# Status of Thermal Scattering Law Data Files

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DE LA RECHERCHE À L'INDUSTRIE

www.cea.fr

| Material number | JEFF-3.1.1 | ENDF/B-VII | JENDL-4.0 |
|---|---|---|---|
| 1 | H(H20) | H(H2O) | H(H2O) |
| 2 | | Para Hydrogen | Para Hydrogen |
| 3 | | Ortho Hydrogen | Ortho Hydrogen |
| 7 | H(ZrH) | H(ZrH) | H(ZrH) |
| 8 | H(CaH2) | | |
| 11 | D(D2O) | D(D20) | D(D2O) |
| 12 | | Para Deuterium | Para Deuterium |
| 13 | | Ortho Deuterium | Ortho Deuterium |
| 26 | Be metal | Be metal | Be metal |
| 27 | | Be(BeO) | Be(BeO) |
| 28 | | O(BeO) | |
| 31 | Graphite | Graphite | Graphite |
| 33 | | Liquid Methane | Liquid Methane |
| 34 | | Solid Methane | Solid Methane |
| 37 | H(CH2) | H(CH2) | |
| 40 | | Benzine | Benzine |
| 45 | | Al metal | |
| 52 | Mg metal | | |
| 56 | | Fe metal | |
| 58 | | Zr(ZrH) | Zr(ZrH) |
| 59 | Ca(CaH2) | | |
| 75 | | O(UO2) | |
| 76 | | U(UO2) | |
| **Number of materials** | 9 | 20 | 14 |

# Thermal scattering law data files for JEFF

**Evaluation work on "thermal scattering data" for JEFF was mainly performed at the Karlsruhe Institute of Technology (KIT) by J. Keinert and M. Mattes**

- 1981-2005 : this group produced Evaluated Nuclear Data Files (MF=7, MT=4) for H in H20, D in D20, H in ZrH, H in polyethylene, Graphite and Be metal

- 2003-2004: Three additional files were produced by CEA (H in CaH2, Ca in CaH2, Mg metal)

see also: "Thermal Scattering Law Data IAEA Nuclear Data Library"
https://www-nds.iaea.org/indltsl/

⇒ **Two different issues of the neutron scattering process as a function of the temperature**

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**Moderator for light and heavy water reactors**

**Cristal lattice effect in UOX fuel**

**Am241 transmission measurements at the GELINA facility, IRMM, Geel**

C. Lampoudis et al. Eur. Phys. J. Plus, 128, 86 (2013)
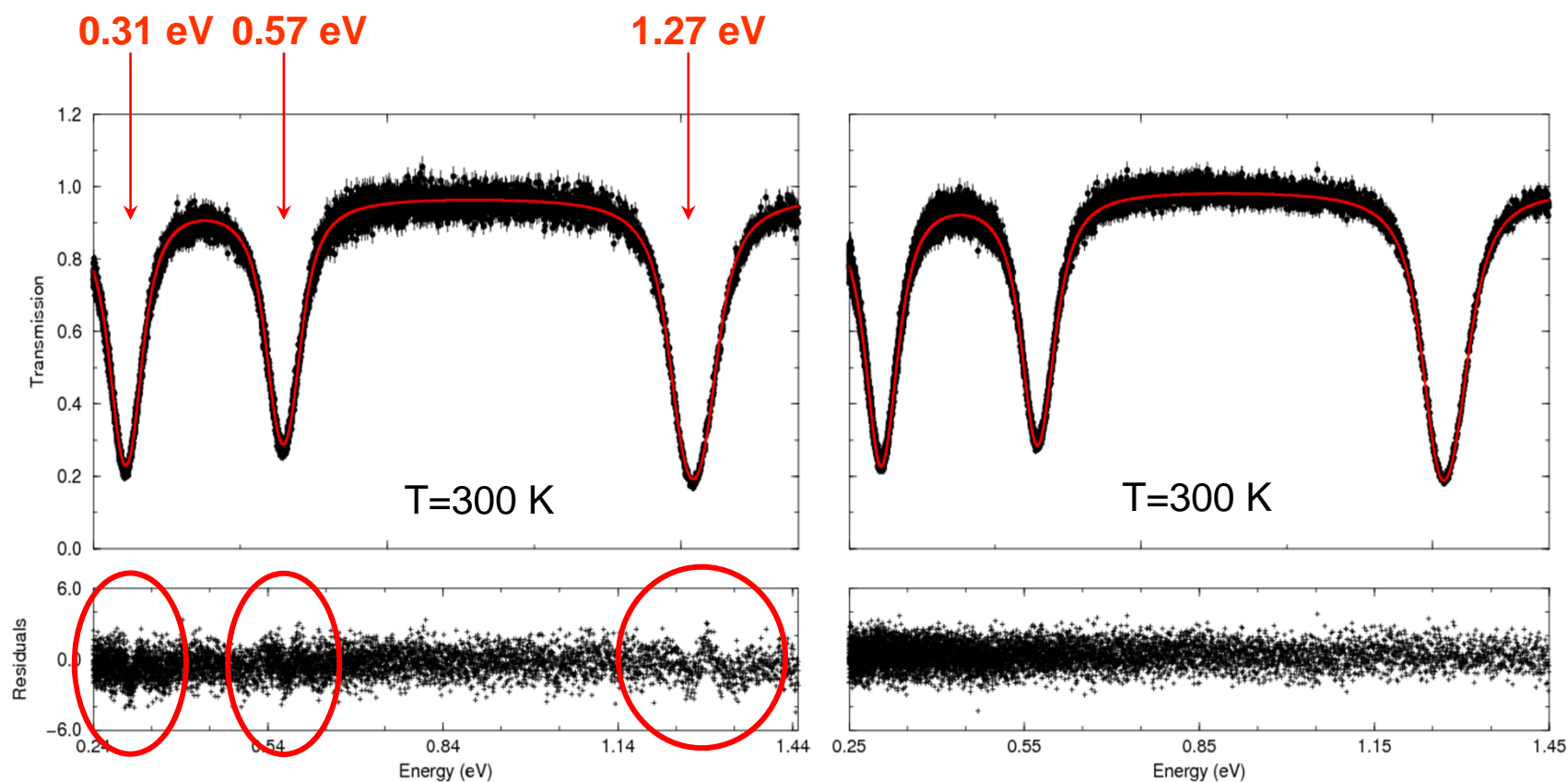


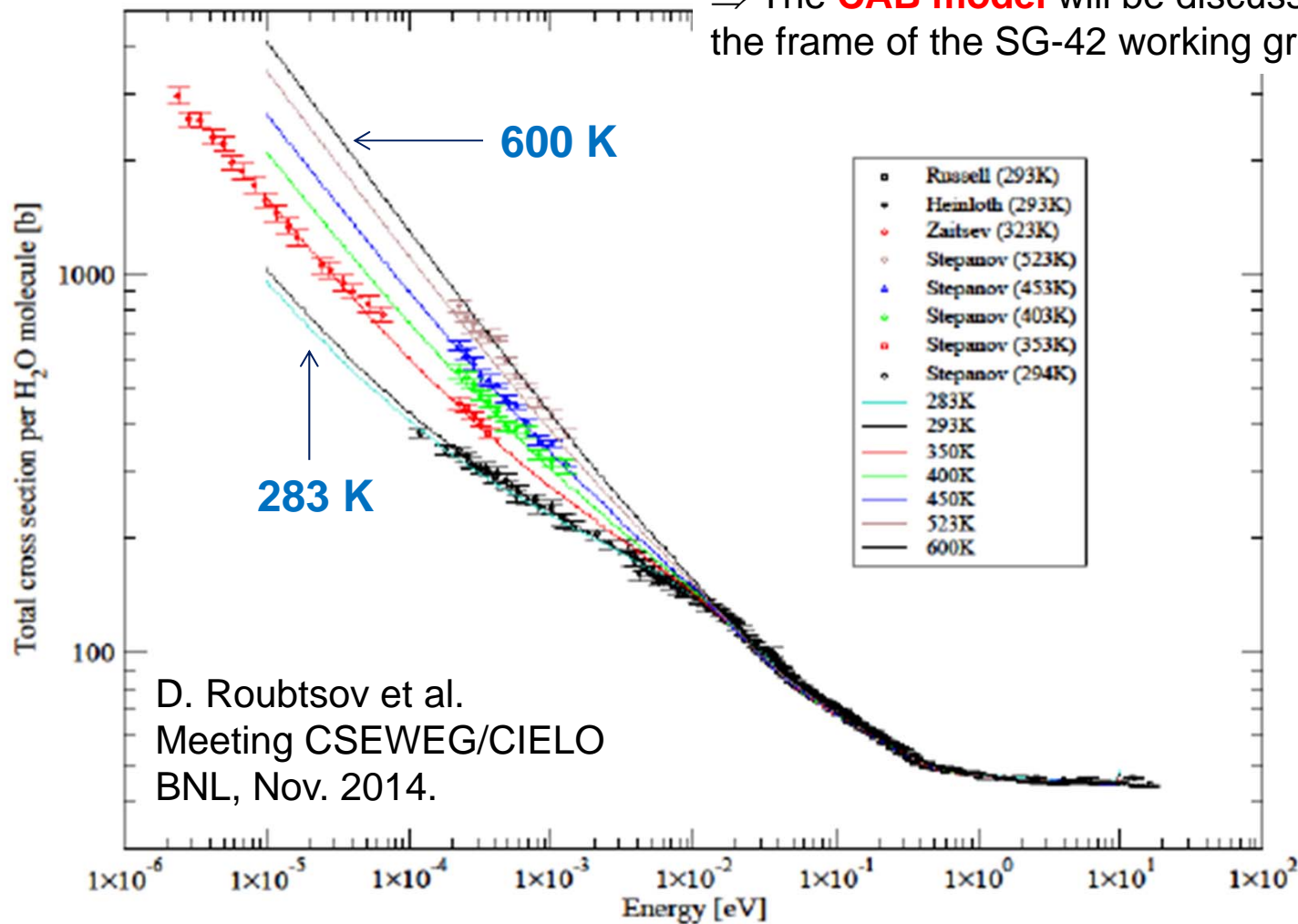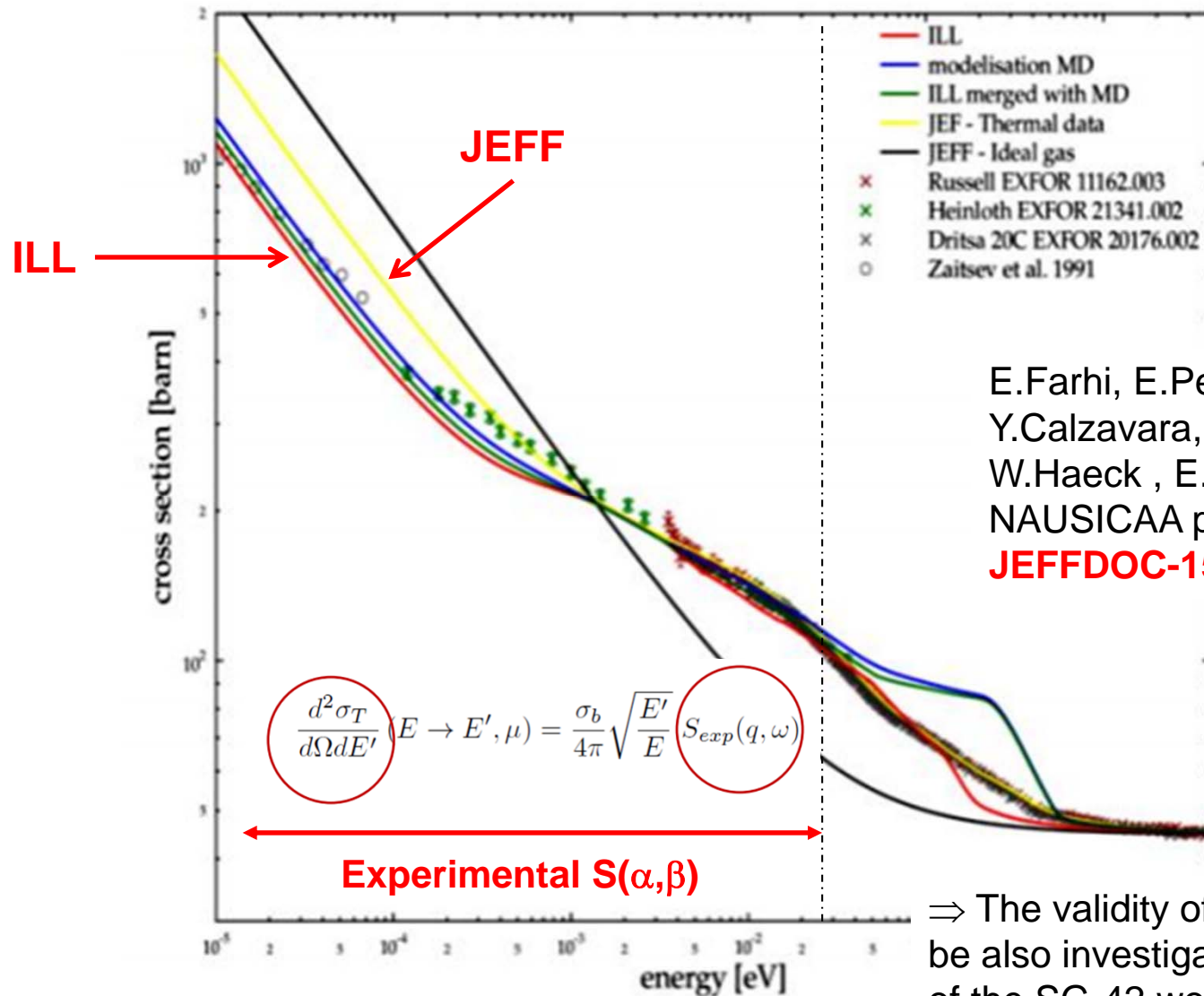Free Gas Model (FGM)
with an effective temperature

Cristal Latice Model (CLM)
with the Dolling's phonon spectrum

⇒ The **CAB model** will be discussed in the frame of the SG-42 working group

D. Roubtsov et al.
Meeting CSEWEG/CIELO
BNL, Nov. 2014.

**JEFF**

**ILL**

Legend:
- ILL
- modelisation MD
- ILL merged with MD
- JEF - Thermal data
- JEFF - Ideal gas
- × Russell EXFOR 11162.003
- × Heinloth EXFOR 21341.002
- × Dritsa 20C EXFOR 20176.002
- ○ Zaitsev et al. 1991

$$\frac{d^2\sigma_T}{d\Omega dE'}(E \to E', \mu) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E'}{E}}S_{exp}(q,\omega)$$

**Experimental S(α,β)**

E.Farhi, E.Pellegrini,
Y.Calzavara, G.Ferran,
W.Haeck , E.Guarini,
NAUSICAA project,
**JEFFDOC-1578**

⇒ The validity of the **ILL data** will
be also investigated in the frame
of the SG-42 working group

Ten years after the release of the latest "scattering data" files, R&D activities on this topic are no longer discussed within the JEFF project.

| Mat. | JEFF-3.1.1 | Temp. (K) | Year | Authors | Institute | Code |
|------|-----------|-----------|------|---------|-----------|------|
| 1 | H(H20) | 293.6<br>323.6<br>373.6<br>423.6<br>473.6<br>523.6<br>573.6<br>623.6<br>647.2<br>800.0<br>1000.0 | Jan. 2004 | J. Keinert<br>M. Mattes | Karlsruhe Institute of Technology | LEAPR NJOY-99.90++ |

Needs for new measurements of the scattering laws + total cross section in « cold » and HZP conditions are needed (steps of 10°C + as a function of pH ?) ⇒ **production of covariance matrices**

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Needs for an improved version of LEAPR (or new code) to account for Molecular Dynamic calculations and new experimental results ?

- **NAUSICAA collaboration:** First workshop in **July 2014** was the kick-off meeting of a collaborative project aiming to increase the accuracy of thermal neutron cross section data thanks to a new way to evaluate these data (ILL initiative)
  $\Rightarrow$ New meeting : **29-30 June 2015** at ILL

- **Wonder 2015, 4th International Workshop on Nuclear Data Evaluation for Reactor Applications**: organized at Aix en Provence **5-8 October** 2015

- **Proposal for a JEFF working group on "thermal scattering law data file":** kick off meeting at the NEA during the JEFF meeting of **November 2015**

- **Consultant's Meeting on Experimental Nuclear Reaction Data (EXFOR) Compilation of Thermal Neutron Scattering Data**: organized in **November 2015** at the AIEA

- A.I. Hawari, Modern Techniques for Inelastic Thermal Neutron Scattering Analysis, Nuclear Data Sheets 118 (2014) 172–175

- J.C. Holmes and A.I. Hawari, Generation of an $S(\alpha, \beta)$ Covariance Matrix by Monte Carlo Sampling of the Phonon Frequency Spectrum, Nuclear Data Sheets 118 (2014) 392–395 (+PhD thesis)

- M.L. Zerkle, Generation of TSL for YH2 using ab initio methods, Transactions of the American Nuclear Society, Vol. 111, Anaheim, California, November 9–13, 2014

- J.I. Marquez Damian, J.R. Granada and D.C. Malaspina, CAB model for water: a new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format, Annals of Nuclear Energy 65 (2014) 280–289

- E. Farhi et al., Light and heavy water dynamic structure factor for neutron transport codes, Journal of Nuclear Science and Technology 52, 844 (2015)

- Y. Abe and S. Tasaki, Molecular dynamics analysis of incoherent neutron scattering from light water via the Van Hove space–time self-correlation function with a new quantum correction, Annals of Nuclear Energy 83 (2015) 302–308

- …

# Detailed time schedule

| year | period | activities |
|------|--------|------------|
| 2015 | May | Start of SG activities at the NEA:<br>• Review of the experimental facilities and on-going work<br>• Review of the existing/new "evaluation methodologies"<br>• Review of the existing Evaluated Nuclear Data File in ENDF-6 format<br>• Selection of the benchmarks of interest |
| | May-June | Collect evaluation in ENDF-6 format |
| | June- Dec. | • Processing and Benchmarking<br>• Status/performance of available data |
| 2016 | Jan-May | Begin to reflect on the generation of covariance data |
| | May | Status of the one-year activity:<br>• Presentation of the experimental programs<br>• Presentation of the benchmark results<br>• Review of the methodologies for producing covariance data<br>• Needs for improving the evaluation |
| | May-July | Collect experimental data of interest for covariance |
| | July-Dec. | Applied methodologies for producing covariance data |
| 2017 | May | Status of the two-year activities:<br>• Presentation of the experimental results<br>• Presentation of the covariance data<br>• Presentation of the improved evaluations |
| | May-Dec. | Begin to reflect on the nuclear data format |
| 2018 | Jan-May | Monte-Carlo and deterministic uncertainty propagation work |
| | May | Status of the three-years activities<br>Proposal for a draft version of the final report that includes recommendation for future experimental works, evaluations and covariance |

Kick off meeting 18-19 May 2015

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- CAB model: $H(H_2O)$, $D(D_2O)$, $O(H_2O)$
- ILL data : $H(H_2O)$, $D(D_2O)$ ?
- …

+ LEAPR model parameters ?

Define a set of dedicated ICSBEP benchmarks ?

Intermediate report end of 2015 ?