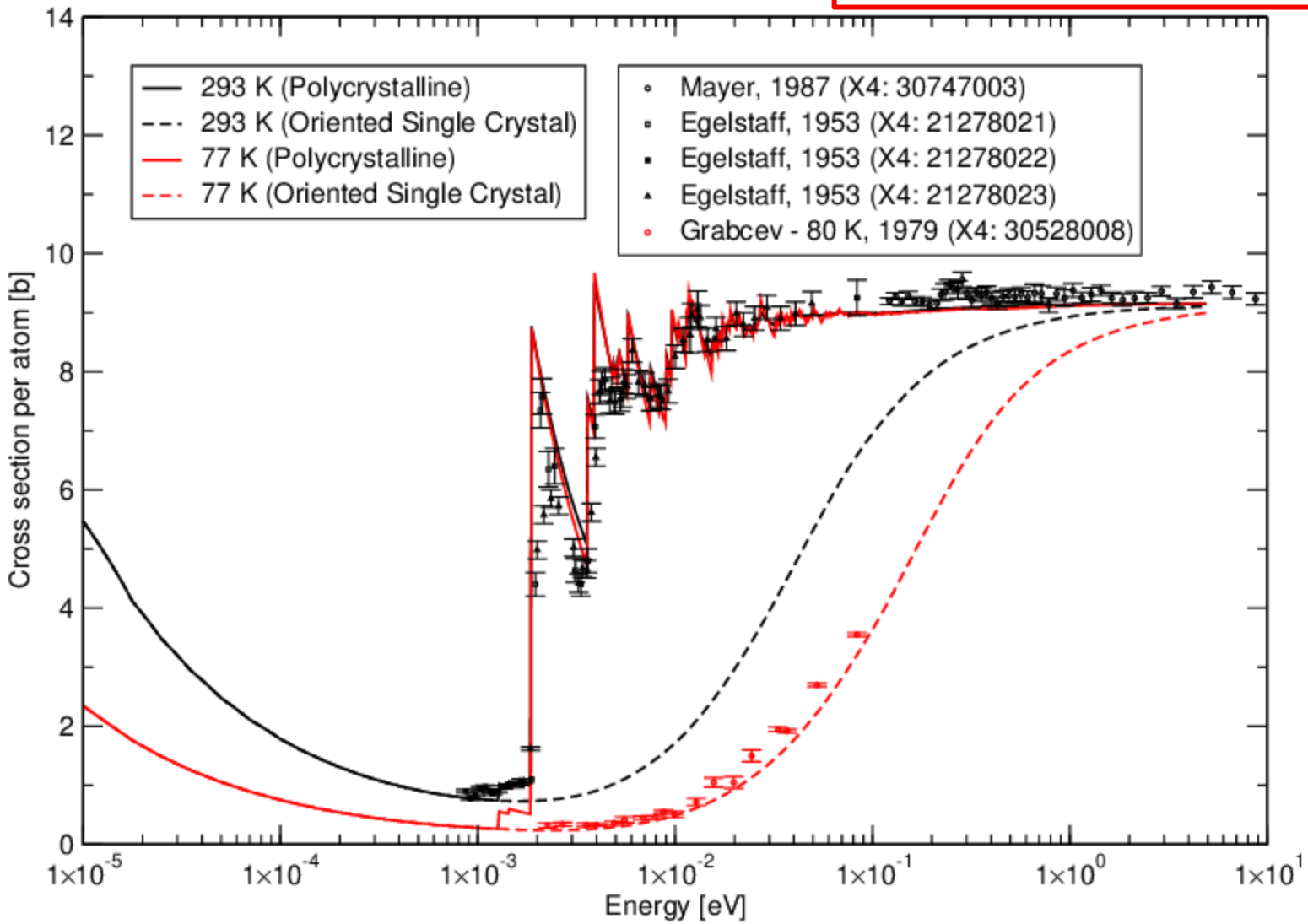


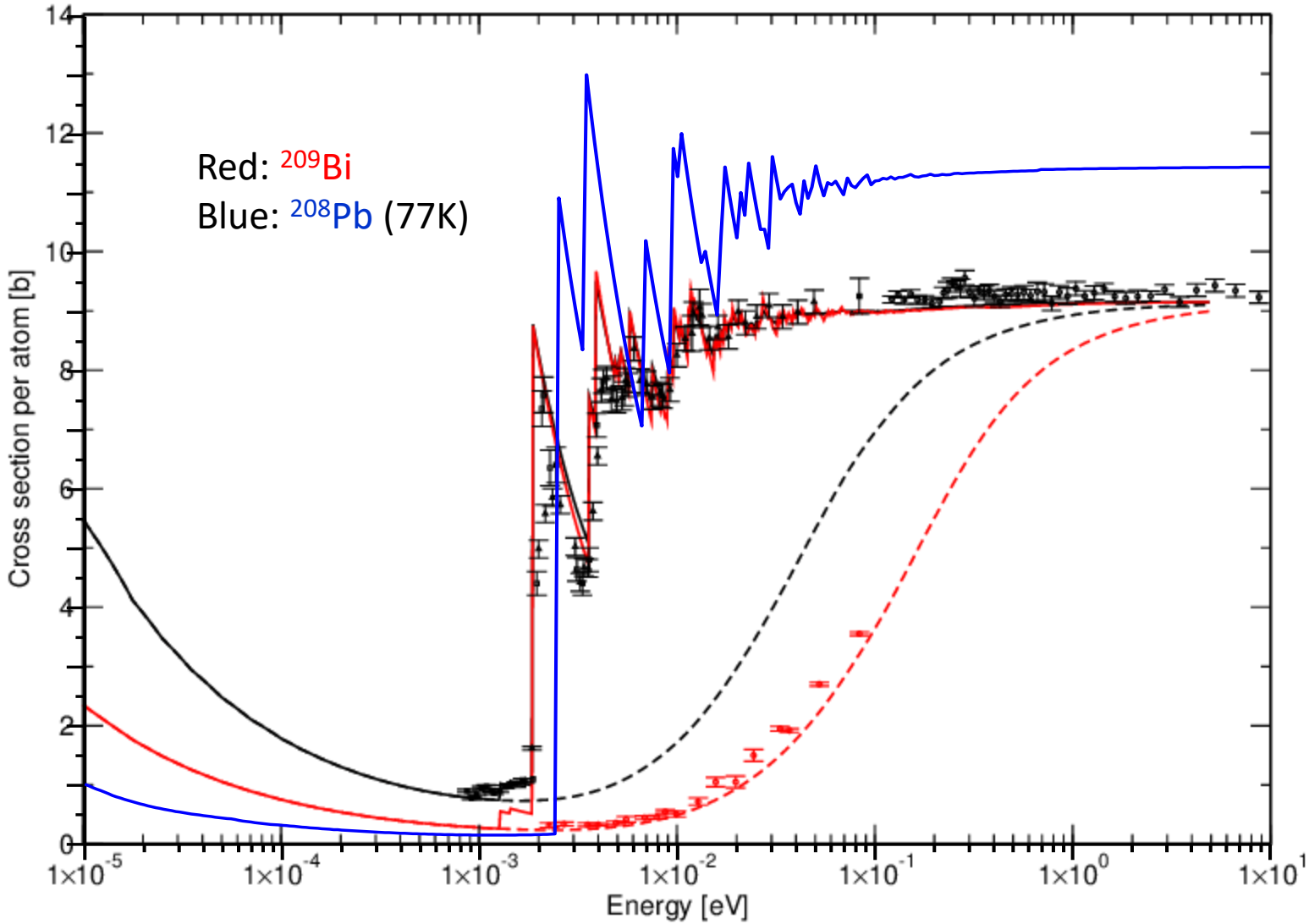


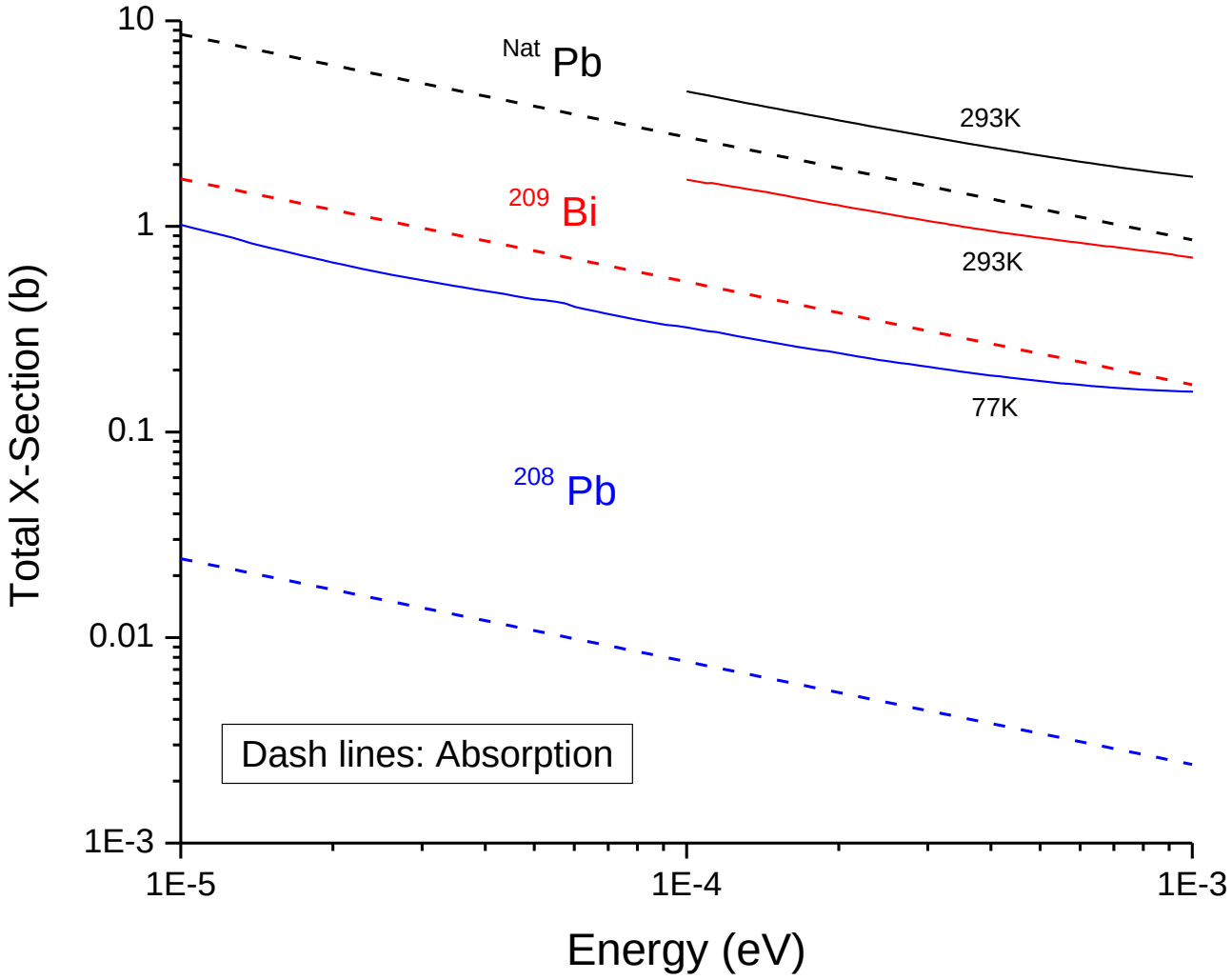
BISMUTH

Nuclear data development at the European Spallation Source

Jose Ignacio Marquez Damian [a,*], Douglas D. DiJulio [a], and Günter Muhrer [a],
[a] *Spallation Physics Group, European Spallation Source ERIC, Lund, Sweden*




Red: ^{209}Bi
Blue: ^{208}Pb (77K)
Cross section per atom [b]
Energy [eV]
0
2
4
6
8
10
12
14
1×10^{-5}
1×10^{-4}
1×10^{-3}
1×10^{-2}
1×10^{-1}
1×10^{0}
1×10^{1}


10
1
0.1
0.01
1E-3
1E-5
1E-4
1E-3
Total X-Section (b)
Energy (eV)
Nat Pb
293K
209 Bi
293K
77K
208 Pb
Dash lines: Absorption

THANKS FOR YOUR ATTENTION