

# Zirconium Hydride Thermal Scattering Law Data

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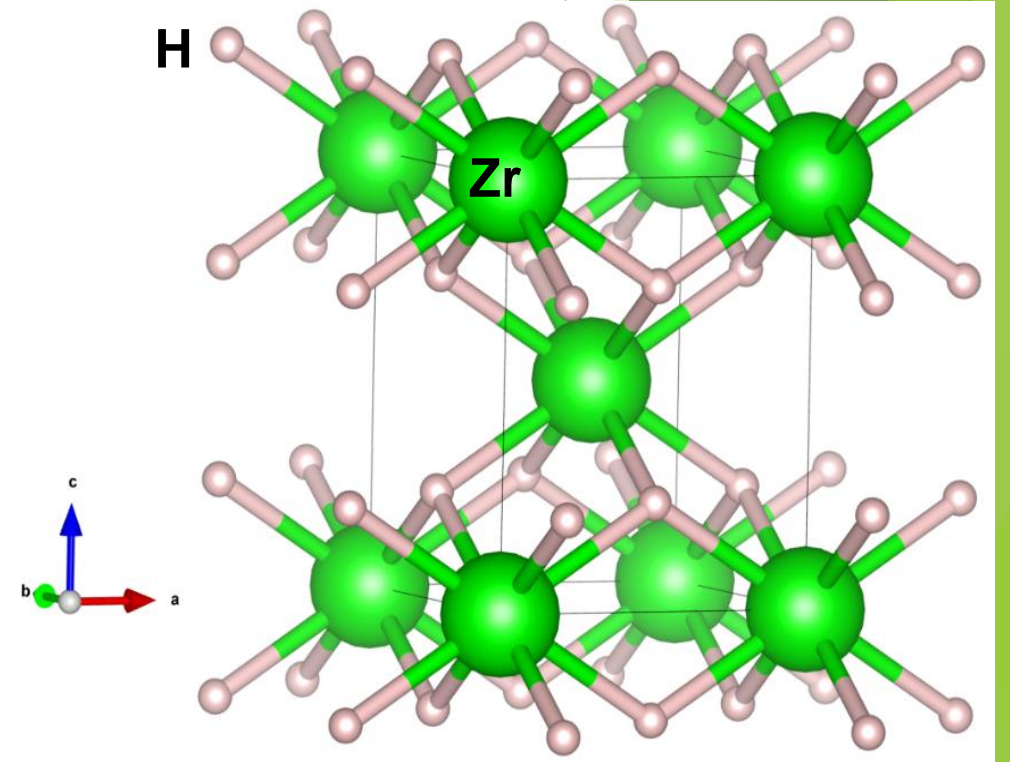
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<sup>3</sup> CEA Cadarache

# ATOMIC STRUCTURE – ZrH<sub>2</sub>

- ▶ Tetragonal crystalline structure (FCT)
- ▶ k point-mesh: 13 x 13 x 13
- ▶ cutoff energy: 675 eV
- ▶ Zr at (0, 0, 0)
- ▶ H at (0, 1/2, 1/4 )

lattice dimension	present work	experiment
a [Å]	3.540	3.522
c [Å]	4.408	4.451



# MECHANICAL PROPERTIES – ZrH<sub>2</sub>

elastic constants:	C <sub>11</sub>	C <sub>12</sub>	C <sub>44</sub>	C <sub>13</sub>	C <sub>33</sub>	C <sub>66</sub>
present work	224.9	90.2	12.5	107.0	149.5	33.6
from *	165.6	140.9	30.5	106.8	145.5	60.6
from **	166	149	26.5	109	149	55.8
from ***	102	20.4	35.6	11.4	108	23.7

Mechanical stability criteria:

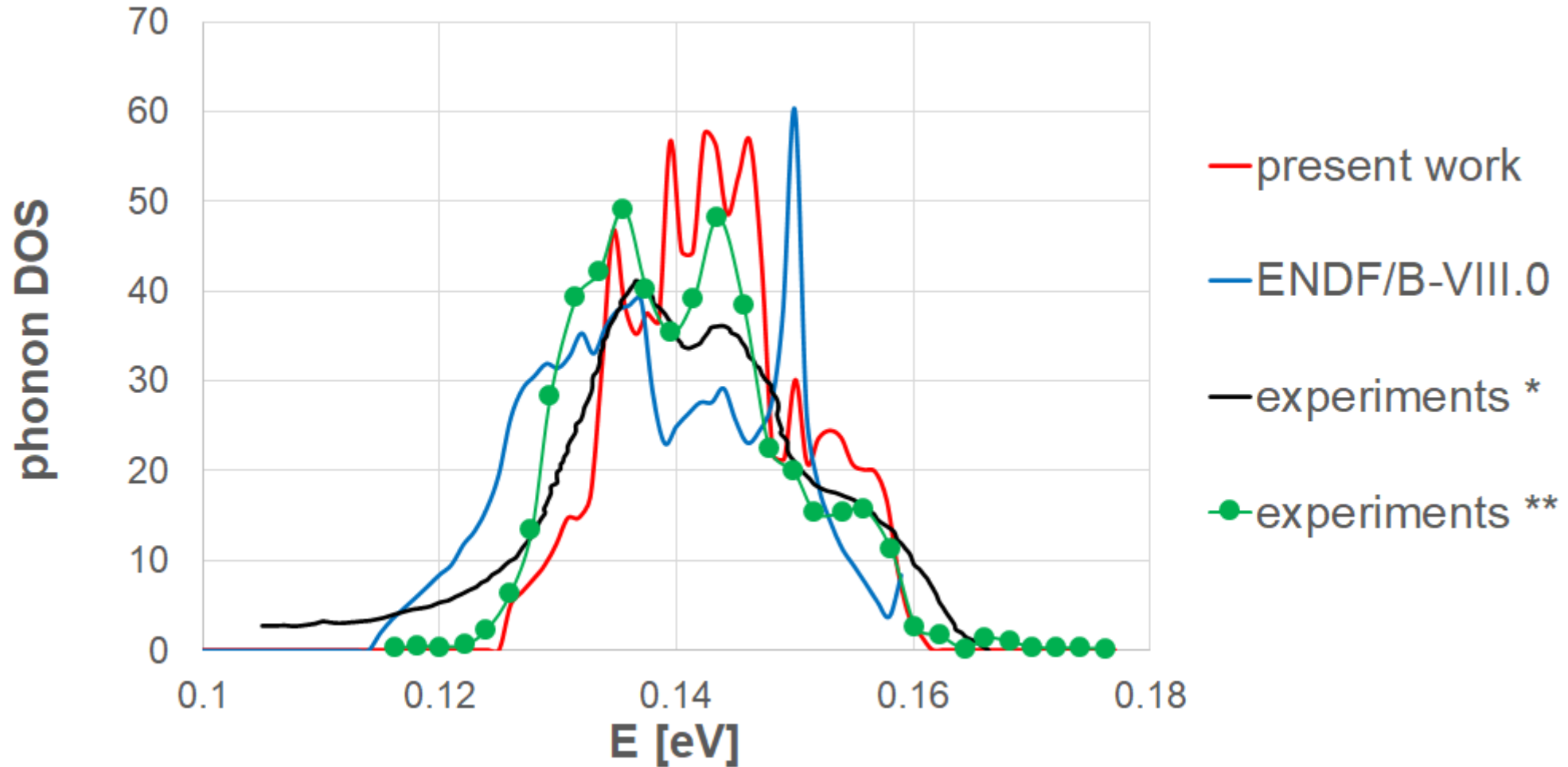
$$\begin{aligned}C_{11} > 0, C_{33} > 0, C_{44} > 0, C_{66} > 0, \\(C_{11} - C_{12}) > 0, (C_{11} + C_{33} - 2C_{13}) > 0, \\(2(C_{11} + C_{12}) + C_{33} + 4C_{13}) > 0.\end{aligned}$$

\* P. Zhang, B. T. Wang, C. H. He, P. Zhang, First-principles study of ground state properties of ZrH<sub>2</sub>, Computational Material Science 50 (2011).

\*\* P. A. T. Olsson, A. R. Massih, J. Blomqvist, A. M. Alvarez Holston, C. Bjerken, Ab initio thermodynamics of zirconium hydrides and deuterides, Computational Materials Science 86 (2014).

\*\*\* W. Zhu, R. Wang, G. Shu, P. Wu, H. Xiao, J. Phys. Chem. C 114 (2010) 22361.

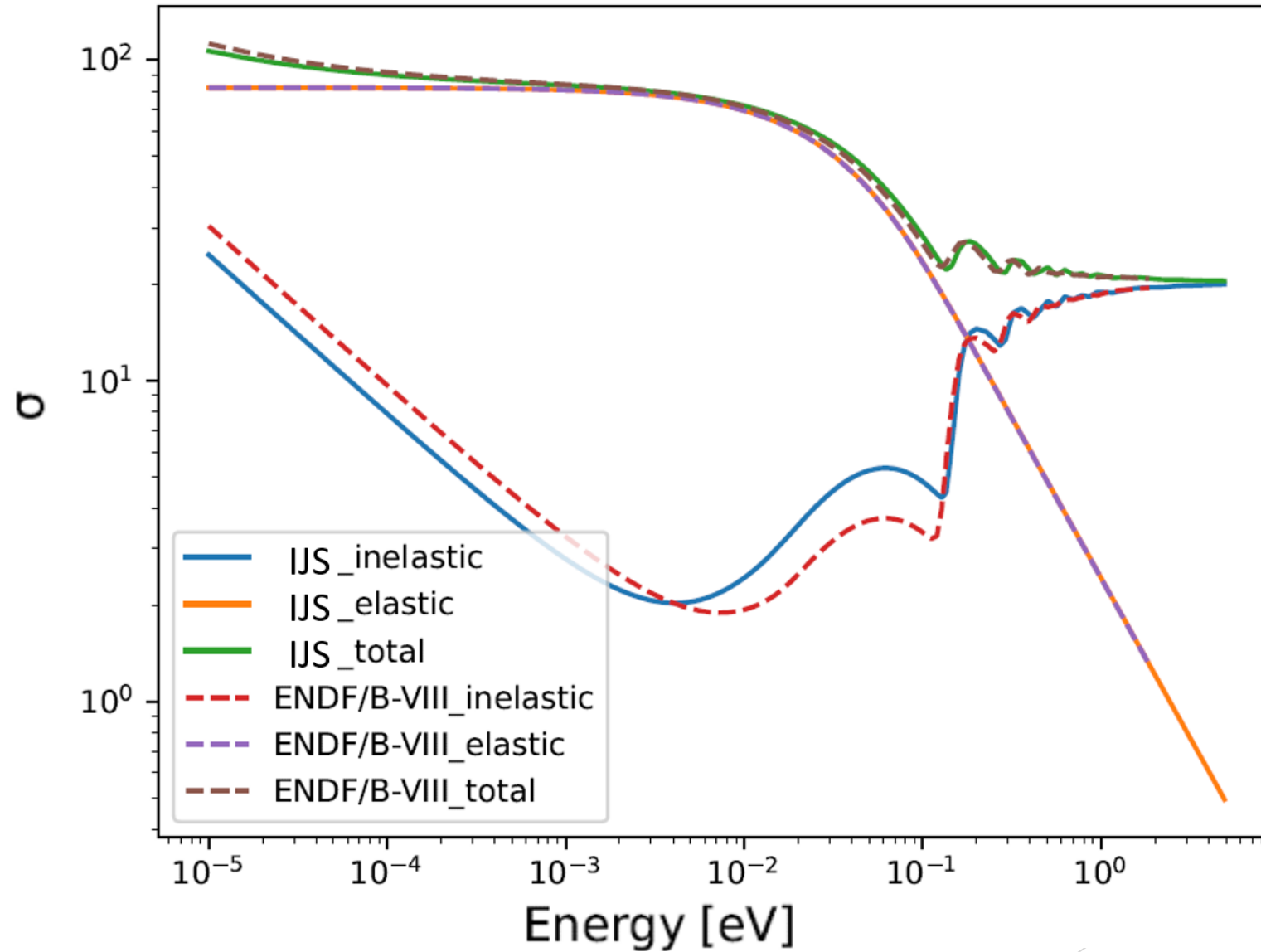
# PHONON DENSITY OF STATES – H in ZrH<sub>2</sub>



\* Weaver J H, Peterman D J, Peterson D T and Franciosi A 1981 *Phys. Rev. B* 23 1692.

\*\* Evans, A., Timms, D., Mayers, J., Bennington, S., 1996. Neutron-scattering study of the impulse approximation in ZrH<sub>2</sub>. *Phys. Rev. B - Condens. Matter Mater. Phys.* 53, 3023–3031.

# CROSS SECTION – H in ZrH

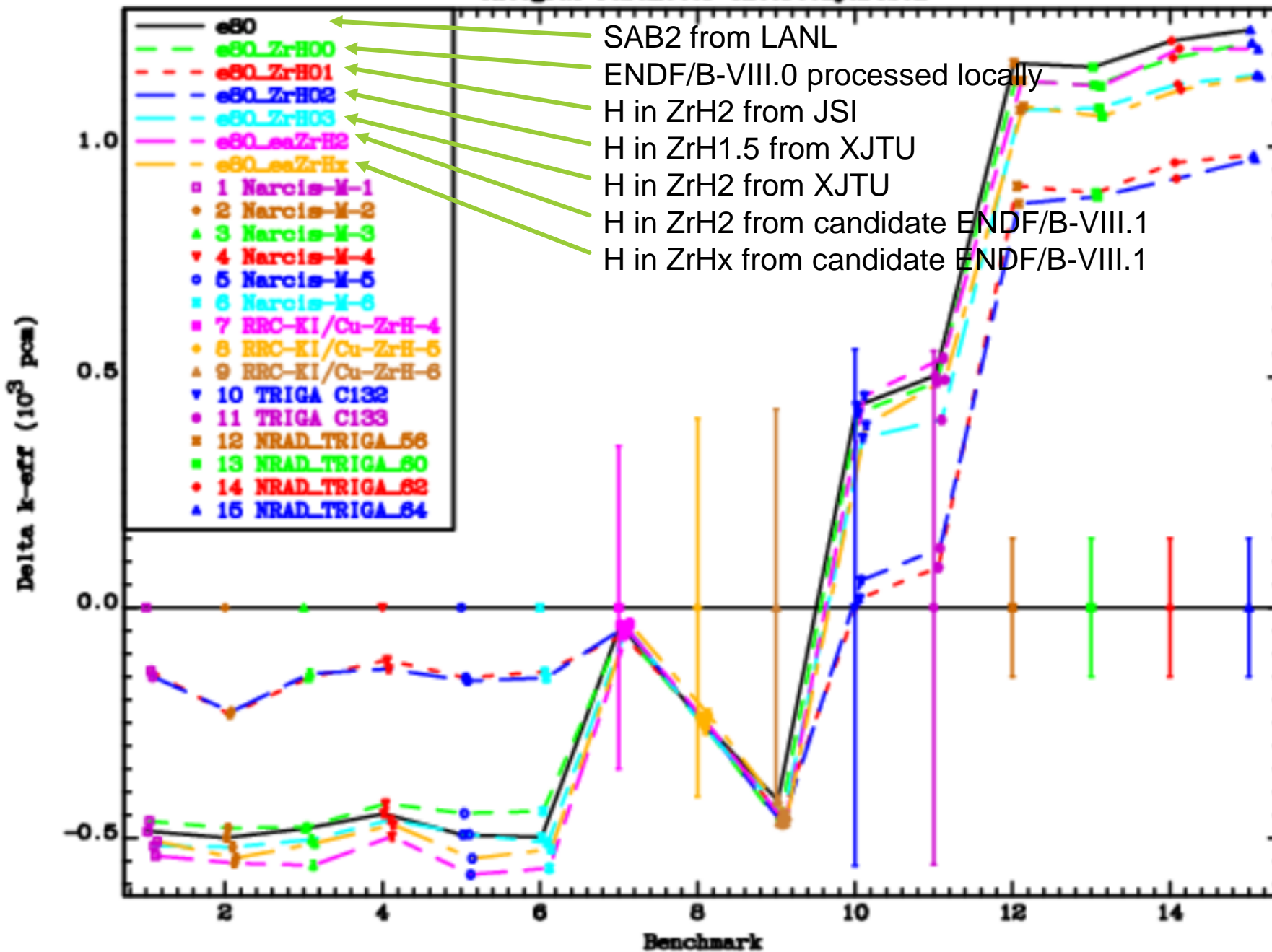


# LIST OF BENCHMARKS

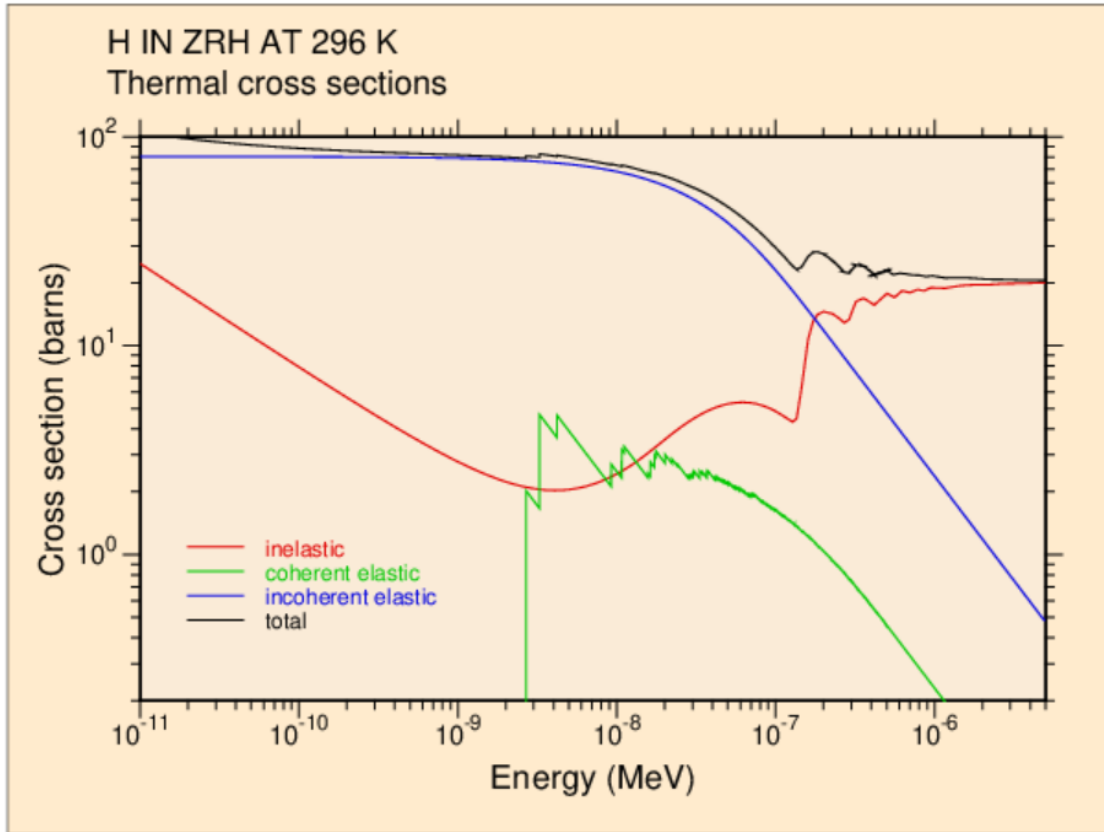
No.	ICSBEP Label	Short name	Common name	Comment
1	HEU-COMP-MIXED-003	hcm003-001	Narcis-M-1	ZrH moderator, H/Zr=1.92
2	HEU-COMP-MIXED-003	hcm003-002	Narcis-M-2 *	ZrH moderator, H/Zr=1.92
3	HEU-COMP-MIXED-003	hcm003-003	Narcis-M-3 *	ZrH moderator, H/Zr=1.92
4	HEU-COMP-MIXED-003	hcm003-004	Narcis-M-4 *	ZrH moderator, H/Zr=1.92
5	HEU-COMP-MIXED-003	hcm003-005	Narcis-M-5 *	ZrH moderator, H/Zr=1.92
6	HEU-COMP-MIXED-003	hcm003-006	Narcis-M-6 *	ZrH moderator, H/Zr=1.92
7	HEU-COMP-THERM-007	hct007-004	RRct-1(cyl)	U-Cu/ZrH fuel, SS_clad
8	HEU-COMP-THERM-007	hct007-005	RRct-2(cyl)	U-Cu/ZrH fuel, SS_clad
9	HEU-COMP-THERM-007	hct007-006	RRct-3(cyl)	U-Cu/ZrH fuel, SS_clad
10	IEU-COMP-THERM-003	ict003-001	TRIGA	SS_clad H(ZrH)
11	IEU-COMP-THERM-003	ict003-002	TRIGA	SS_clad H(ZrH)
12	IEU-COMP-THERM-013	ict013-001	NRAD_TRIGA_56	ZrH Er U(20)
13	IEU-COMP-THERM-013	ict013-002	NRAD_TRIGA_60	ZrH Er U(20)
14	IEU-COMP-THERM-013	ict013-003	NRAD_TRIGA_62	ZrH Er U(20)
15	IEU-COMP-THERM-013	ict013-004	NRAD_TRIGA_64	ZrH Er U(20)

(\*) Input models provided by Yongqiang Tang, Xi'an Jiaotong University (XJTU)

ICSBEF ZrH Benchmarks  
Integral Parameter Intercomparison



# CINEL

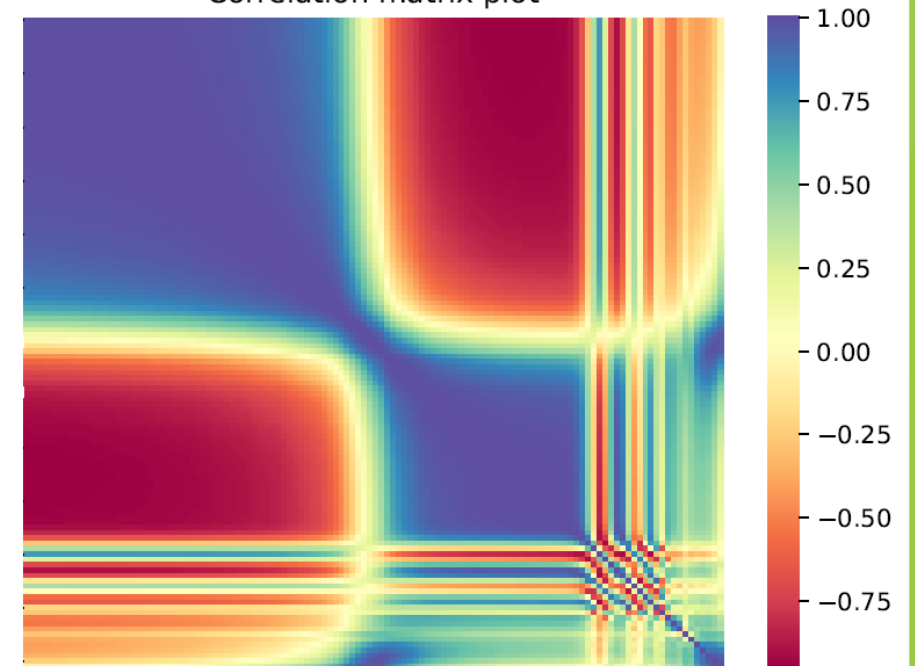
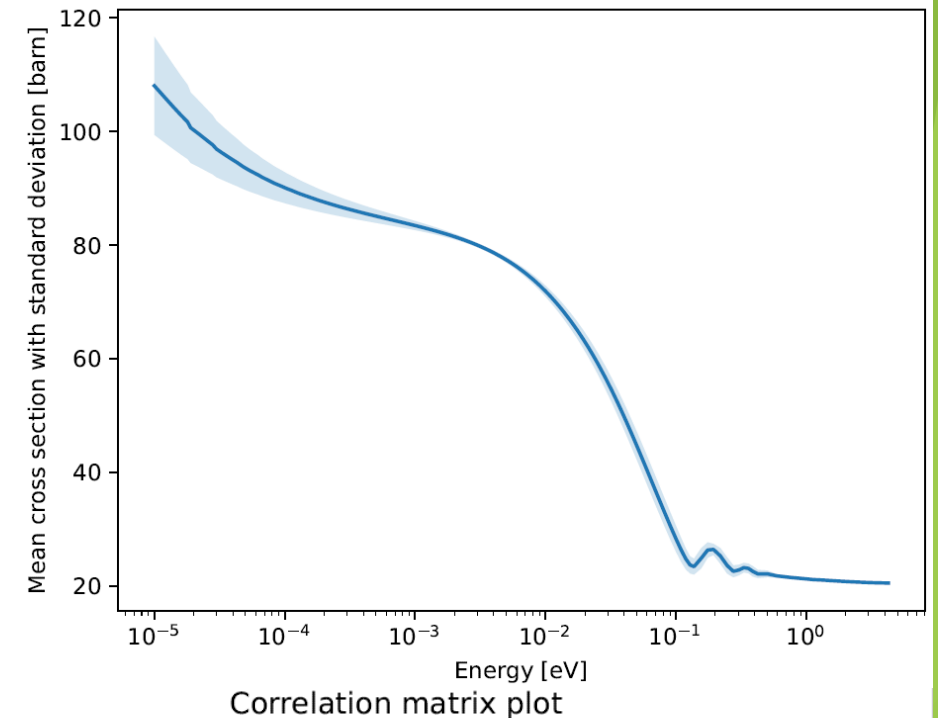


- ▶ Collaboration with CEA Cadarache.
- ▶ **CINEL** is able to generate temperature-dependent TSLs for solid, liquid and free gas materials in ENDF format with mixed elastic format.
- ▶ In the thermal range, coherent elastic cross section and inelastic cross section are in the same order of magnitude.



# TSL Uncertainties

- ▶ Developed python tool to generate random ZrH<sub>2</sub> LEAPR (modul of Njoy) files: free atom cross section for principal scatterer and energy interval randomly generated according to the Gaussian function.
- ▶ Created covariance matrices for S(a,b) and cross sections.
- ▶ Create random ACE files for MCNP by using NJOY modules.
- ▶ Test on simple benchmarks.



# TSL Uncertainties – preliminary results

- According to the Gaussian function randomly generated:
  - ▶ free atom cross section for principal scatterer:
    - ▶ Mean value: 20.43608
    - ▶ FWHM: 0.0001
  - ▶ and energy interval:
    - ▶ Mean value: 0.001
    - ▶ FWHM: 0.0965
- 100 created random ACE files

# TSL Uncertainties – preliminary results

	hcm003-002	ict003-001	ict013-001
$k_{\text{eff}}^1$	$0.99560 \pm 0.00140$	$1.00230 \pm 0.00373$	$1.01095 \pm 0.00316$
ENDF/B-VIII.0 <sup>2</sup>	$0.99430 \pm 0.00010$	$1.00496 \pm 0.00010$	$1.01300 \pm 0.00005$
mean values <sup>3</sup>	$0.99710 \pm 0.00010$	$1.00100 \pm 0.00010$	$1.01040 \pm 0.00005$

<sup>1</sup> results calculated with 100 created random ACE files and cross section calculated at JSI.

<sup>2</sup> results calculated with ENDF/B-VIII.0 cross section (uncertainty is MC statistical only).

<sup>3</sup> results calculated with cross section calculated at JSI using nominal values of free atom cross section for principal scatterer and energy interval (uncertainty is MC statistical only).

# CONCLUSIONS

- ▶ At JSI calculated phonon density of states for H in ZrH<sub>2</sub> is in good agreement with experiments.
- ▶ The results from TSL for H in ZrH<sub>2</sub> from IJS are not in agreement with H in ZrH<sub>2</sub> from ENDF/B-VIII.1 candidate.
- ▶ ICT013 benchmarks remain strongly discrepant with all TSL data (H/Zr 1.58), possibly due to Er content.
- ▶ keff and its standard deviation calculated using IJS cross section 100 randomly generated ACE files are all in the range of keff calculated with ENDF/B-VIII.0 cross section.