Zirconium Hydride Thermal Scattering Law Data

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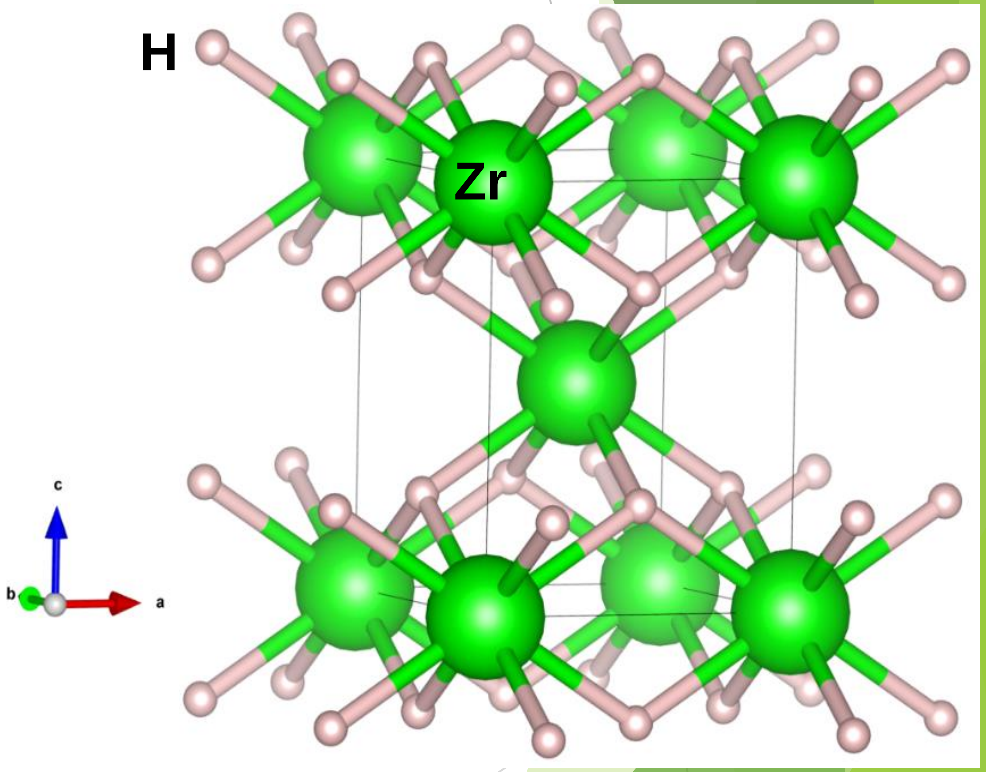
ATOMIC STRUCTURE – ZrH_2

- Tetragonal crystalline structure (FCT)
- k point-mesh: 13 x 13 x 13
- cutoff energy: 675 eV
- Zr at (0, 0, 0)
- H at (0, ½, ¼)

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



MECHANICAL PROPERTIES – ZrH_2

elastic constants:	C_{11}	C_{12}	C_{44}	C_{13}	C_{33}	C_{66}
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:

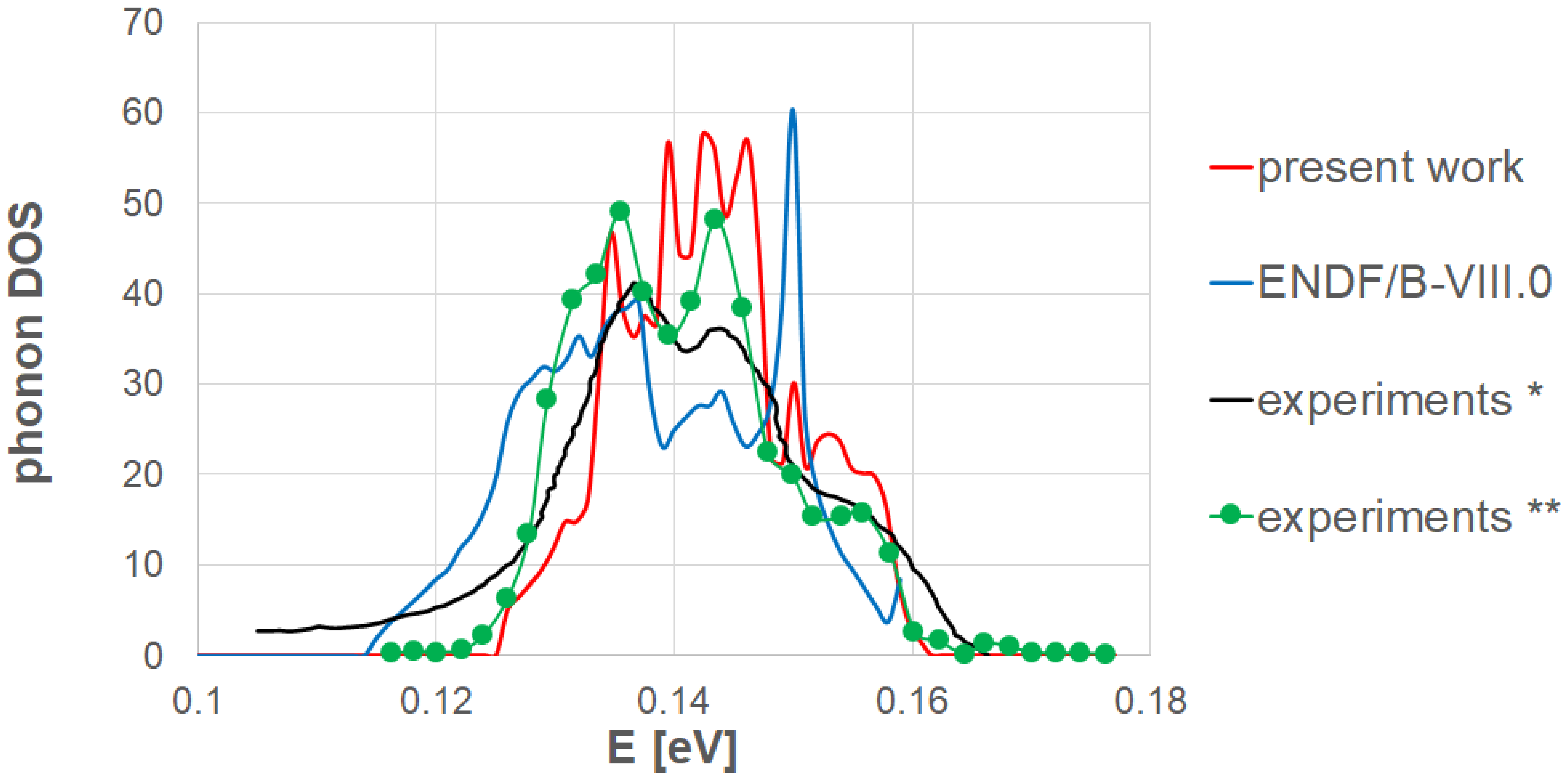
$$C_{11} > 0, C_{33} > 0, C_{44} > 0, C_{66} > 0,$$
$$(C_{11} - C_{12}) > 0, (C_{11} + C_{33} - 2C_{13}) > 0,$$
$$(2(C_{11} + C_{12}) + C_{33} + 4C_{13}) > 0.$$

* P. Zhang, B. T. Wang, C. H. He, P. Zhang, First-principles study of ground state properties of ZrH_2, 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.

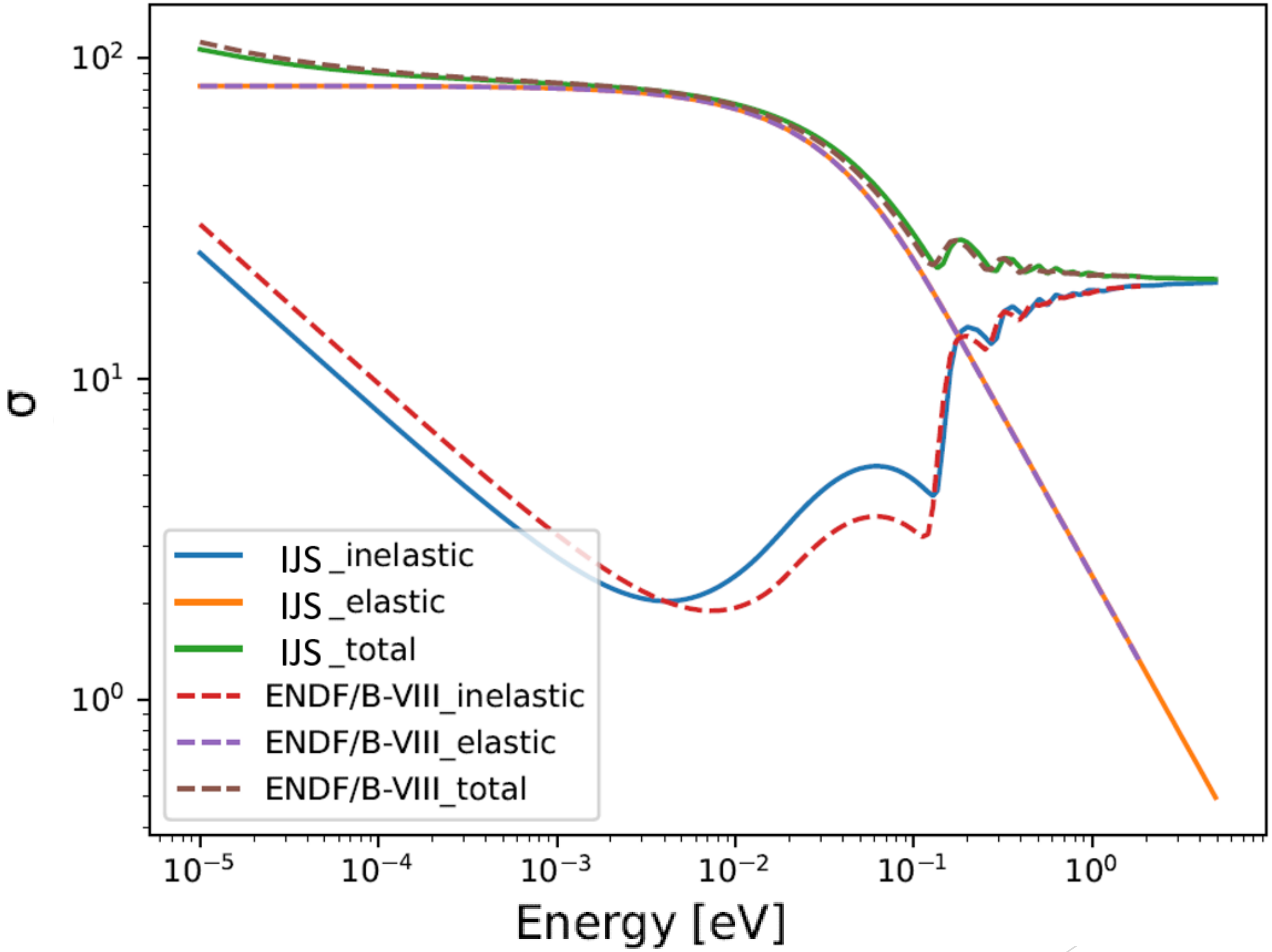
PHONON DENSITY OF STATES – H in ZrH_2



* 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 ZrH2. Phys. Rev. B - Condens. Matter Mater. Phys. 53, 3023–3031.

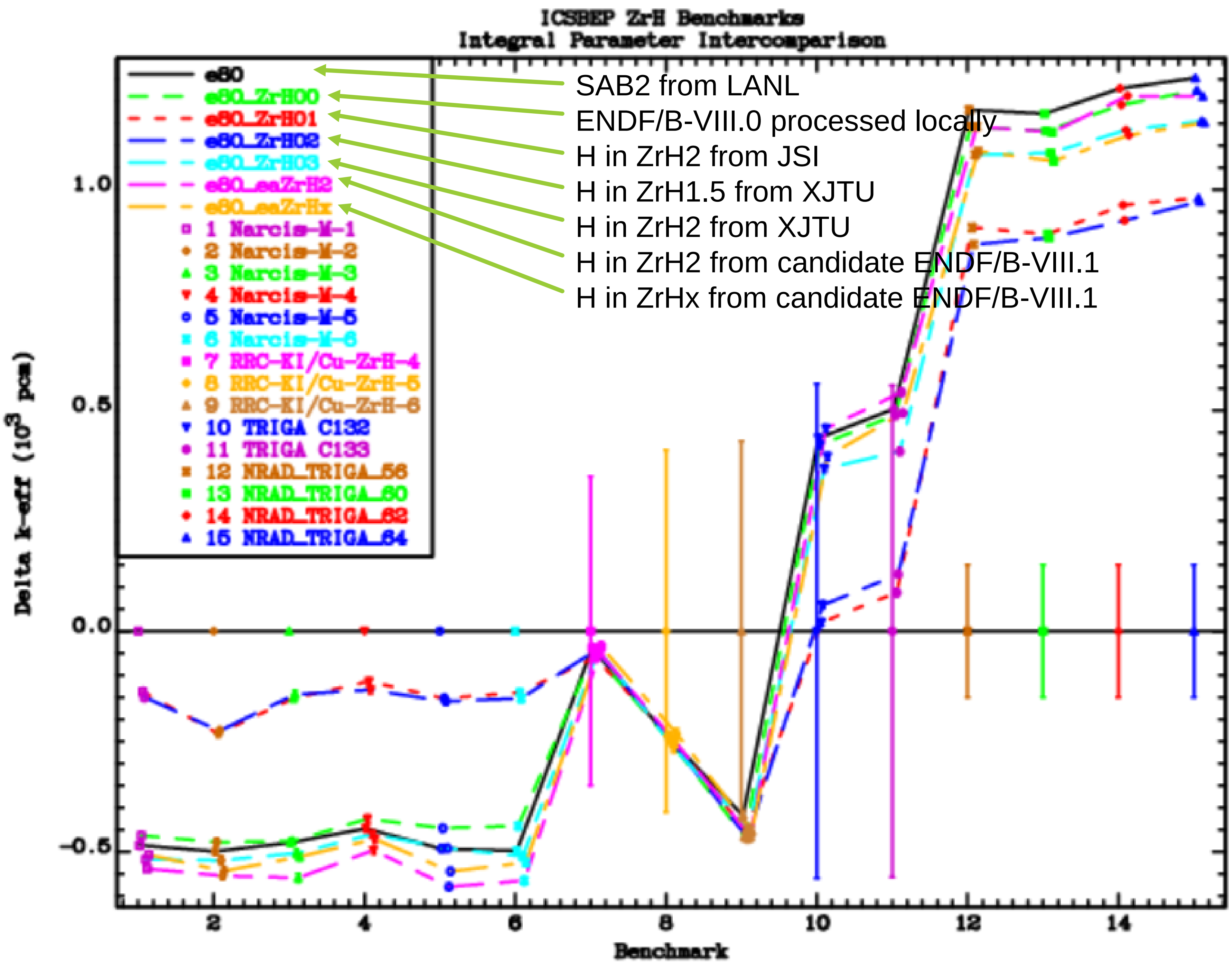
CROSS SECTION – H in ZrH



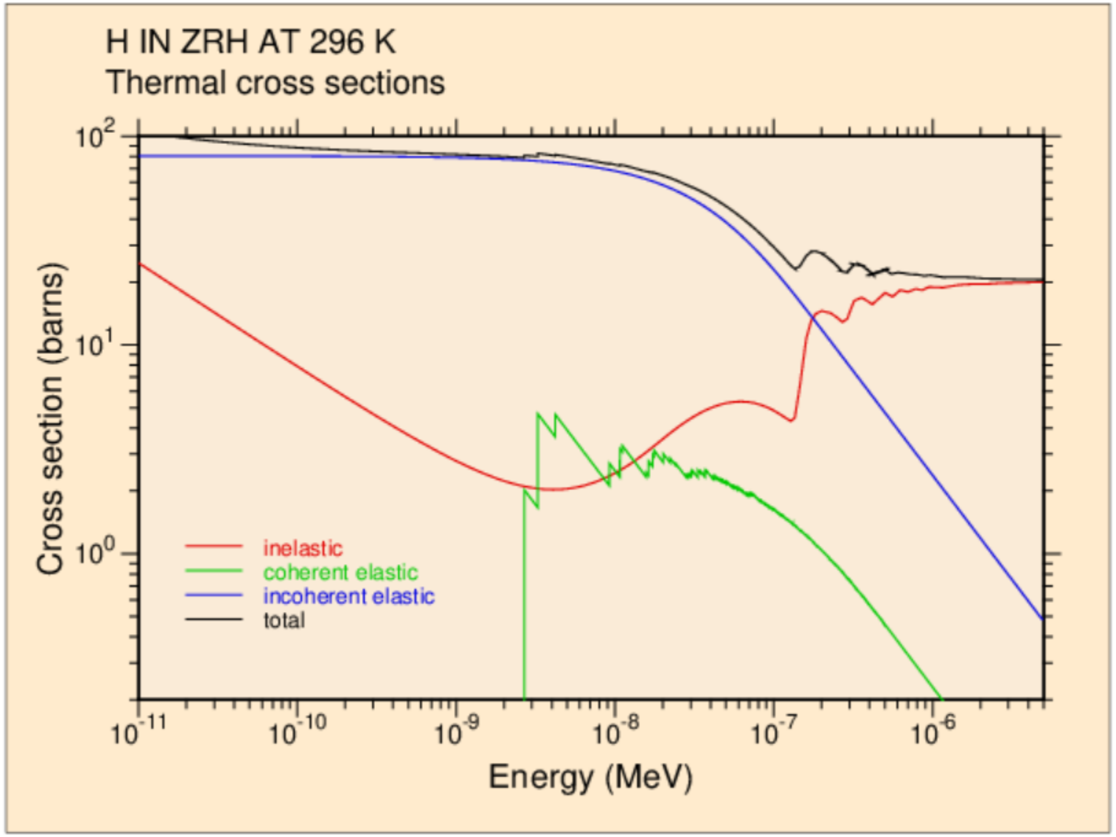
LIST OF BENCHMARKS

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)


ICSBEP ZrH Benchmarks
Integral Parameter Intercomparison
e80
e80_ZrH00
e80_ZrH01
e80_ZrH02
e80_ZrH03
e80_eaZrH2
e80_eaZrHx
1 Narcis-M-1
2 Narcis-M-2
3 Narcis-M-3
4 Narcis-M-4
5 Narcis-M-5
6 Narcis-M-6
7 RRC-KI/Cu-ZrH-4
8 RRC-KI/Cu-ZrH-5
9 RRC-KI/Cu-ZrH-6
10 TRIGA C132
11 TRIGA C133
12 NRAD_TRIGA_56
13 NRAD_TRIGA_60
14 NRAD_TRIGA_62
15 NRAD_TRIGA_64
SAB2 from LANL
ENDF/B-VIII.0 processed locally
H in ZrH2 from JSI
H in ZrH1.5 from XJTU
H in ZrH2 from XJTU
H in ZrH2 from candidate ENDF/B-VIII.1
H in ZrHx from candidate ENDF/B-VIII.1
Delta k-eff (10^3 pcm)
1.0
0.5
0.0
-0.5
2
4
6
8
10
12
14
Benchmark

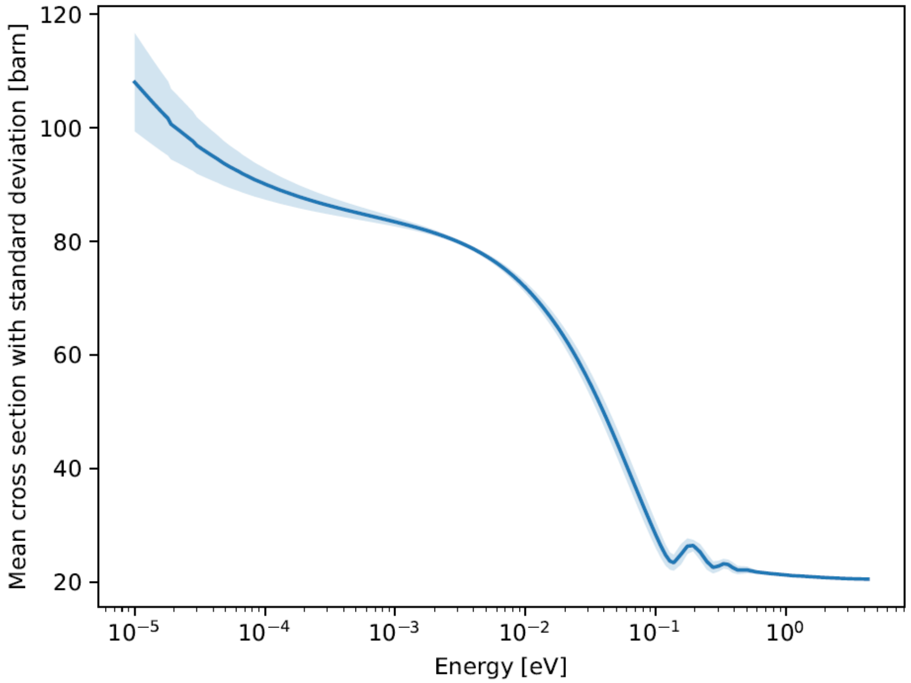
CINEL



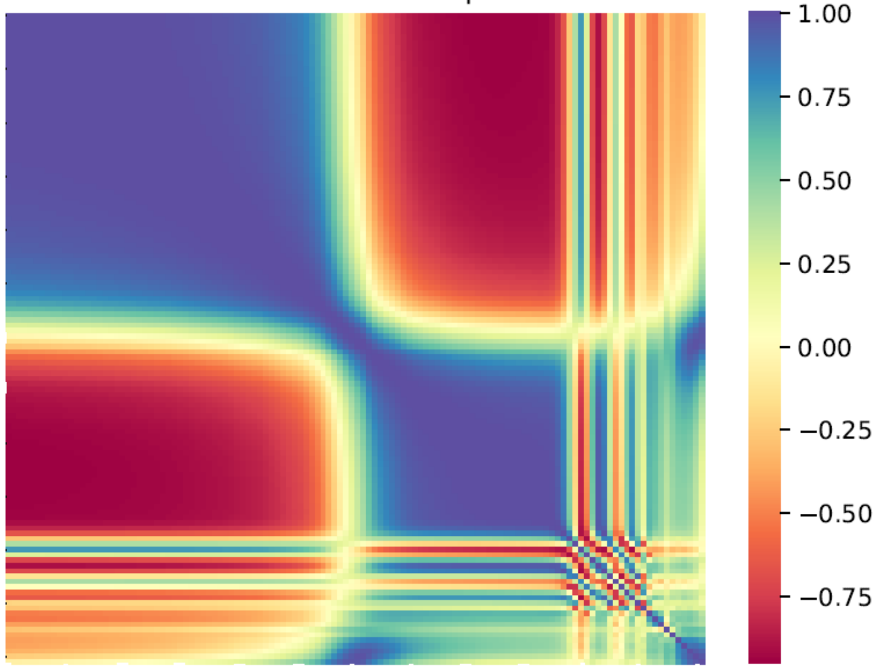
- Collaboration with CEA Cadarache.
- **CINEL** is able to generate temperature-dependent TSLs for solid, liquid and free gas materials in ENDF format with mixed elastic format.
- In the thermal range, coherent elastic cross section and inelastic cross section are in the same order of magnitude.

TSL Uncertainties

- Developed python tool to generate random ZrH2 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.



Correlation matrix plot



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

	ict003-001	hcm003-002	ict013-001
k_{eff}[1]	1.0023 ± 3.7213e-03	0.9956 ± 1.4192e-03	1.01095 ± 3.1561e-03
ENDF/B-VIII.0[2]	1.00496 ± 0.0001	0.9943 ± 0.0001	1.0130 ± 0.00005
mean values[3]	1.0010 ± 0.0001	0.9971 ± 0.0001	1.0104 ± 0.00005

[1] results calculated with 100 created random ACE files and cross section calculated at JSI.

[2] results calculated with ENDF/B-VIII.0 cross section.

[3] results calculated with cross section calculated at JSI using mean values of free atom cross section for principal scatterer and energy interval.

CONCLUSIONS

- At JSI calculated phonon density of states for H in ZrH2 is in good agreement with experiments.
- The results from TSL for H in ZrH2 from IJS are not in agreement with H in ZrH2 from ENDF/B-VIII.1 candidate.
- ICT013 benchmarks remain strongly discrepant with all TSL data (H/Zr 1.58).
- 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.