^{56}Fe Evaluation for the CIELO Project

G.P.A. Nobre[1) & M. Herman[1)
for the CIELO Collaboration[2)

[1) National Nuclear Data Center, Brookhaven National Laboratory, USA
[2) Subgroup 40 (Iron), Working Party on Evaluation Collaboration (WPEC), OECD/NEA Data Bank, Paris, France

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Status of ^{56}Fe CIELO evaluation

Collaboration: BNL, CNDC, IAEA, IRM, JSI, LANL, ORNL, RPI

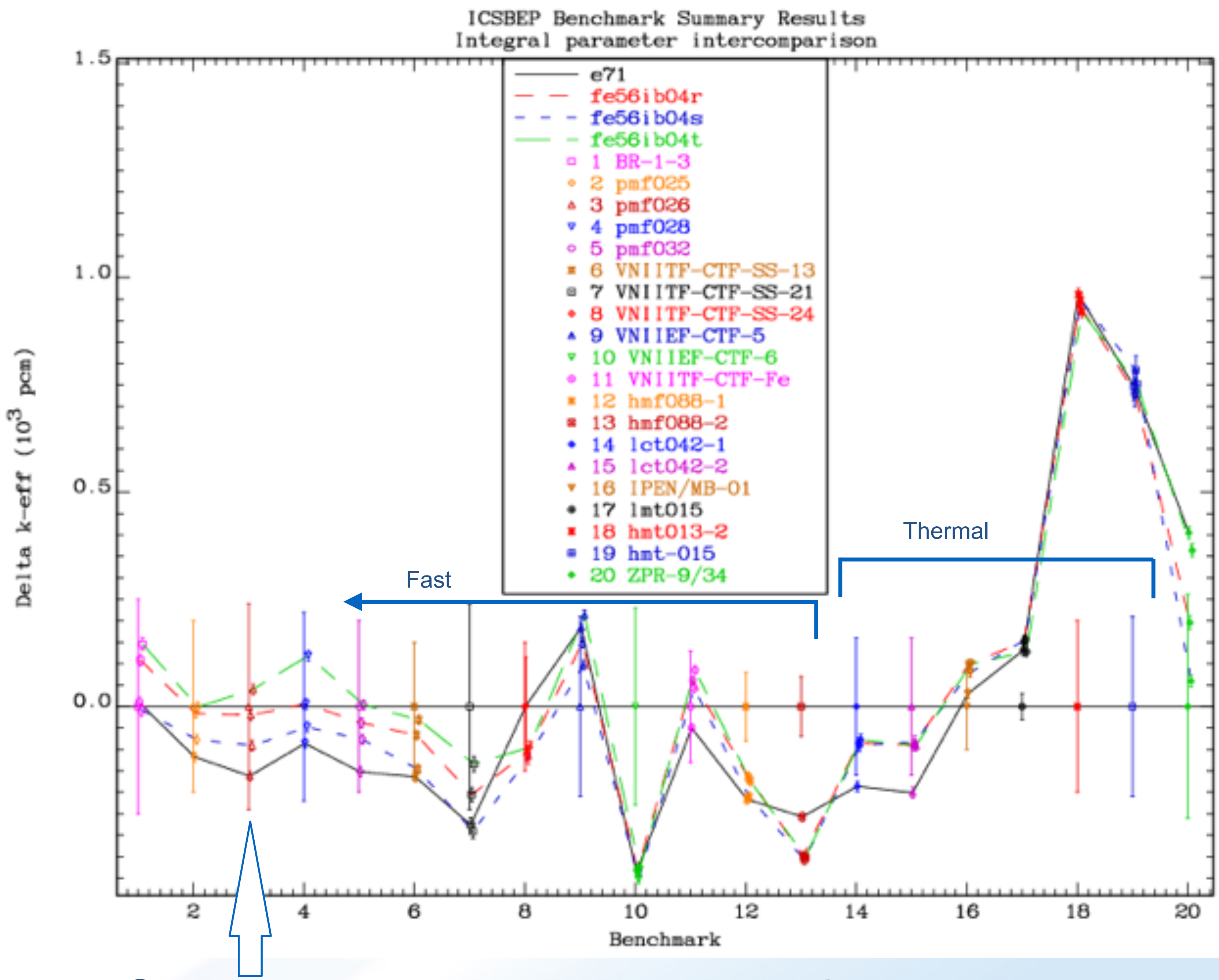
- Exp. data analysis CNDC
- Resonance range ORNL
- Fast neutron range EMPIRE (BNL, IAEA)
- File assembly IAEA, BNL
- Testing IAEA, RPI, BNL, LANL, JSI

- First test release: rev.49
  - RR - ORNL rev.43 up to 2 MeV
  - Fast - EMPIRE calculations with HFB level dens. rev.48
  - X-sec fluctuations ignored
  - Elastic ang. distr. - RR reconstructed and smoothed ORNL (~JENDL-4.0)
  - Selection of 24 benchmarks by JSI and IAEA
  - Benchmarking by IAEA and RPI (semi-integral exp.)

Benchmark results for rev.49

- Criticality benchmarks by A. Trkov comparable to ENDF/B-VII.1

	ICSBEP name	Common name
1	PU-MET-FAST-015	BR-1-3
2	PU-MET-FAST-025	pmf025
3	PU-MET-FAST-026	pmf026
4	PU-MET-FAST-028	pmf028
5	PU-MET-FAST-032	pmf032
6	HEU-MET-FAST-013	VNIITF-CTF-SS-13
7	HEU-MET-FAST-021	VNIITF-CTF-SS-21
8	HEU-MET-FAST-024	VNIITF-CTF-SS-24
9	IEU-MET-FAST-005	VNIITF-CTF-SS-5
10	IEU-MET-FAST-006	VNIITF-CTF-SS-6
11	HEU-MET-FAST-087	VNIITF-CTF-Fe
12	HEU-MET-FAST-088	hmf088-1
13	HEU-MET-FAST-088	hmf088-2
14	LEU-COMP-THERM-042	lct042-1
15	LEU-COMP-THERM-042	lct042-2
16	LEU-COMP-THERM-043	IPEN/MB-01
17	LEU-MET-THERM-015	lmt015
18	HEU-MET-THERM-013	hmt013-2
19	HEU-MET-THERM-015	hmt015
20	HEU-MET-INTER-001	ZPR-9/34
21	PU-MET-INTER-002	ZPR-6/10
22	MIX-COMP-FAST-001	ZPR-6/7
23	MIX-COMP-FAST-005	ZPR-9/31
24	MIX-COMP-FAST-006	ZPPR-2



Certain sensitivity to degree of smoothing of elastic angular distributions

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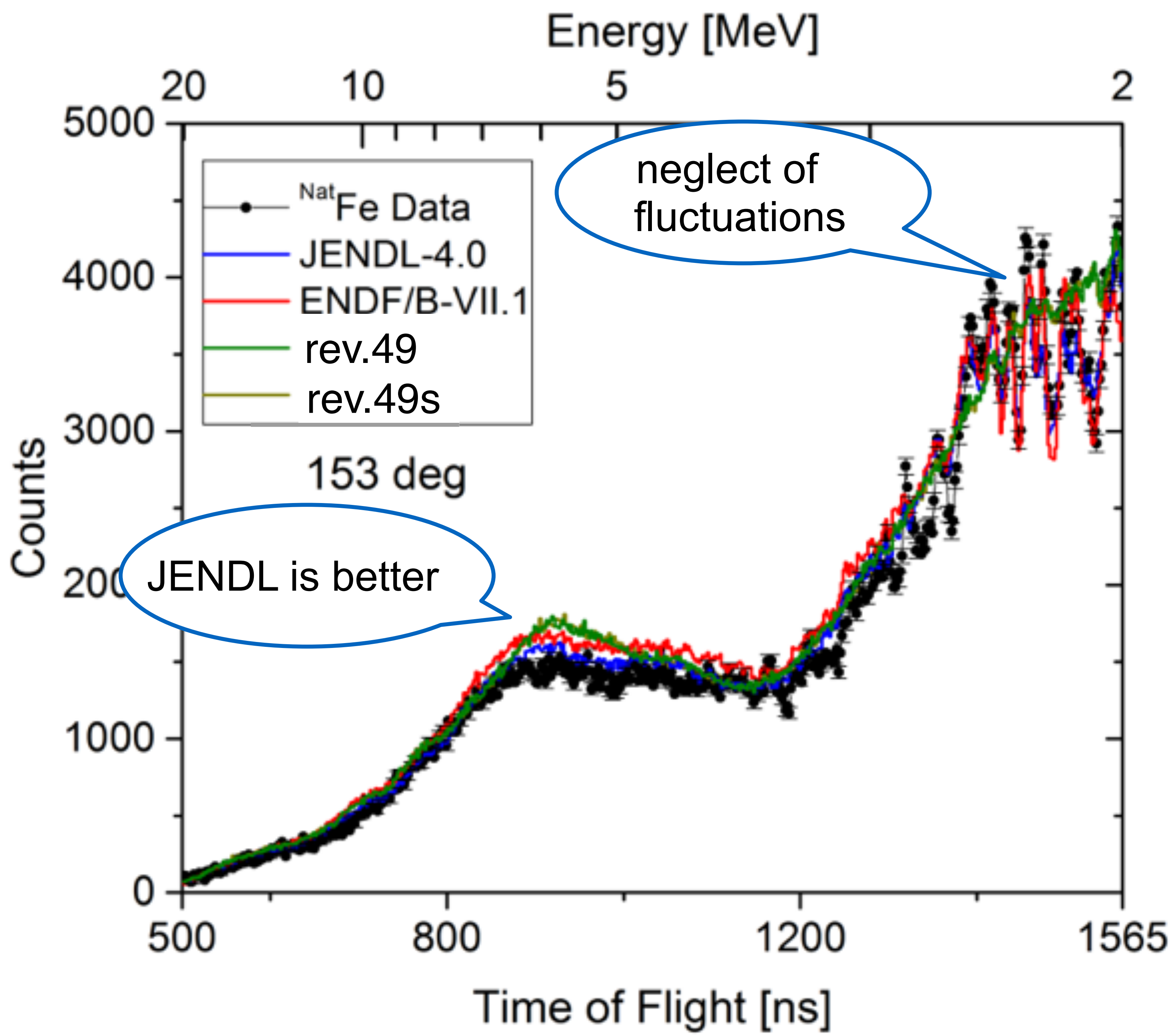
RPI semi-integral experiments

- Preference to JENDL-4.0 and ENDF/B-VII.1
  - neglect of fluctuations
  - angular distributions in RR
  - discrepancies in the fast region



CIELO-iron rev.88

Cross sections:

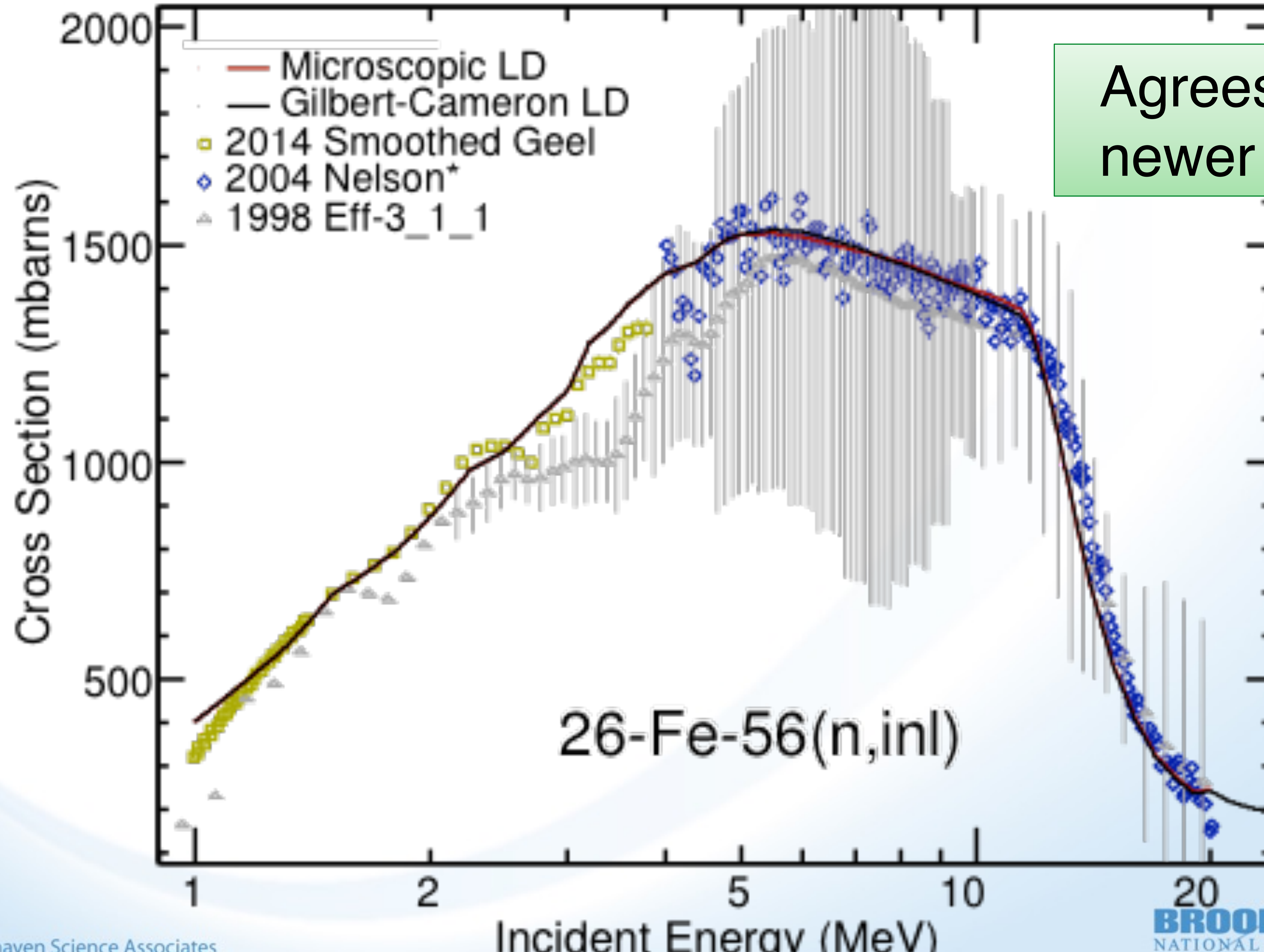
- RR up to 846 keV: Luiz Leal (ORNL) rev.43
- Total 846 keV - 4 MeV: JEFF-3.2 (smoothed Berthold/ Weigmann experimental data)
- MT51,52 up to 4 MeV: Negret (Geel) data
- All the rest except elastic: EMPIRE calculations with **GC** level densities
- Elastic: total - sum of all the channels

- Angular distributions:
  - RR up to 846 keV: JENDL-4.0
  - All the rest: EMPIRE calculations

Summary of EMPIRE calculations

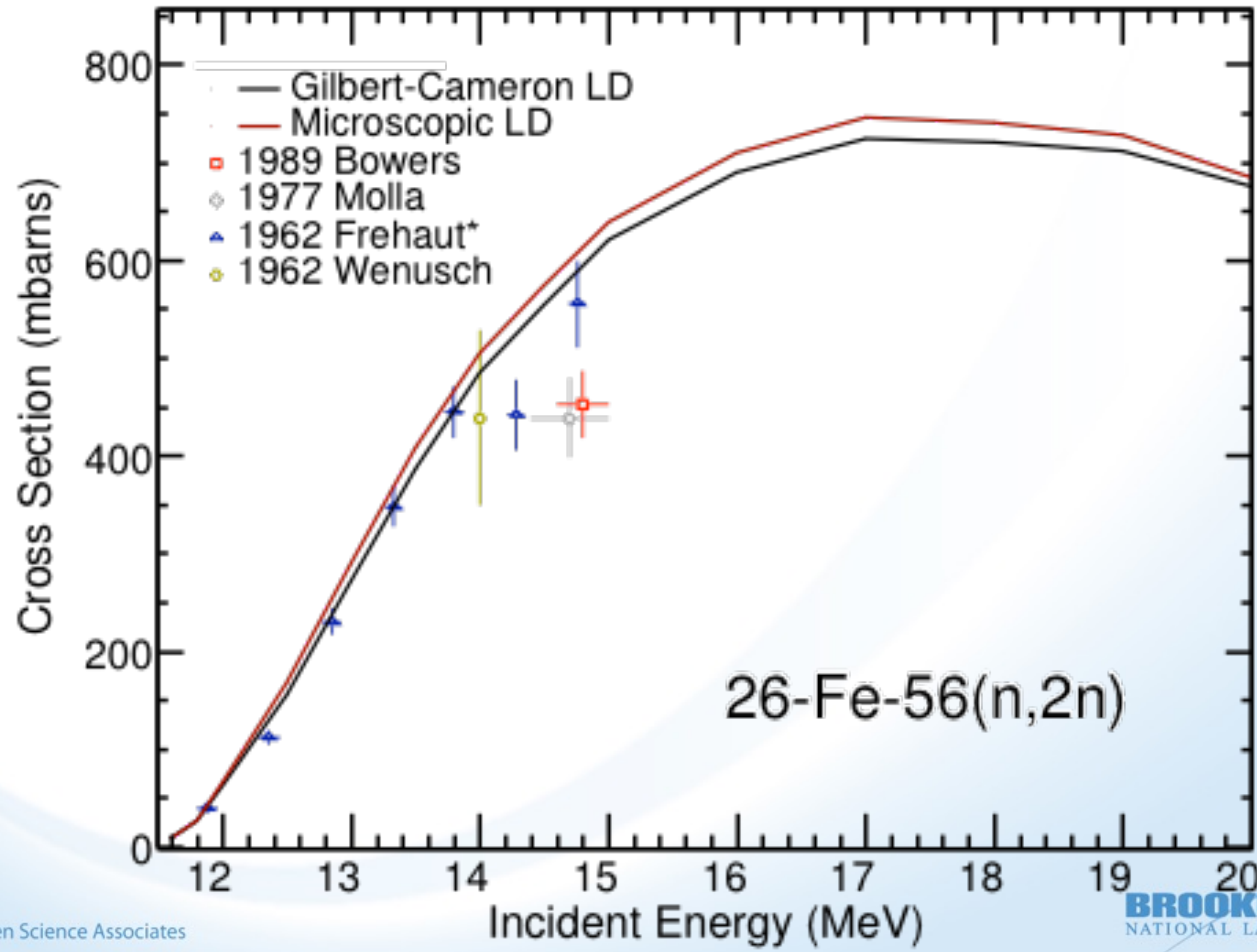
- CC for incident/outgoing channels + DWBA to uncoupled levels
- Lane-consistent dispersive OMP by Soukhovitskii & Capote
- Rev. 88 replaces microscopic HFB level densities with Gilbert-Cameron (open issue of parity distribution)
- Width fluctuation correction (HRTW) up to 8 MeV (difference HRTW v. Moldauer <1%)
- Default gamma-ray strength function (Plujko MLO1)
- TUL Multistep Direct >3 MeV plus Multistep Compound
- Exciton model (PCROSS) for *p*- and *γ*-emission
- Iwamoto-Harada model for PE cluster emission
- Fitted LD parameters to IRDFF for (n,p) and to experimental data for α production

Small differences for inelastic channel

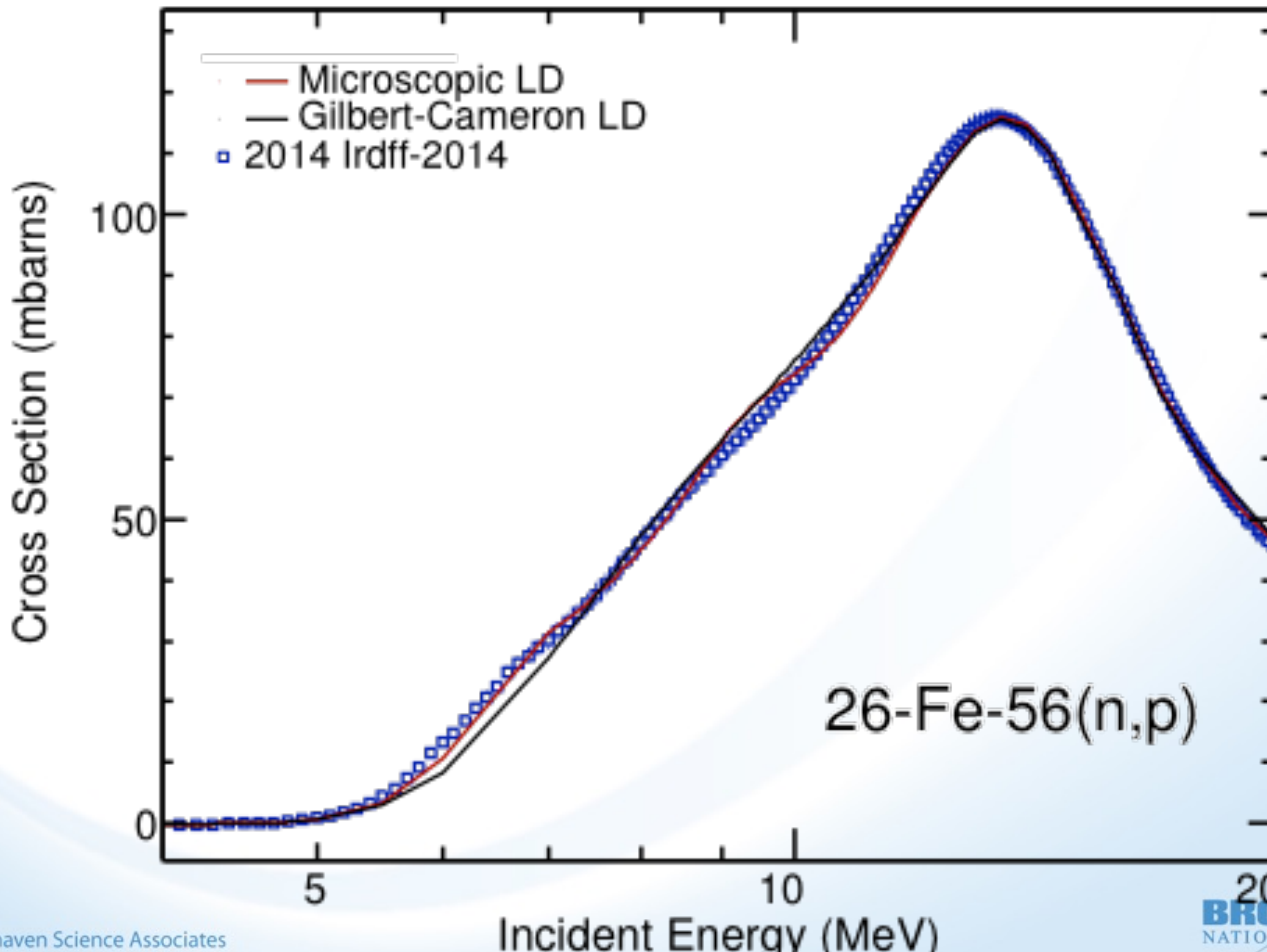


Agrees with newer data!

Slight improvement for $^{56}Fe(n,2n)$



$^{56}Fe(n,p)$: Not as great as before, but still very good and… can be fine-tuned



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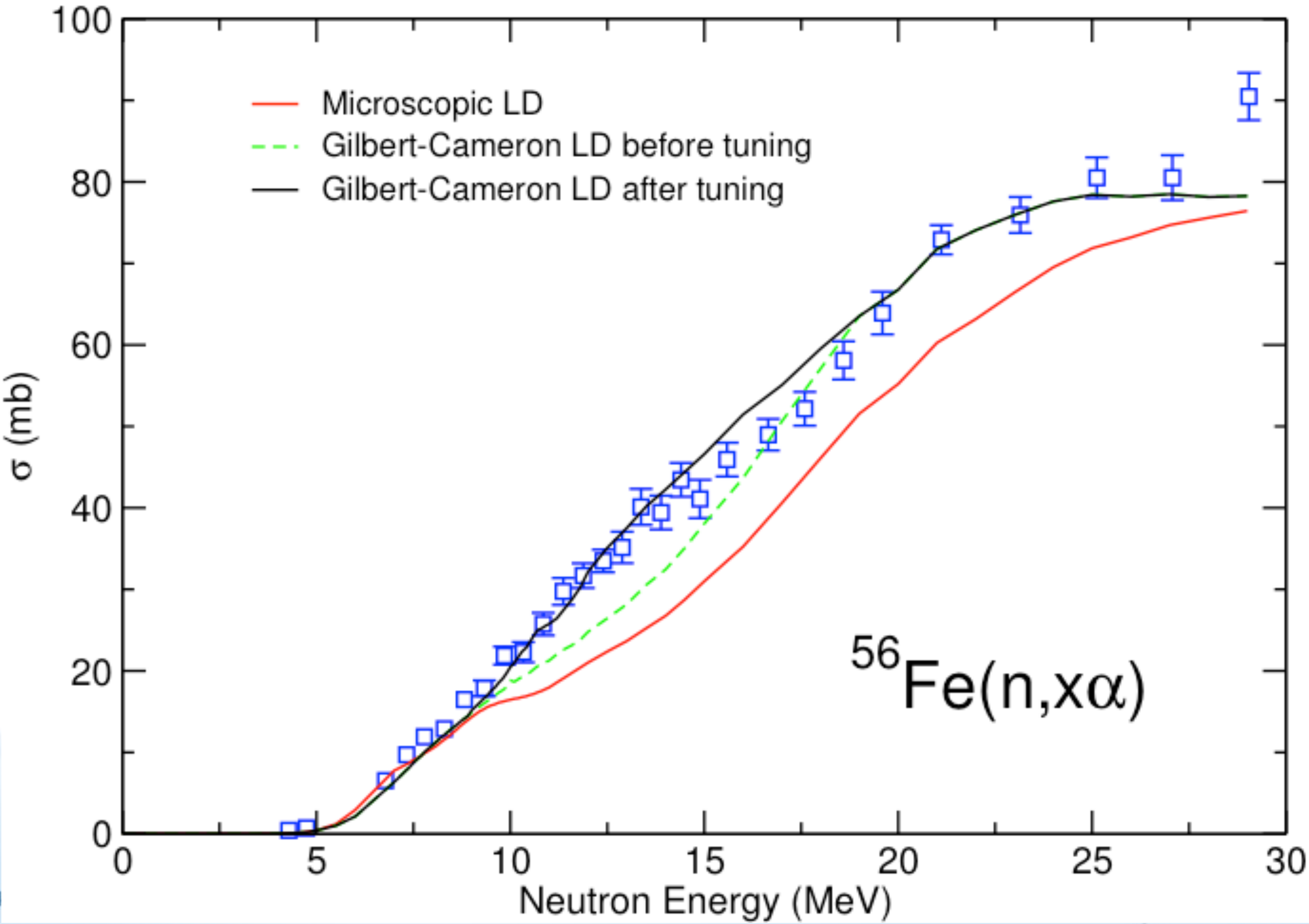
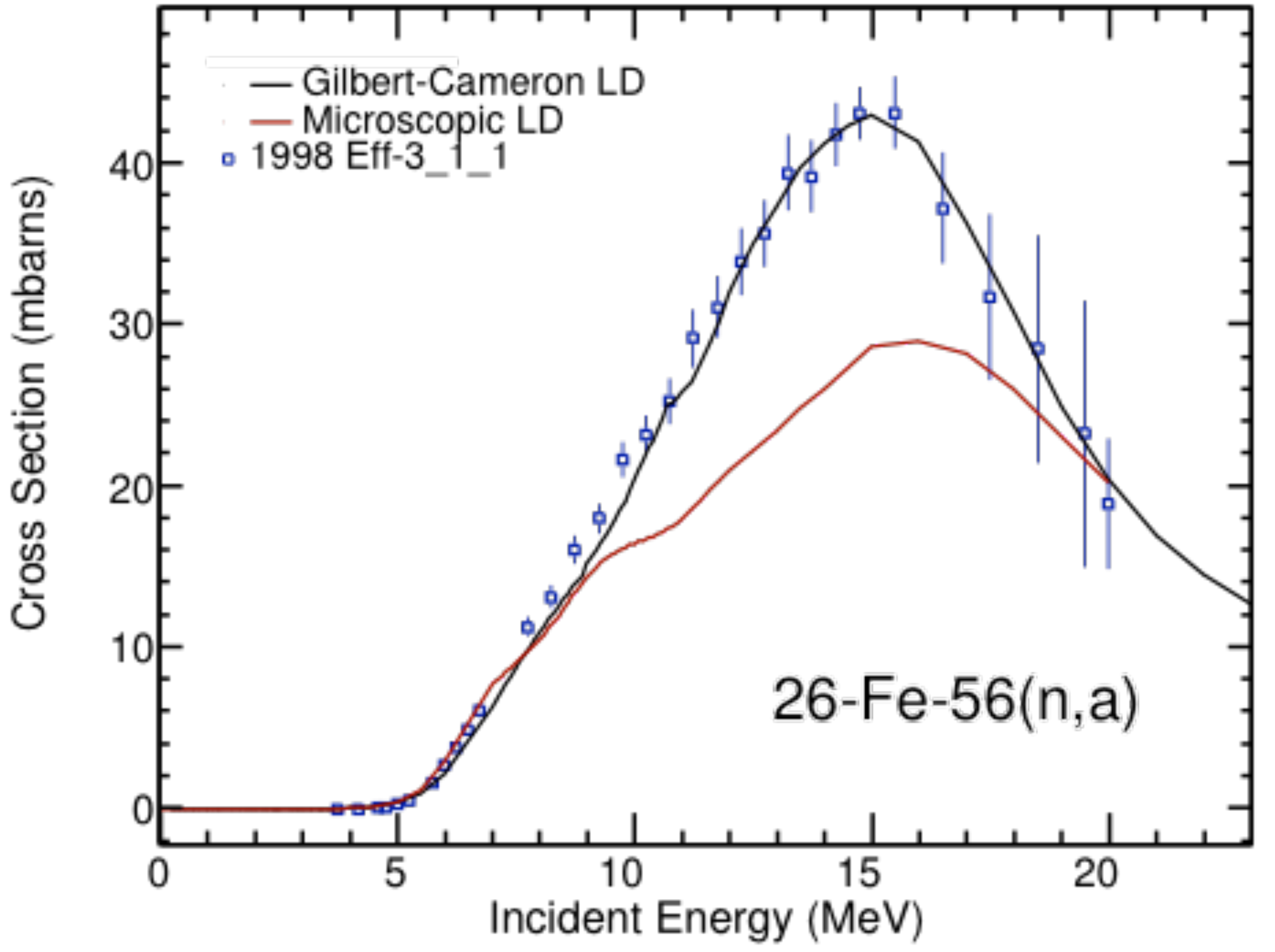
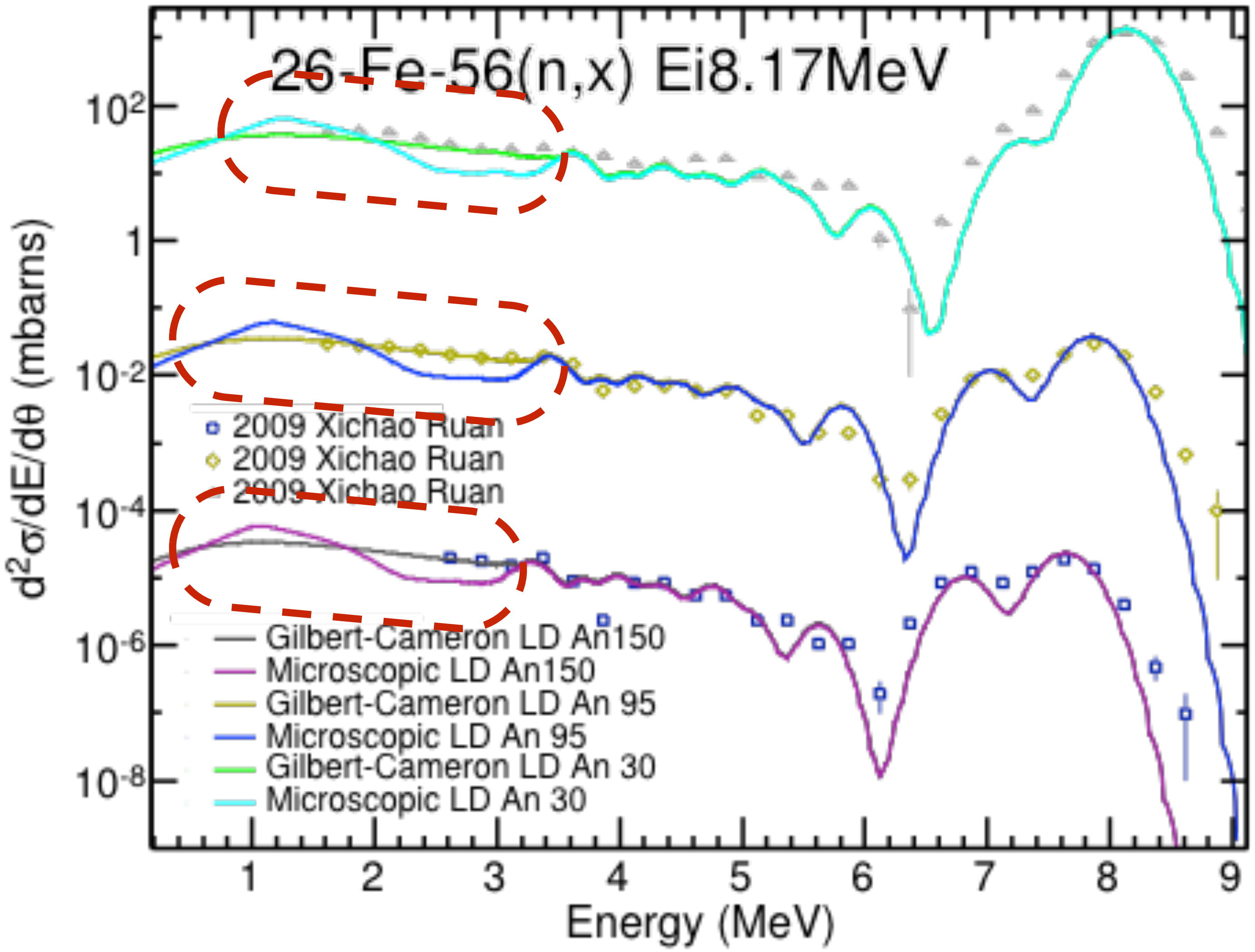
Improved α production

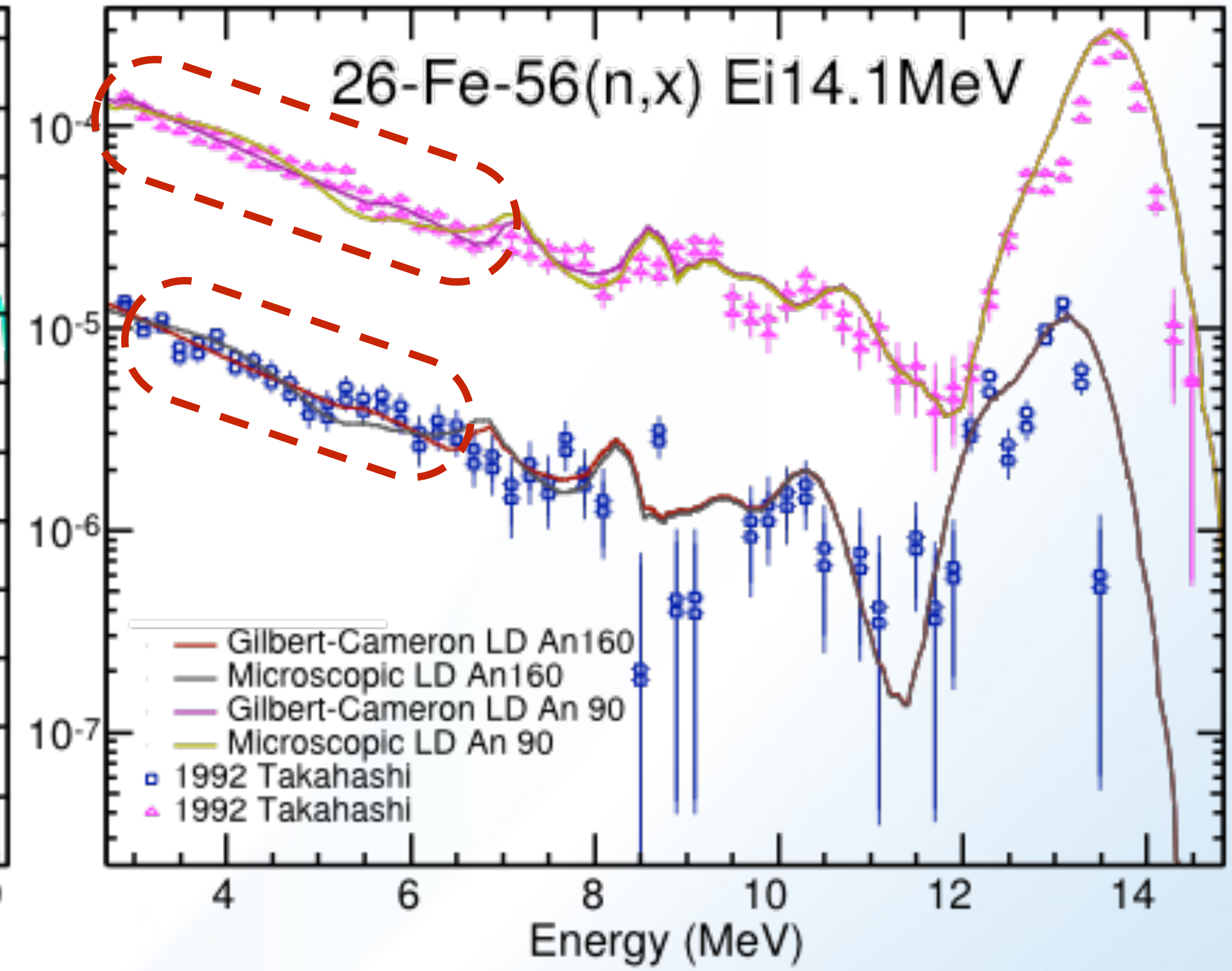


Agreement of (n,α) with JEFF

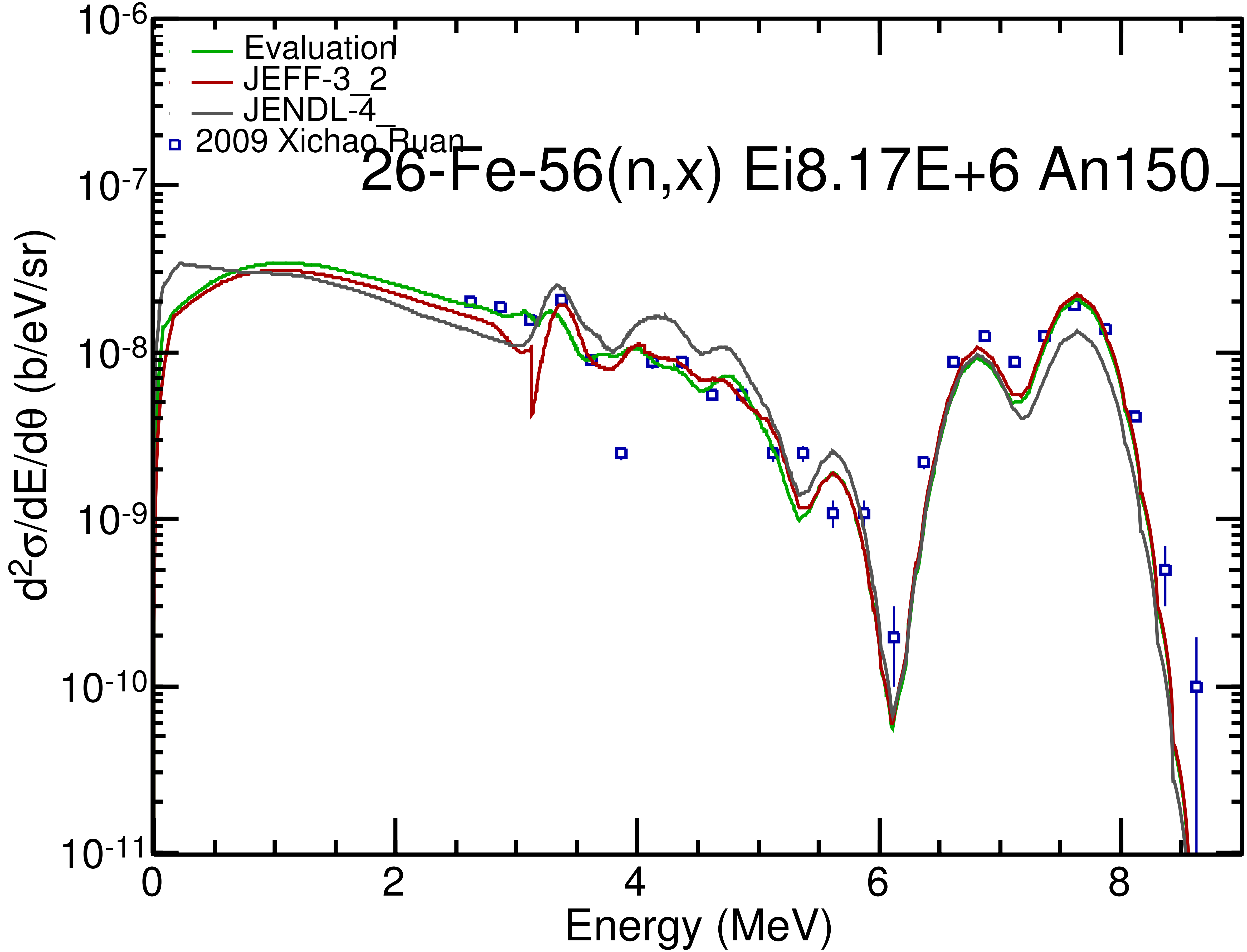


Double-differential spectra

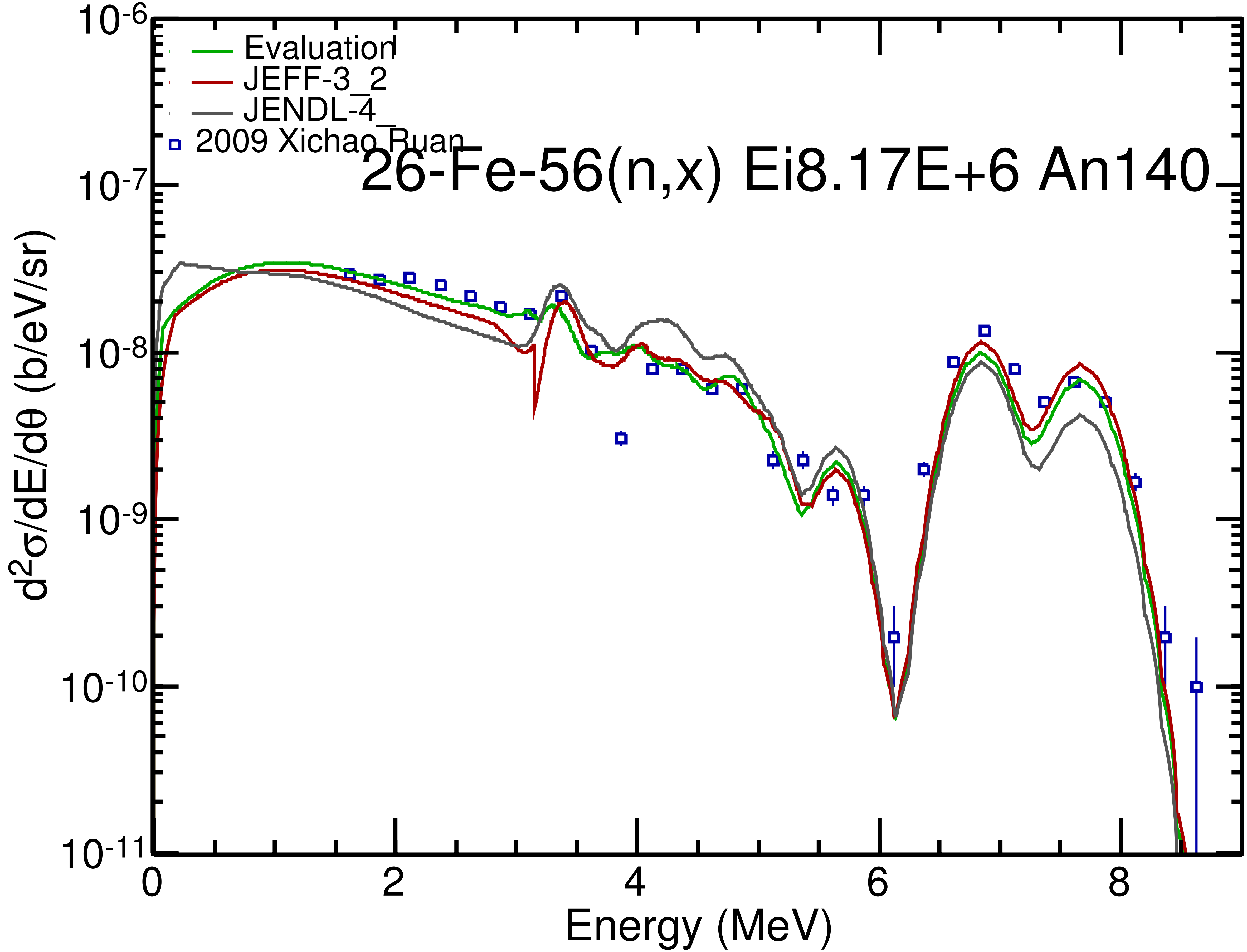




Improved non-physical oscillation of double-differential spectra at low energies!



26-Fe-56(n,x) Ei8.17E+6 An150
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
$d^2\sigma/dE/d\theta$ (b/eV/sr)
Energy (MeV)
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
0
2
4
6
8



26-Fe-56(n,x) Ei8.17E+6 An140
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
$d^2\sigma/dE/d\theta$ (b/eV/sr)
Energy (MeV)
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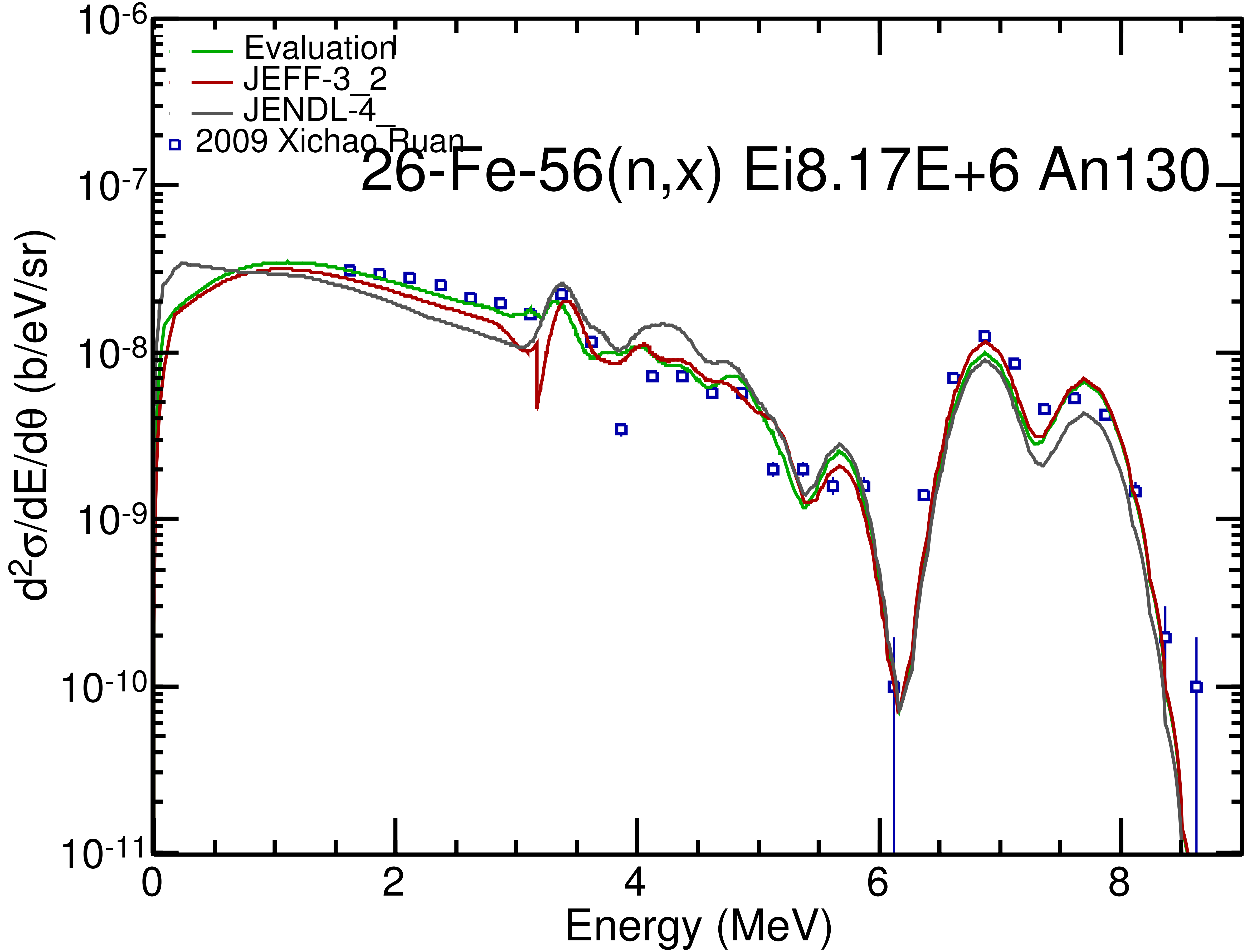
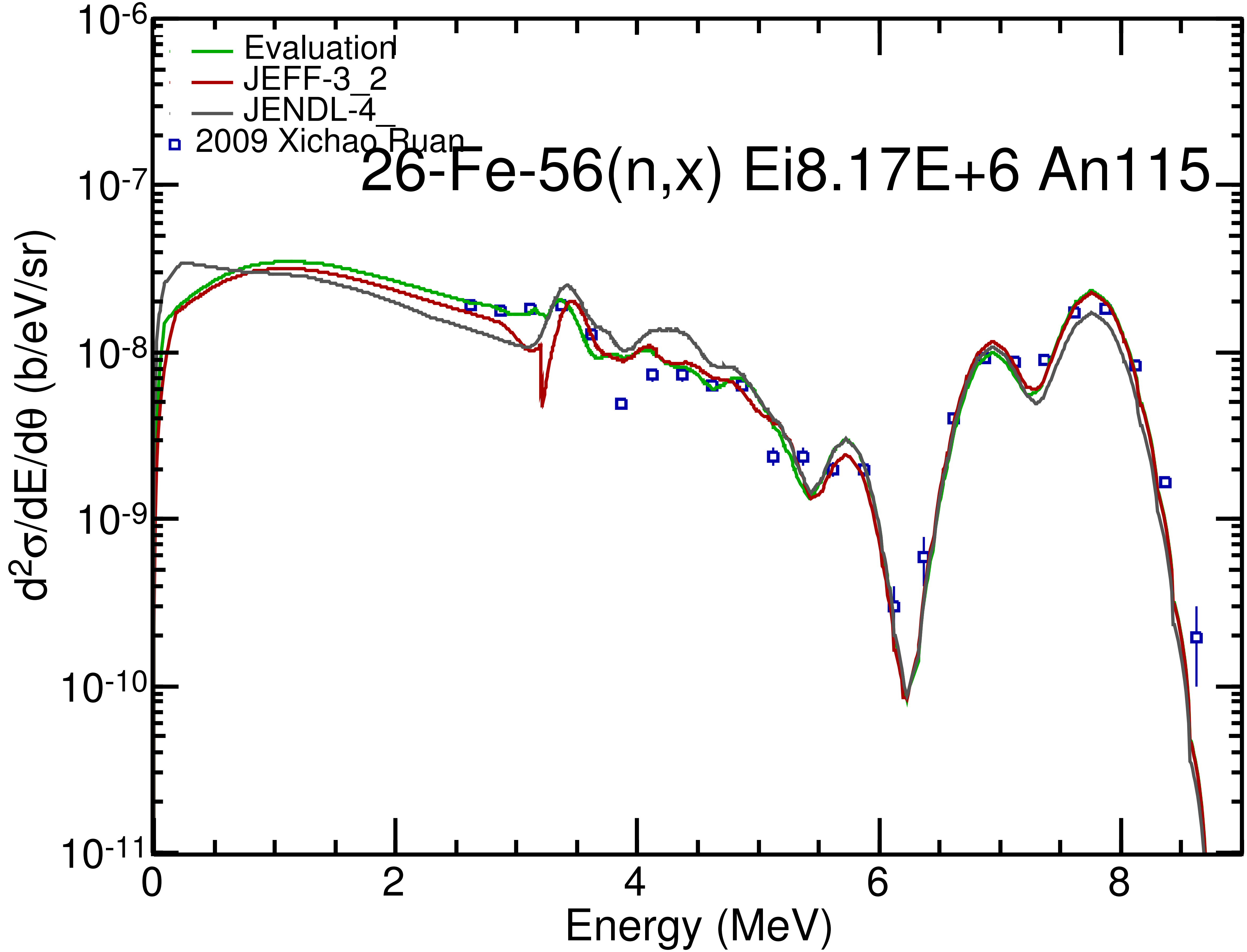
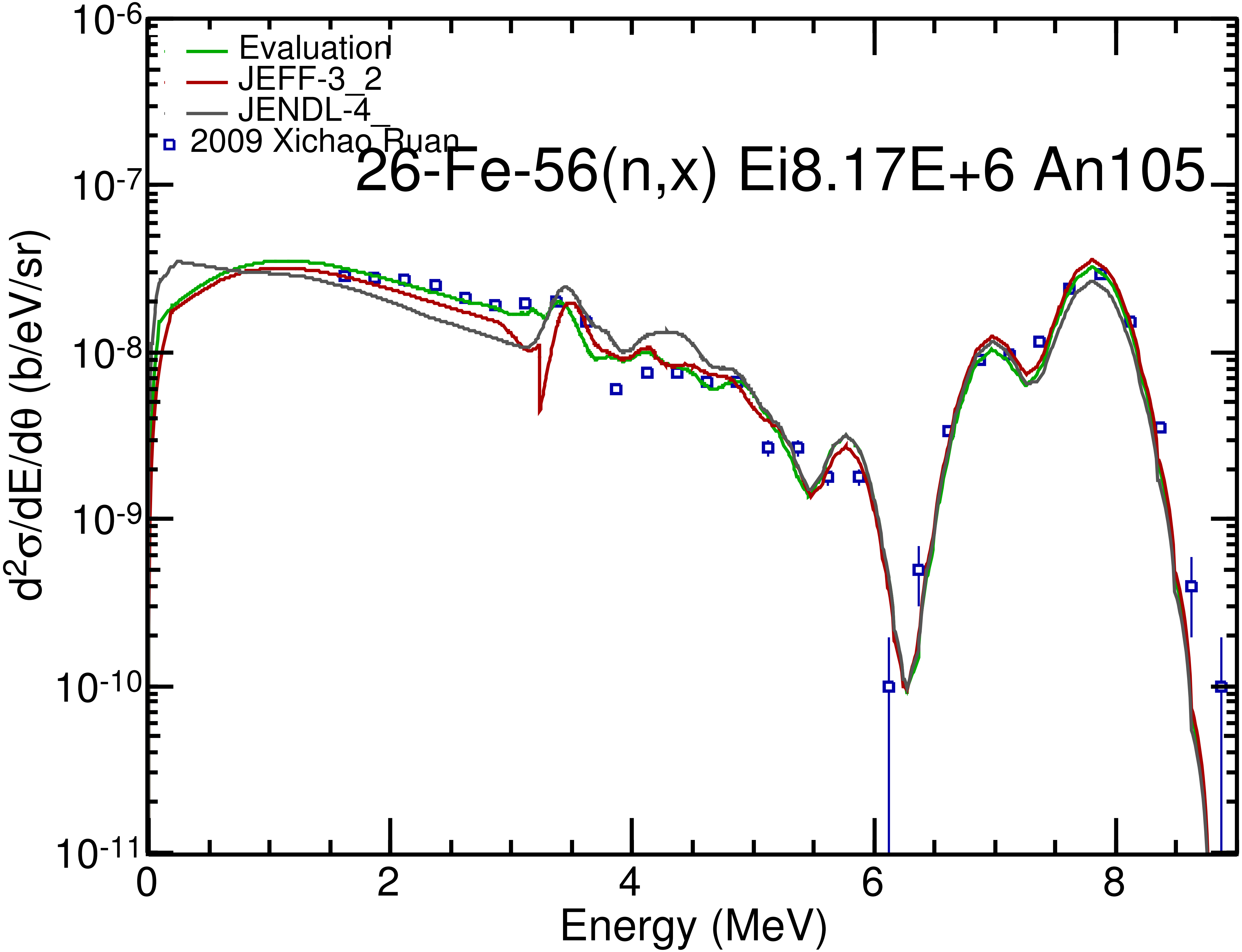
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
0
2
4
6
8



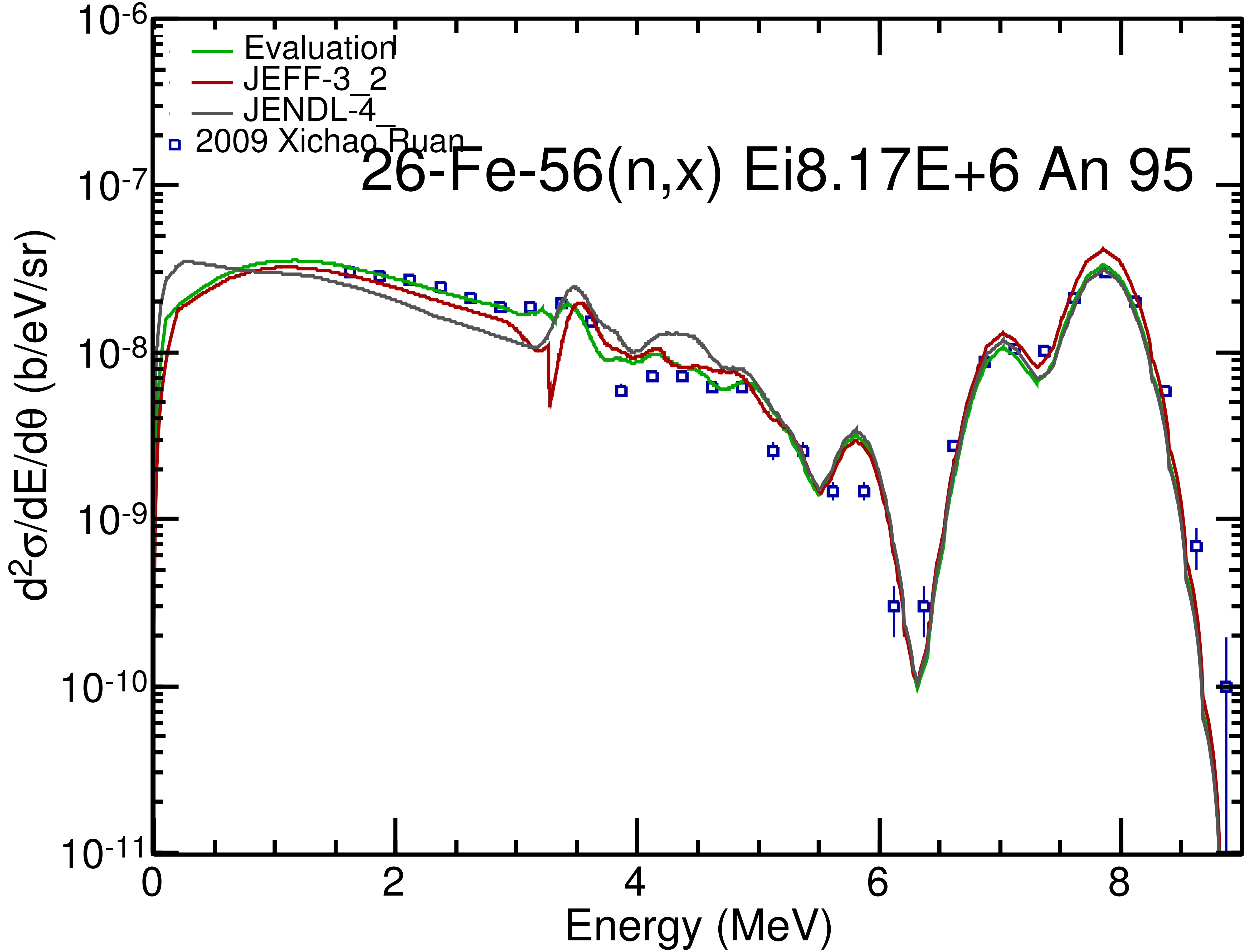
26-Fe-56(n,x) Ei8.17E+6 An130
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao_Ruan
$d^2\sigma/dE/d\theta$ (b/eV/sr)
Energy (MeV)
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
0
2
4
6
8



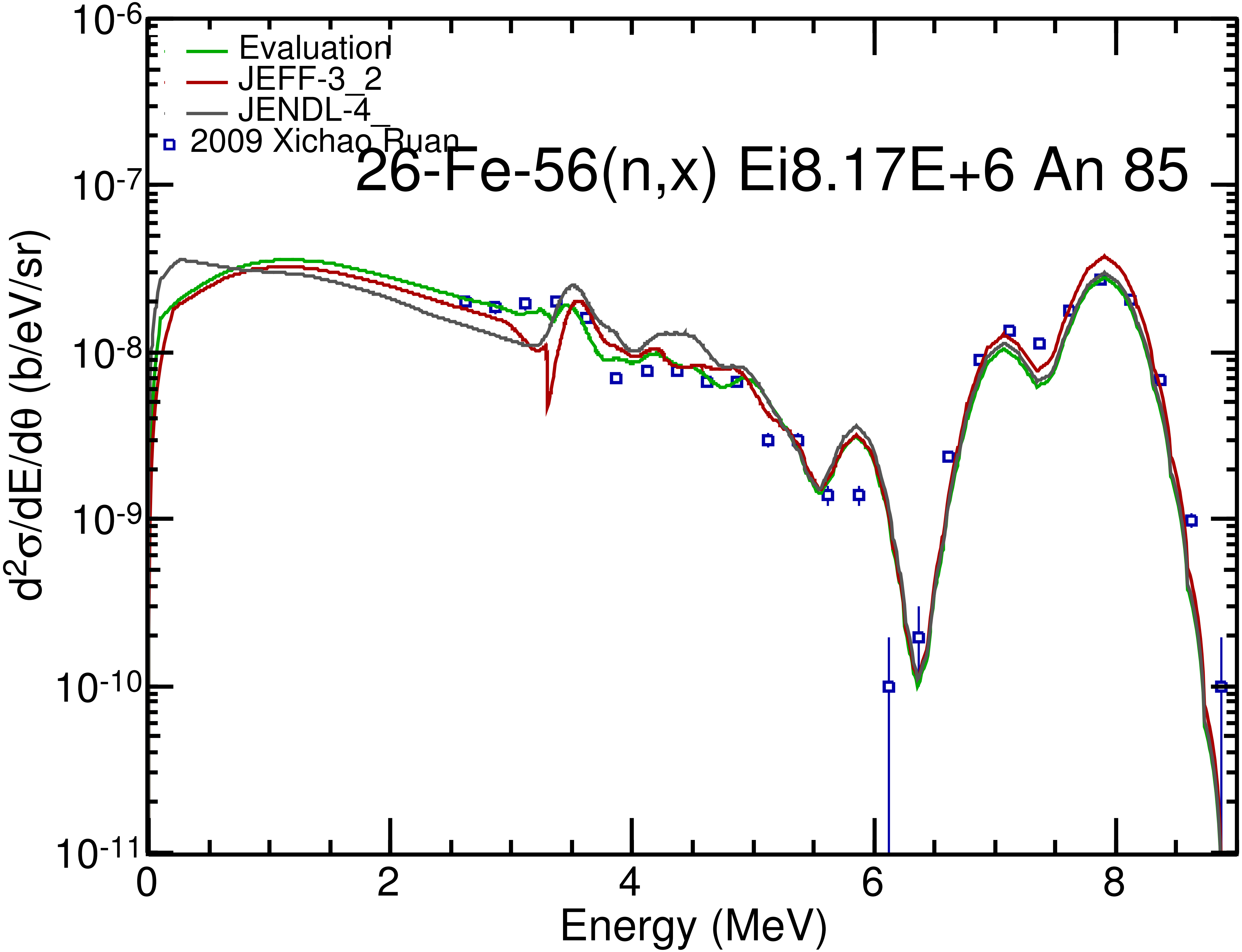
26-Fe-56(n,x) Ei8.17E+6 An115
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
$d^2\sigma/dE/d\theta$ (b/eV/sr)
Energy (MeV)
10-6
10-7
10-8
10-9
10-10
10-11
0
2
4
6
8



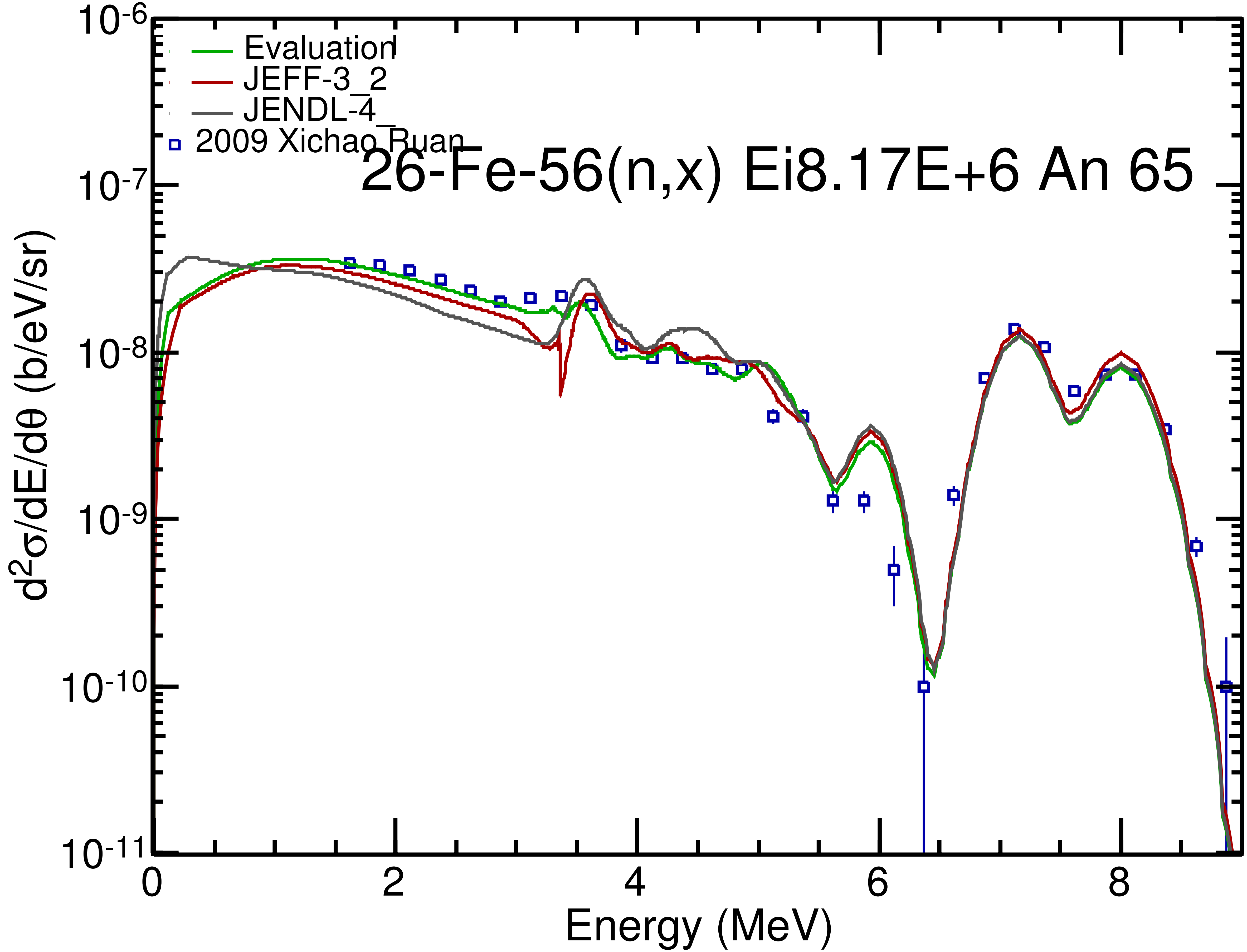
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
26-Fe-56(n,x) Ei8.17E+6 An105
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
$d^2\sigma/dE/d\theta$ (b/eV/sr)
0
2
4
6
8
Energy (MeV)



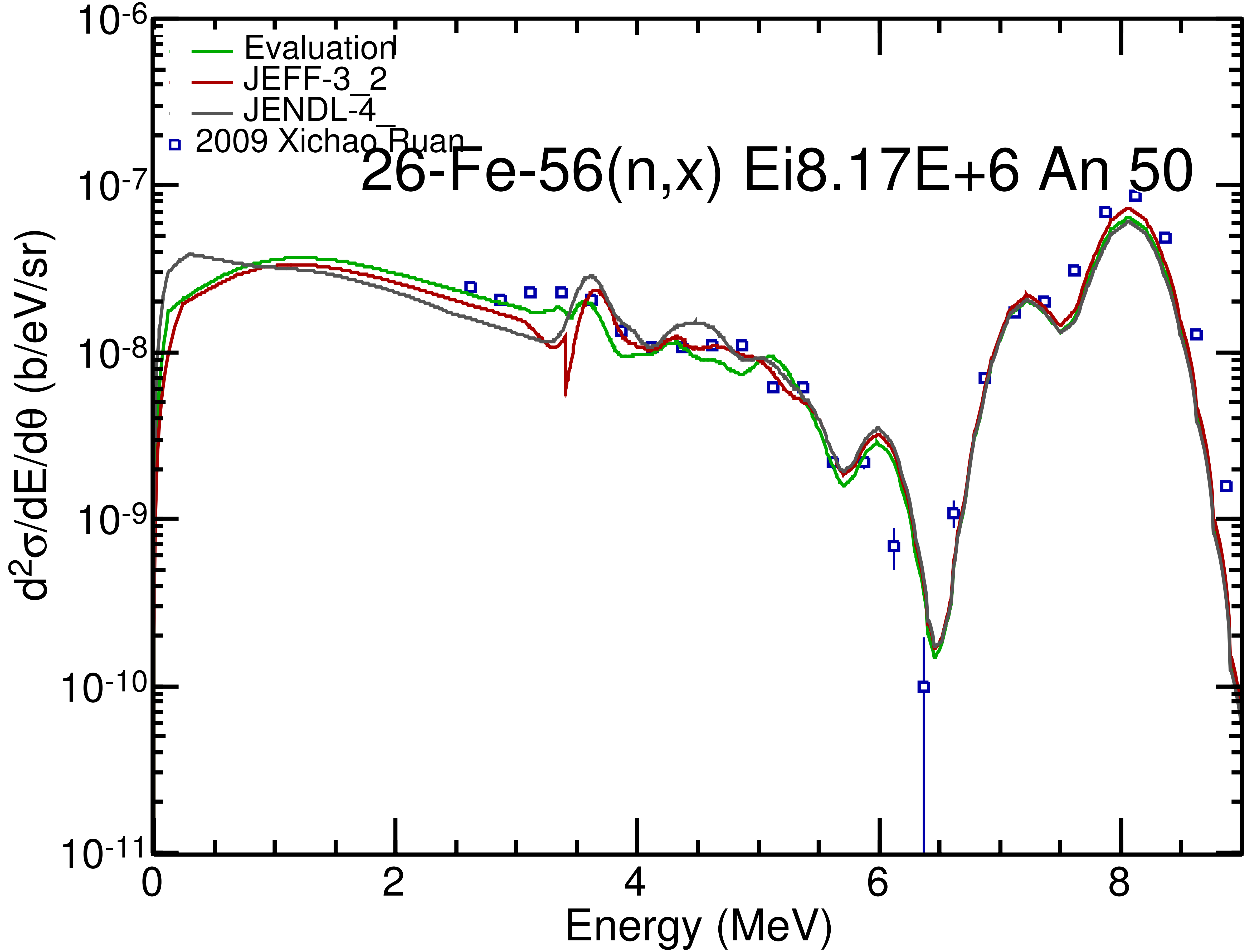
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
26-Fe-56(n,x) Ei8.17E+6 An 95
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
$d^2\sigma/dE/d\theta$ (b/eV/sr)
0
2
4
6
8
Energy (MeV)



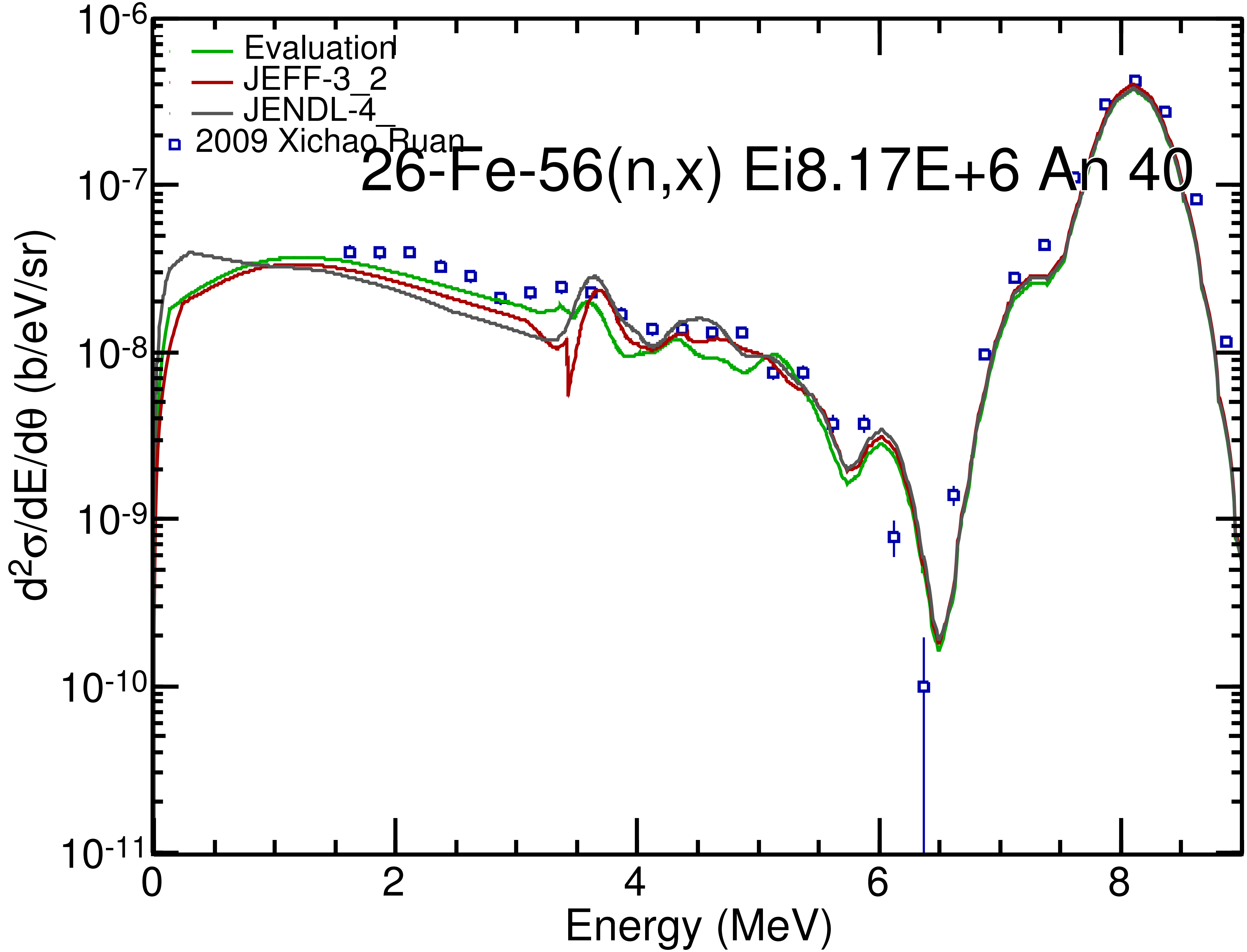
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao_Ruan
26-Fe-56(n,x) Ei8.17E+6 An 85
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
$d^2\sigma/dE/d\theta$ (b/eV/sr)
0
2
4
6
8
Energy (MeV)



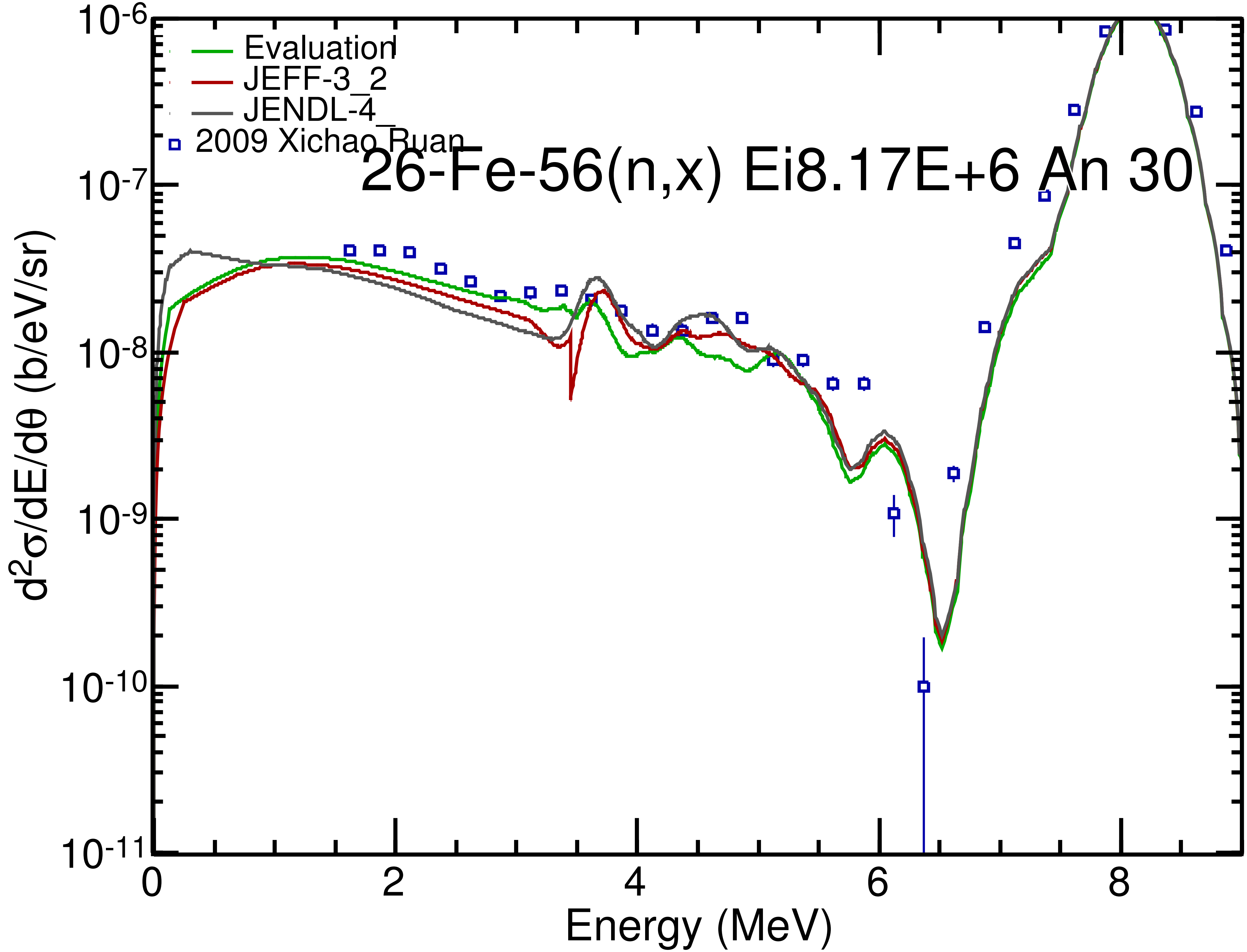
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
26-Fe-56(n,x) Ei8.17E+6 An 65
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
$d^2\sigma/dE/d\theta$ (b/eV/sr)
0
2
4
6
8
Energy (MeV)



Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
26-Fe-56(n,x) Ei8.17E+6 An 50
$d^2\sigma/dE/d\theta$ (b/eV/sr)
Energy (MeV)
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
0
2
4
6
8



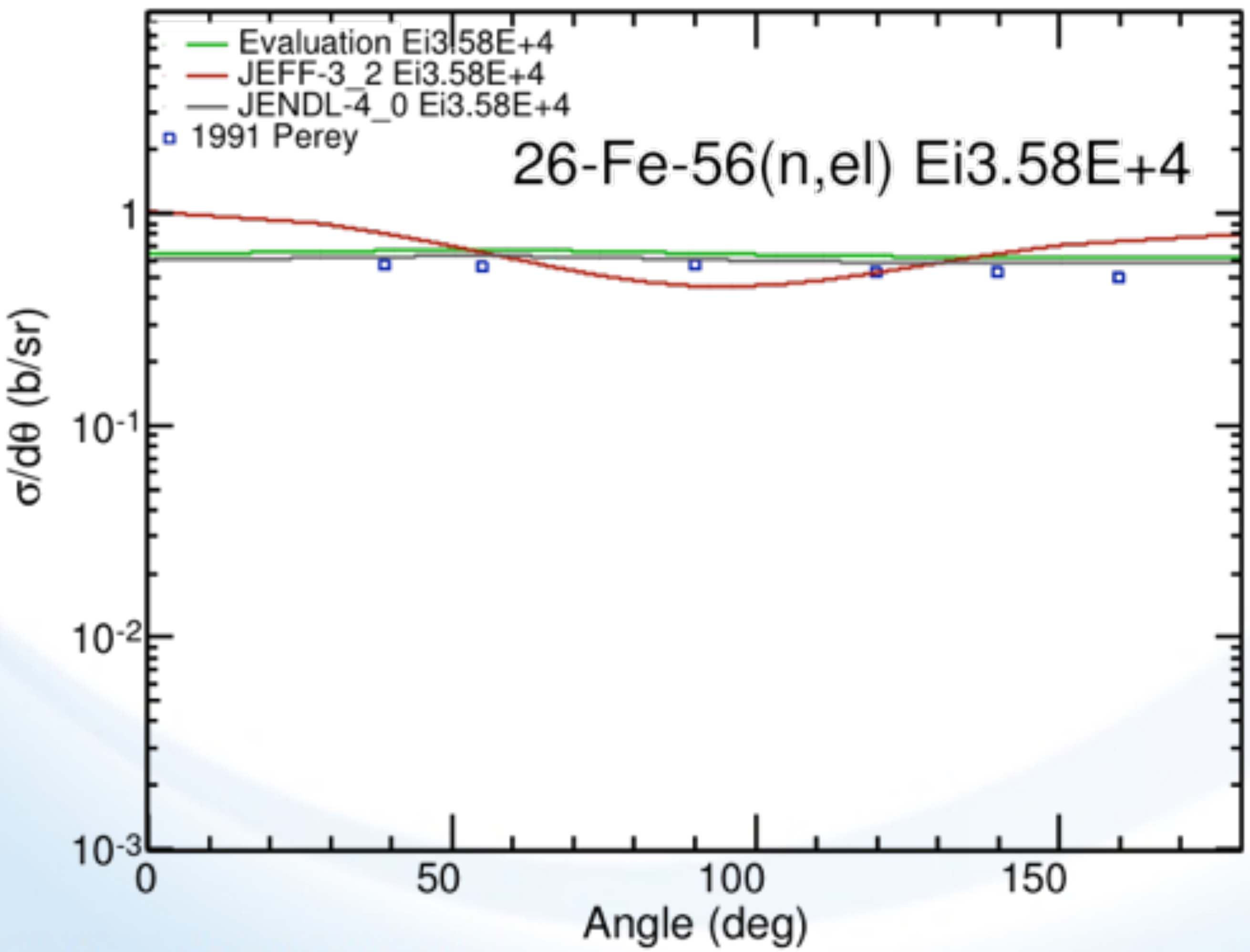
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
26-Fe-56(n,x) Ei8.17E+6 An 40
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
$d^2\sigma/dE/d\theta$ (b/eV/sr)
0
2
4
6
8
Energy (MeV)

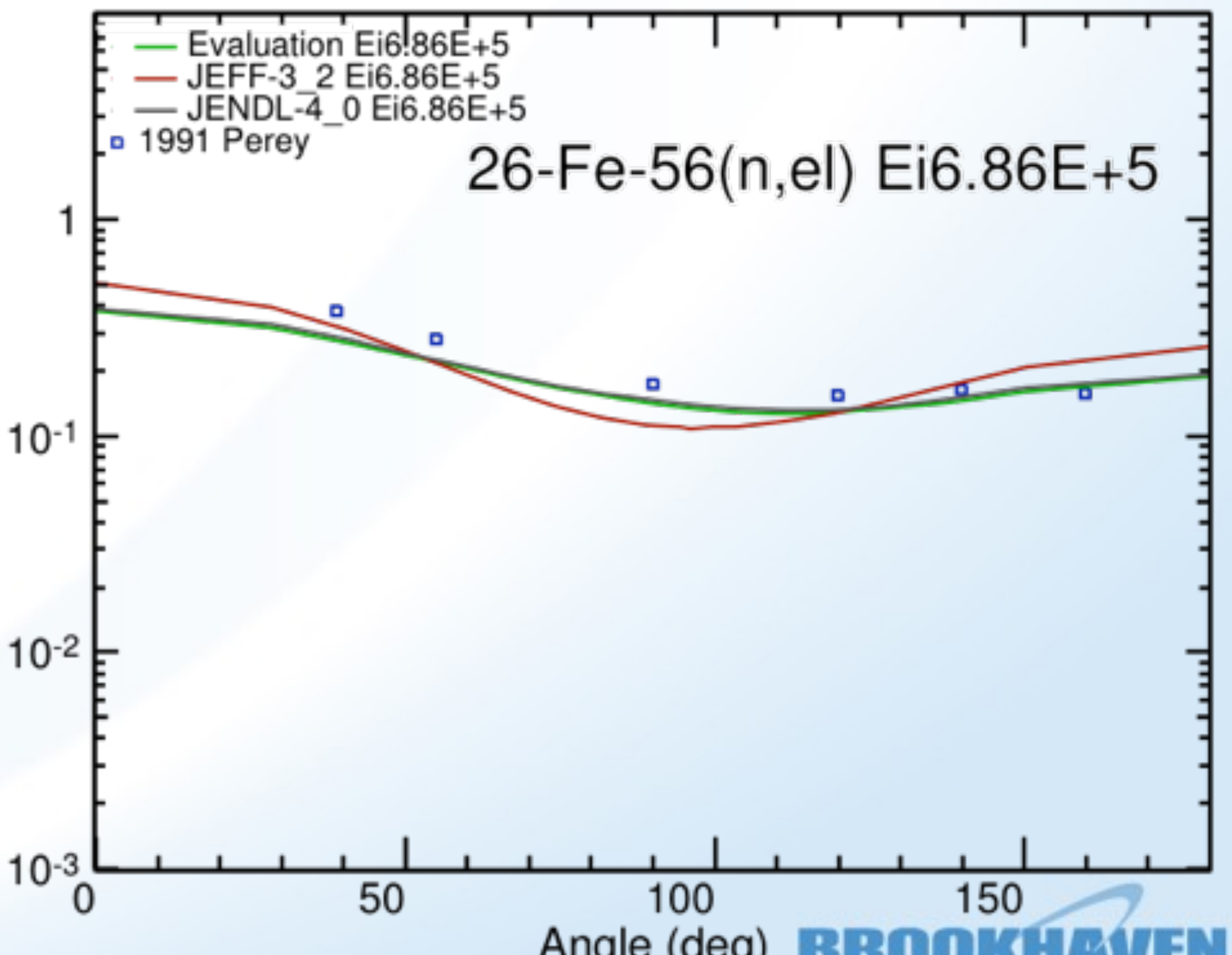


26-Fe-56(n,x) Ei8.17E+6 An 30
Evaluation
JEFF-3_2
JENDL-4_
2009 Xichao Ruan
d²σ/dE/dθ (b/eV/sr)
Energy (MeV)
10-6
10-7
10-8
10-9
10-10
10-11
0
2
4
6
8

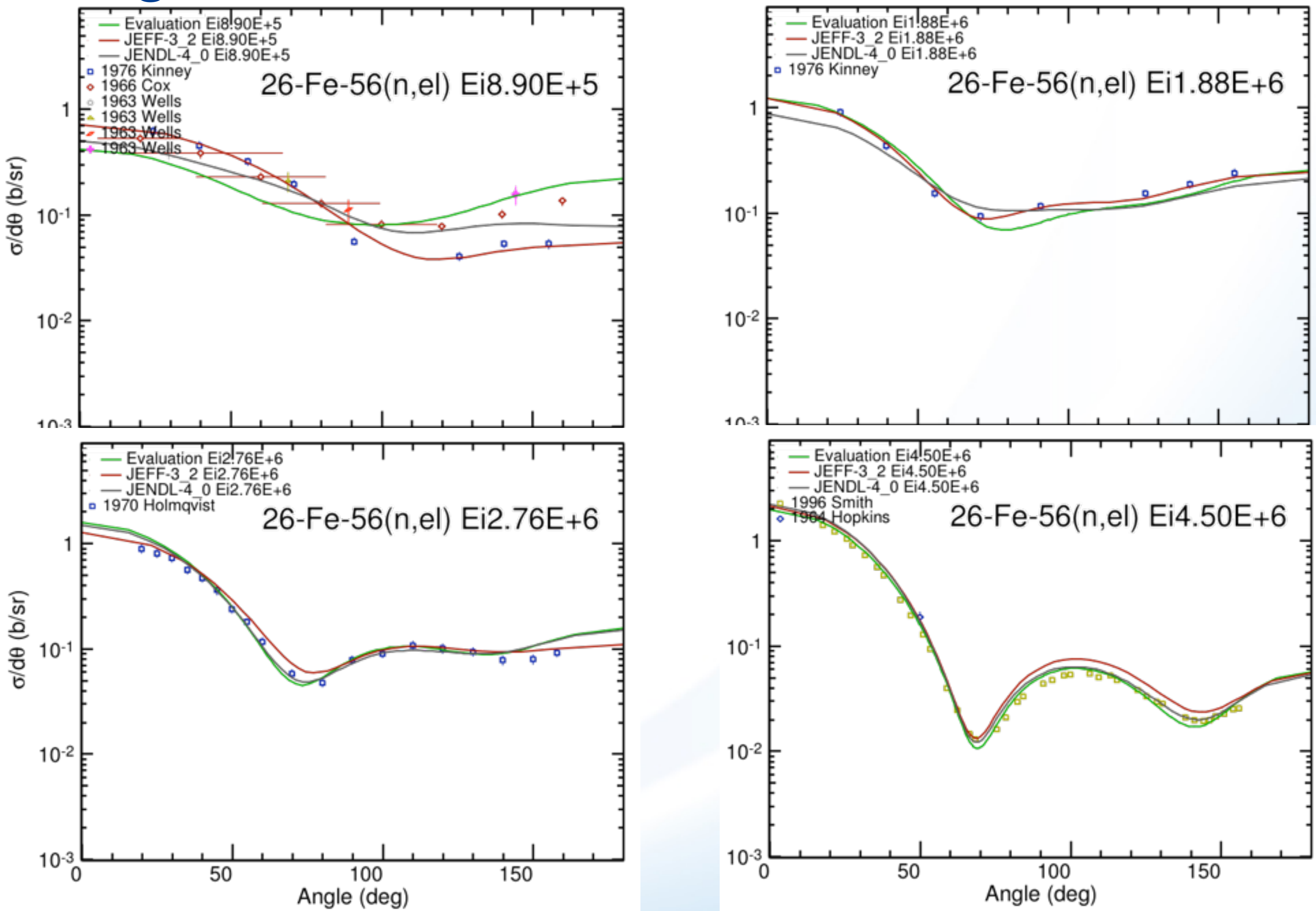
Angular distributions

- HUGE amount of experimental data: 2824 plots!
- Some examples…
- Comparison with JEFF and JENDL

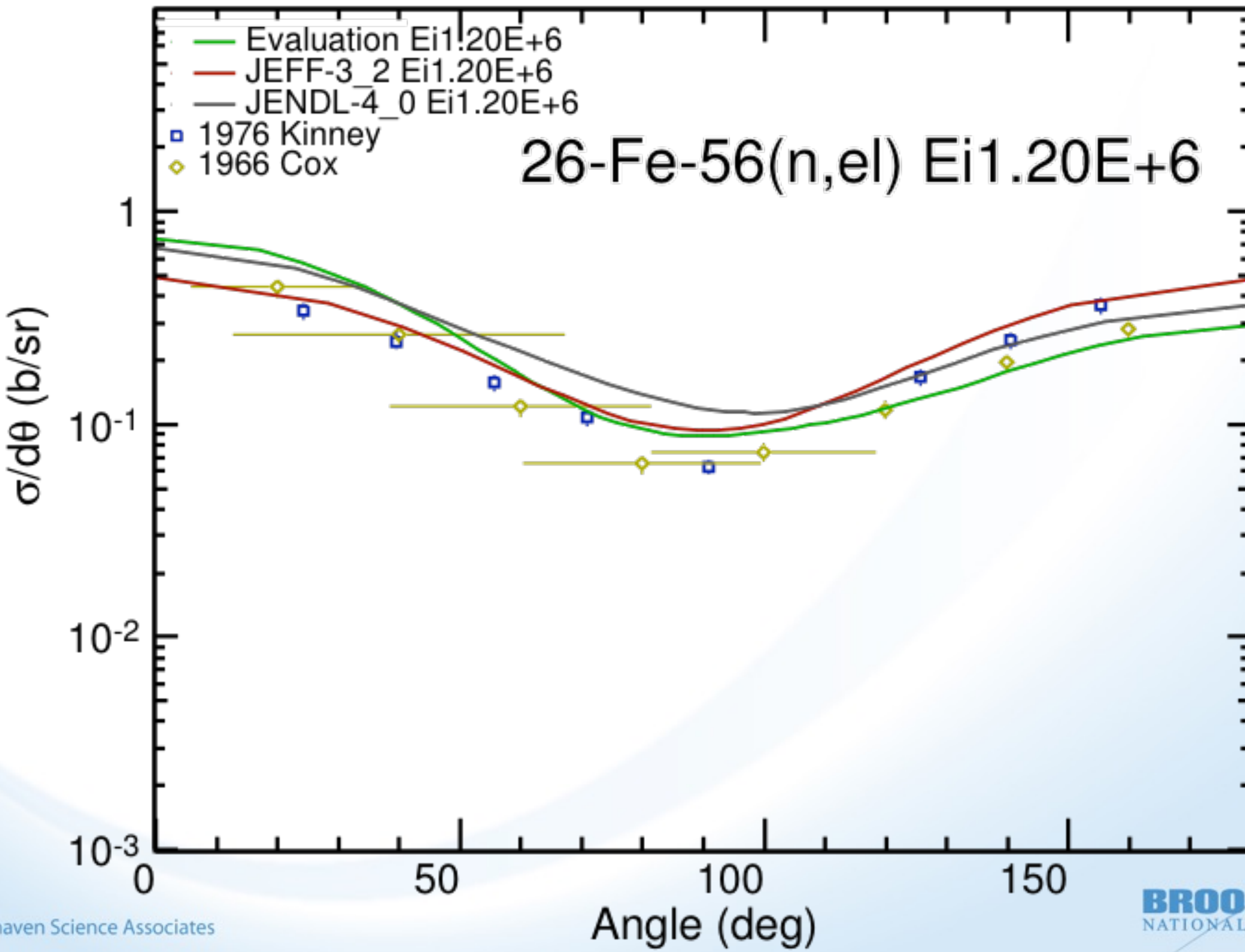




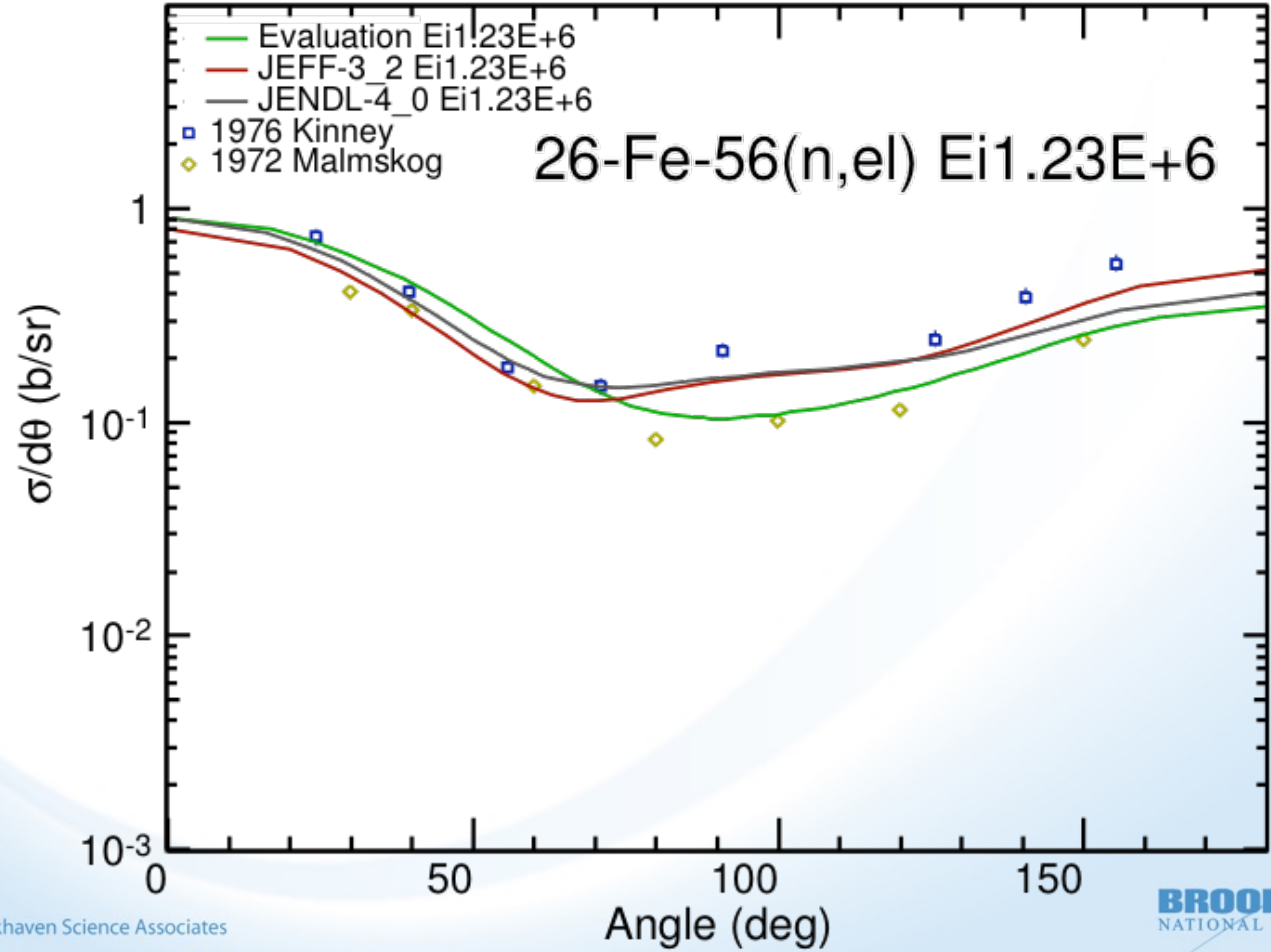
Angular distributions



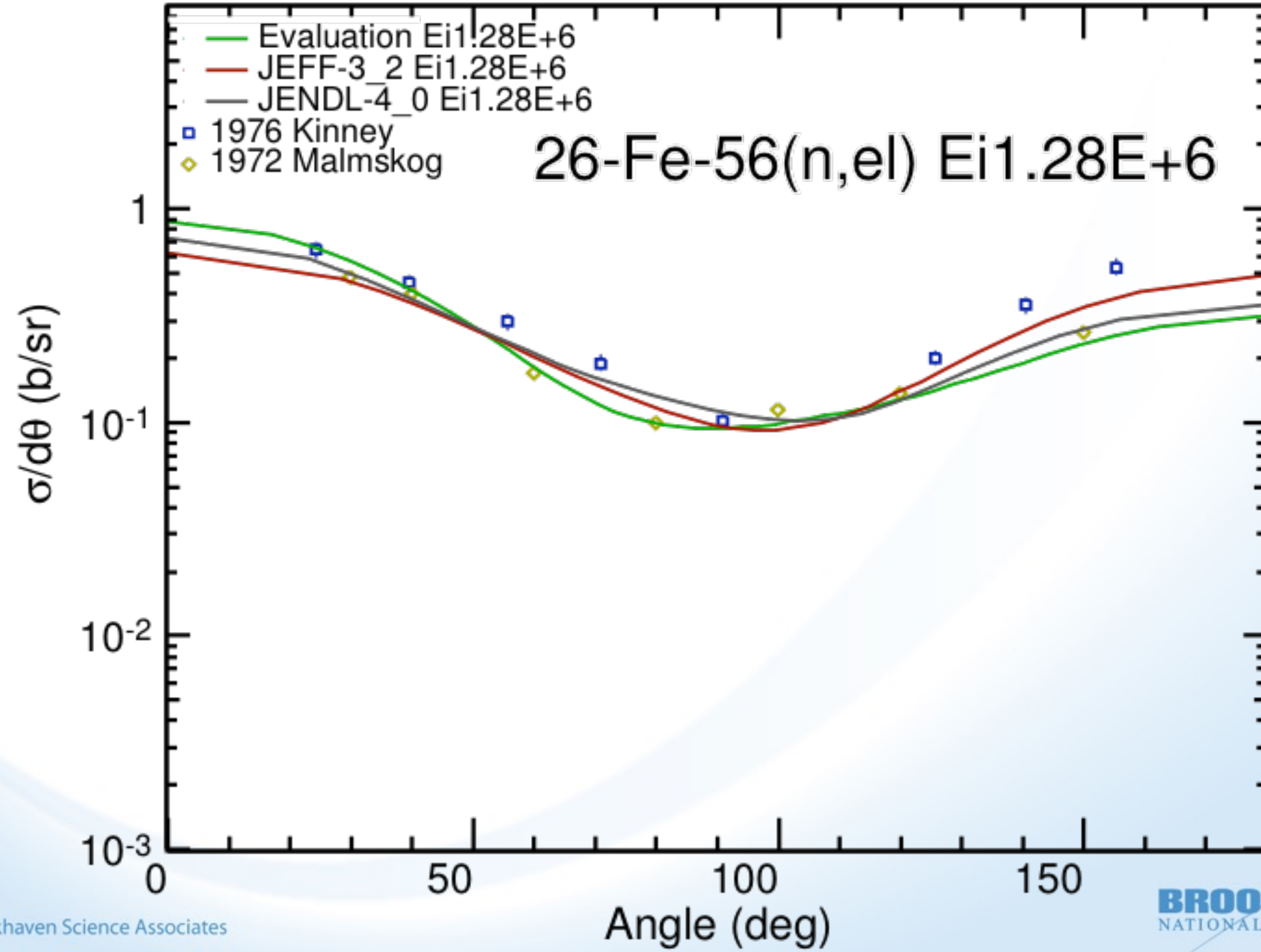
Angular distributions – Kinney data



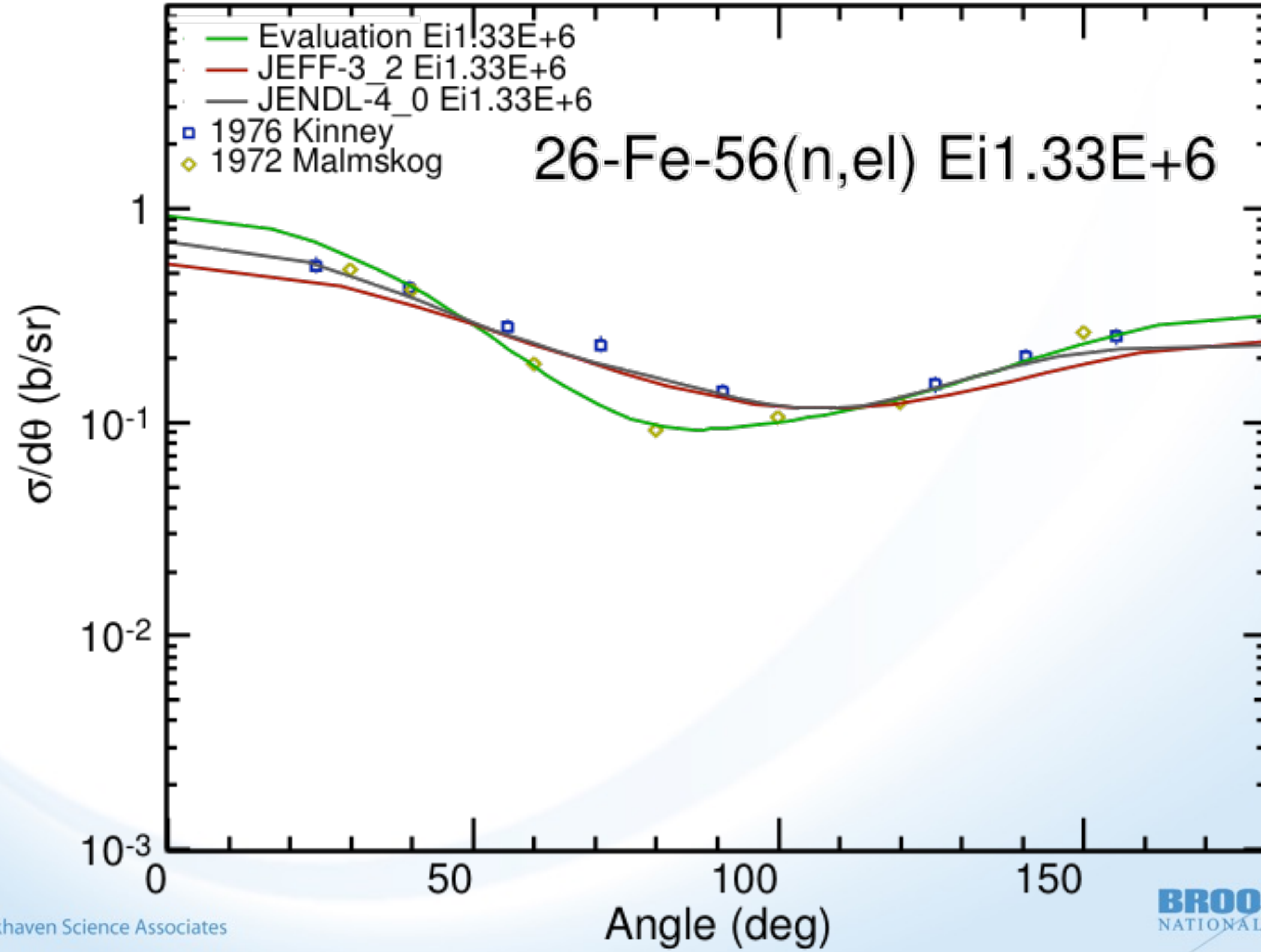
Angular distributions – Kinney data



Angular distributions – Kinney data



Angular distributions – Kinney data



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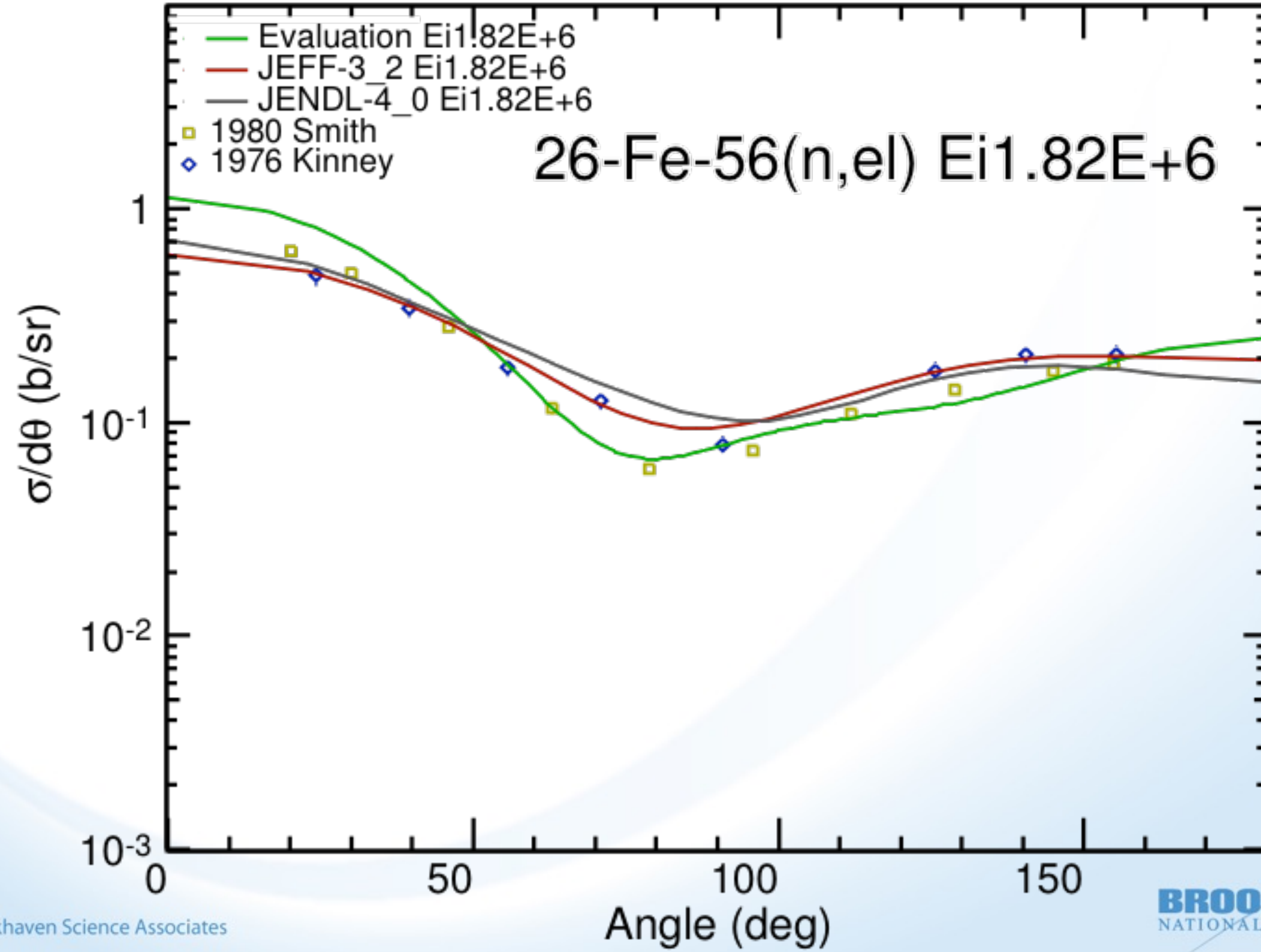
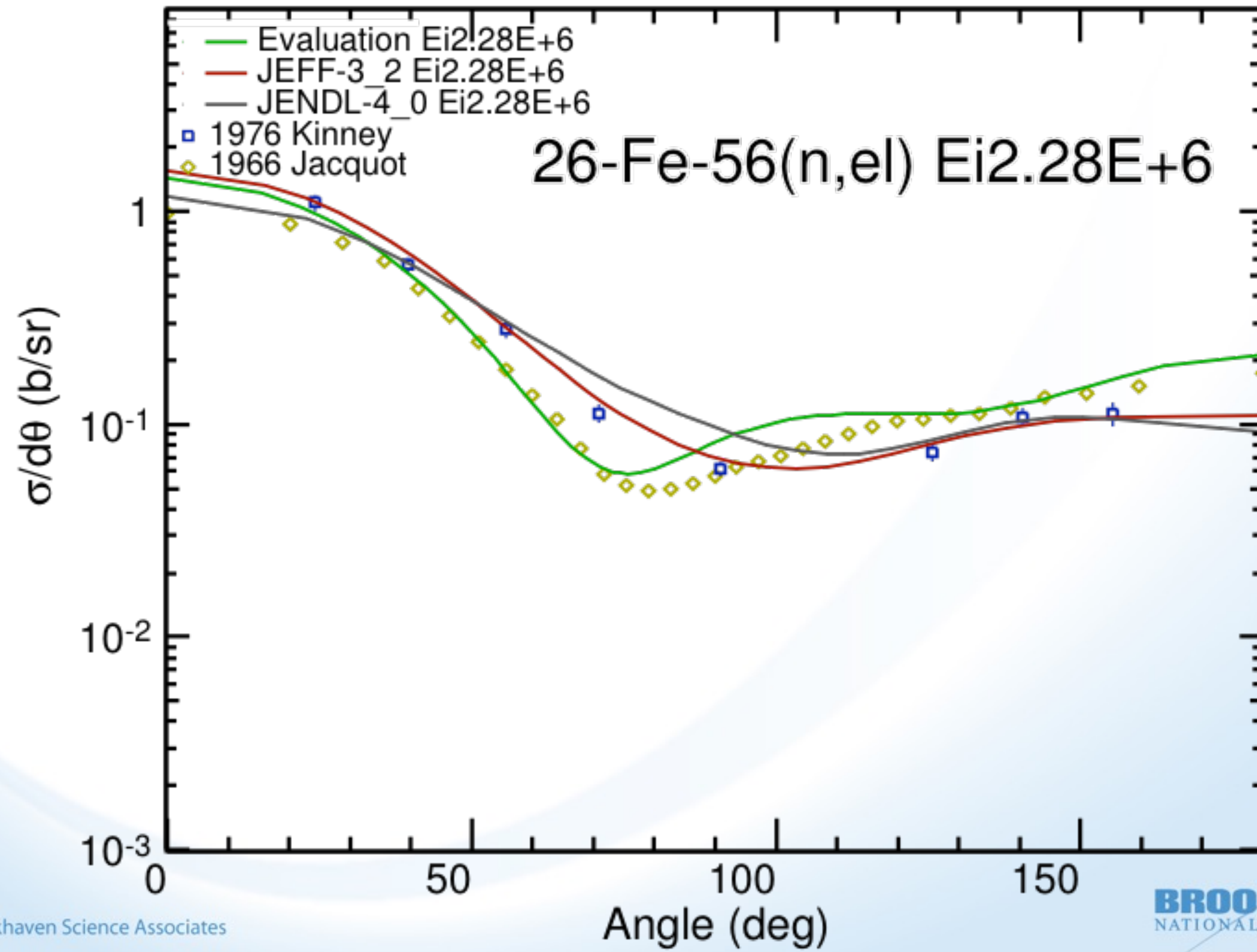
Angular distributions – Kinney data



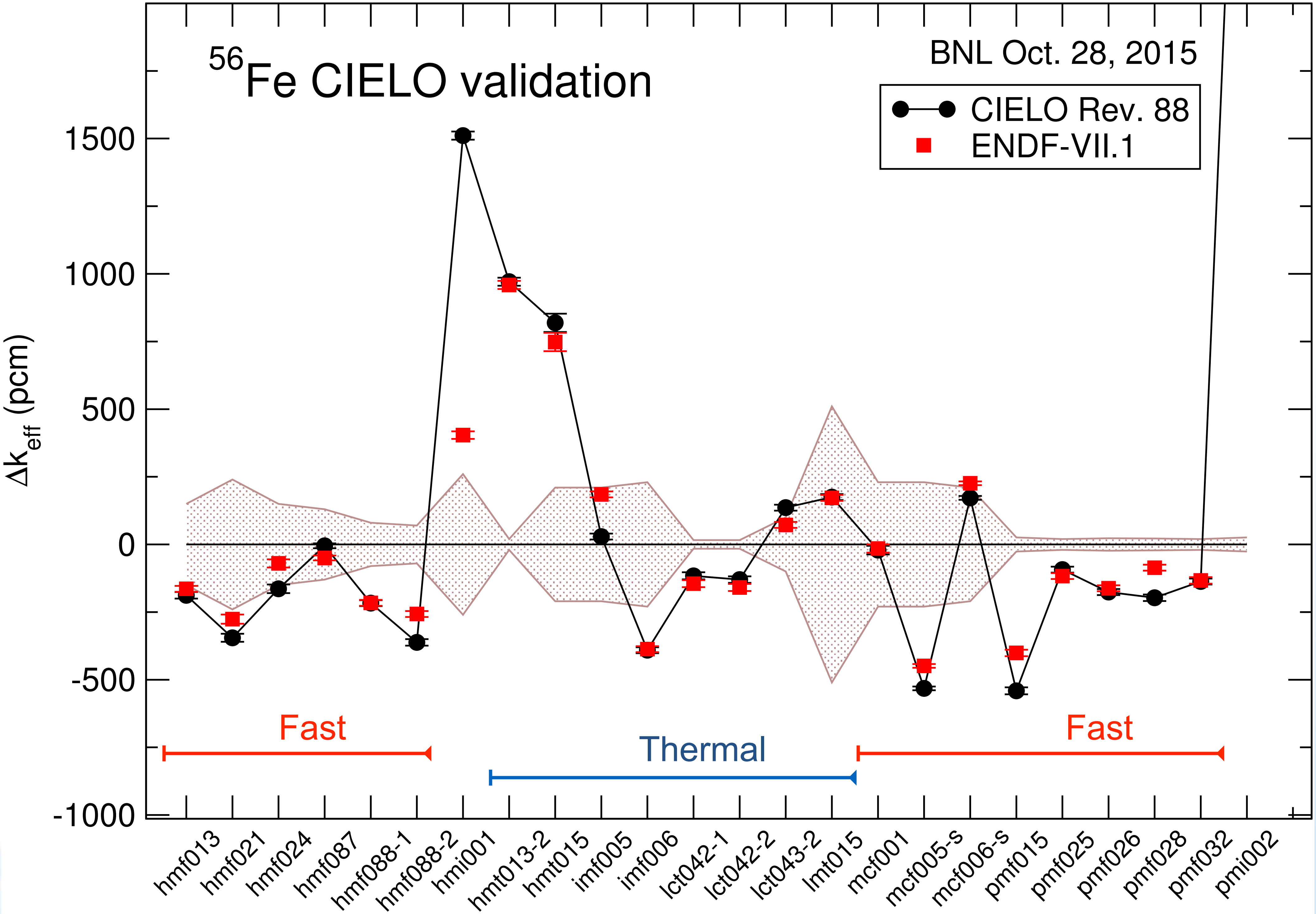
Angular distributions – Kinney data



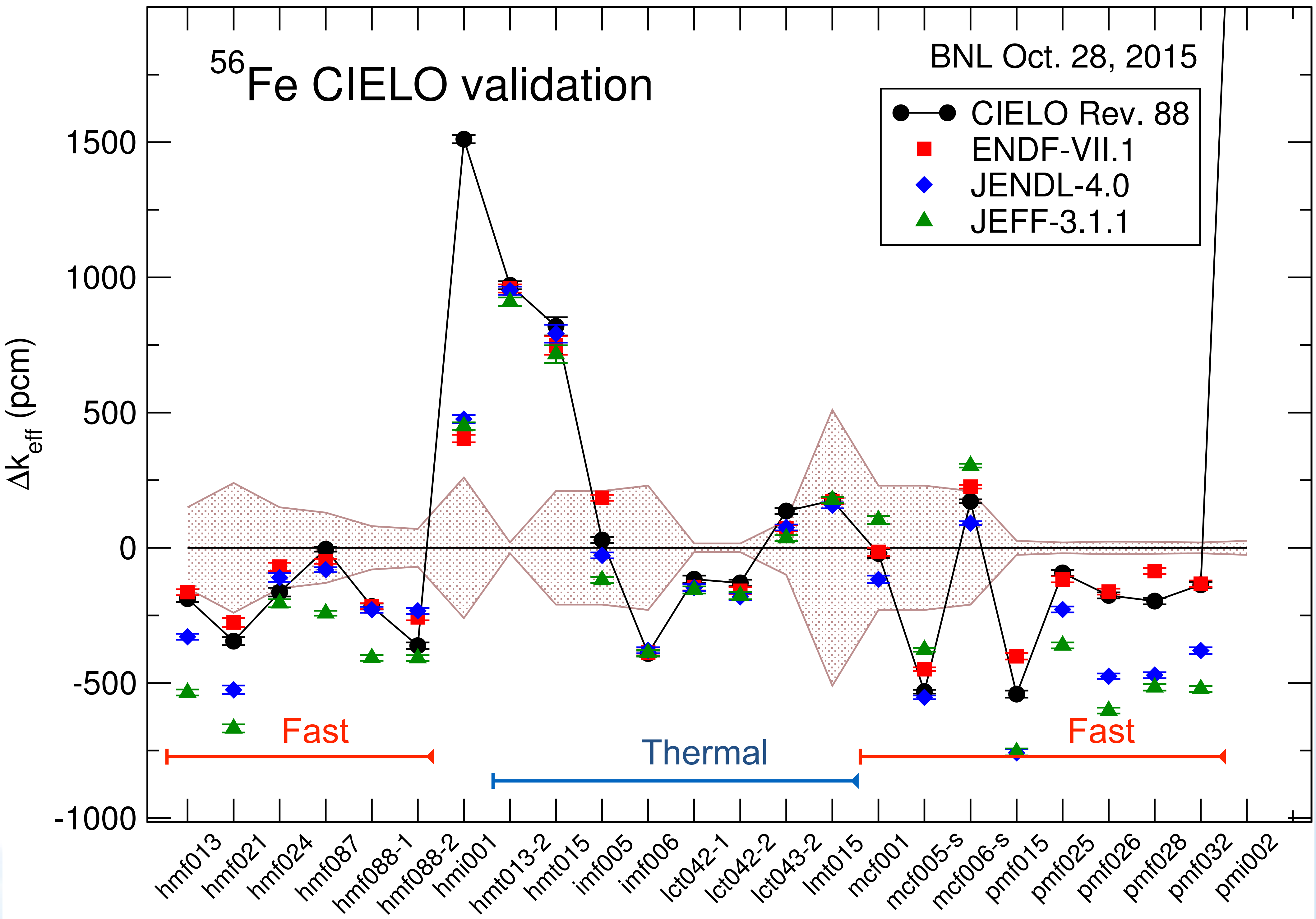
Elastic angular distributions

- Kinney data are the most extensive and detailed above the inelastic threshold
- JEFF-3.1 ang. distr. are fitted to the Kinney data
- Whenever other experimental data are available they are closer to EMPIRE calculations than to Kinney
- These data are usually taken with lower energy resolution than Kinney's

Validation
CIELO rev.88 versus ENDF/B-VII.1



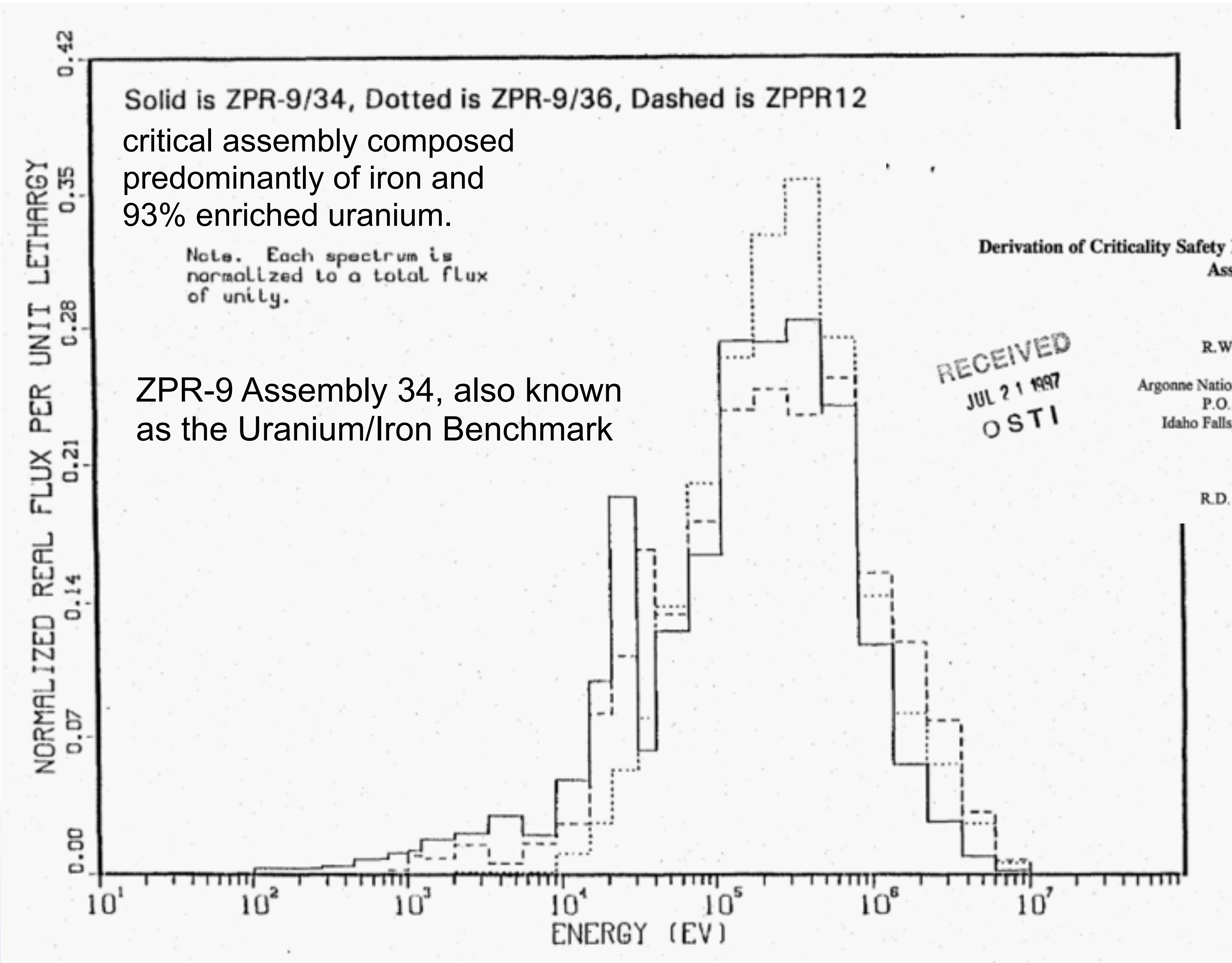
Comparison with JEFF-3.1.1 & JENDL-4.0



Neutron spectrum hmi01 = ZPR-9/34

critical assembly composed predominantly of iron and 93% enriched uranium.

ZPR-9 Assembly 34, also known as the Uranium/Iron Benchmark



ANL/ED/CP-93644
CONF-971125--

Derivation of Criticality Safety Benchmarks from ZPR Fast Critical Assemblies

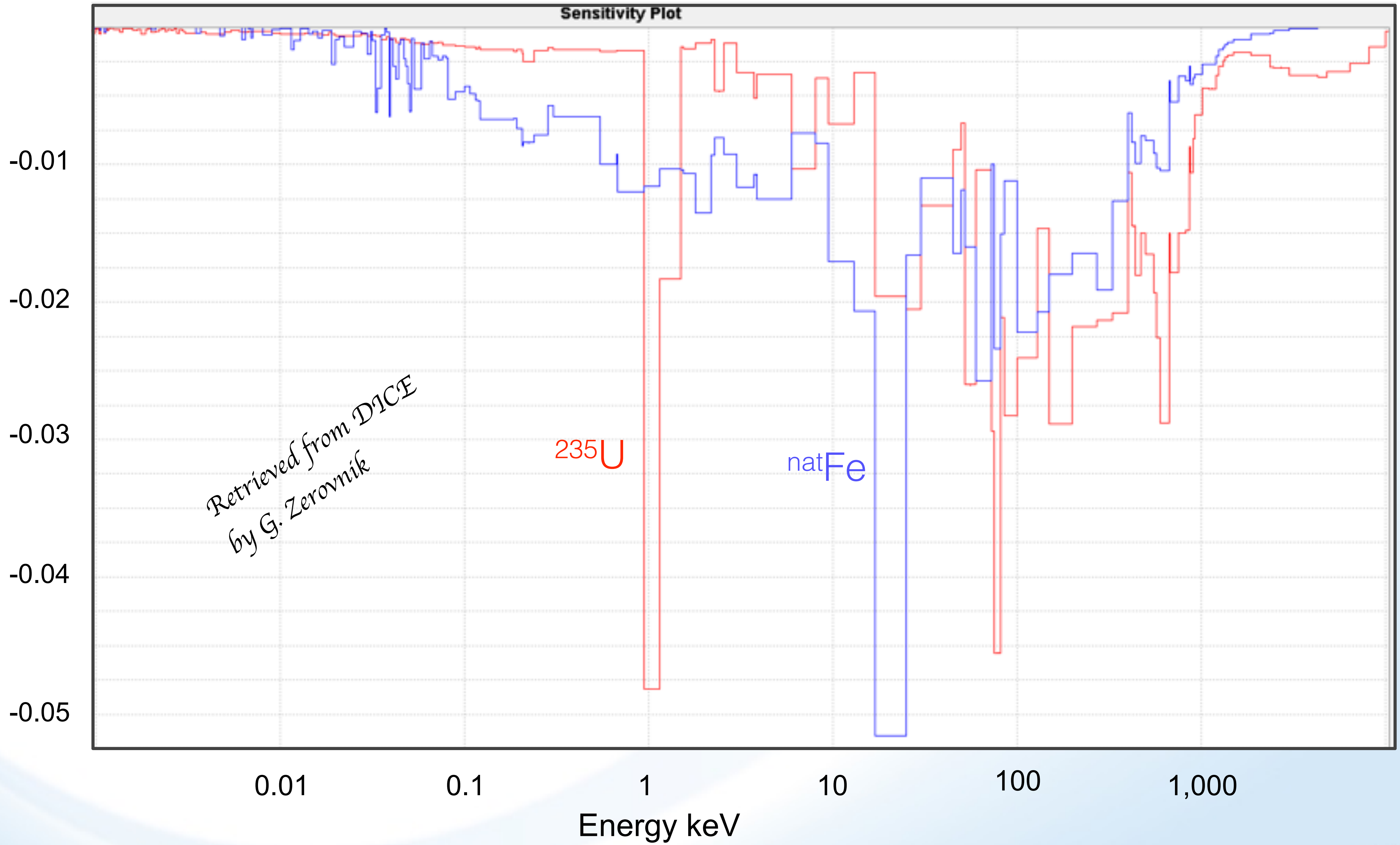
by

R.W. Schaefer
Argonne National Laboratory-West
P.O. Box 2528
Idaho Falls, ID 83403-2528

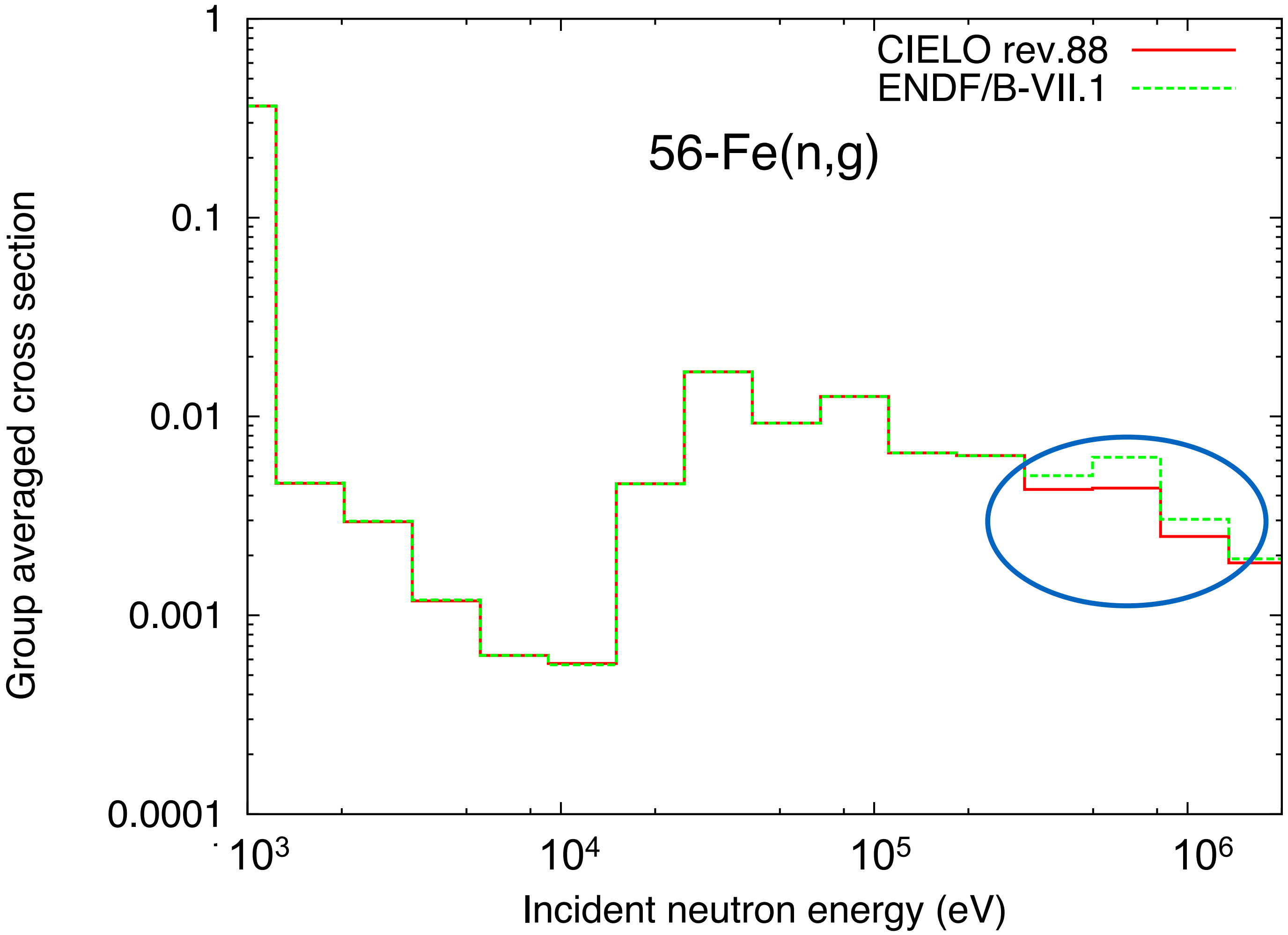
and

R.D. McKnight

Sensitivity of ZPR-9/34 (hmi001) to capture in U-235 and Fe-nat

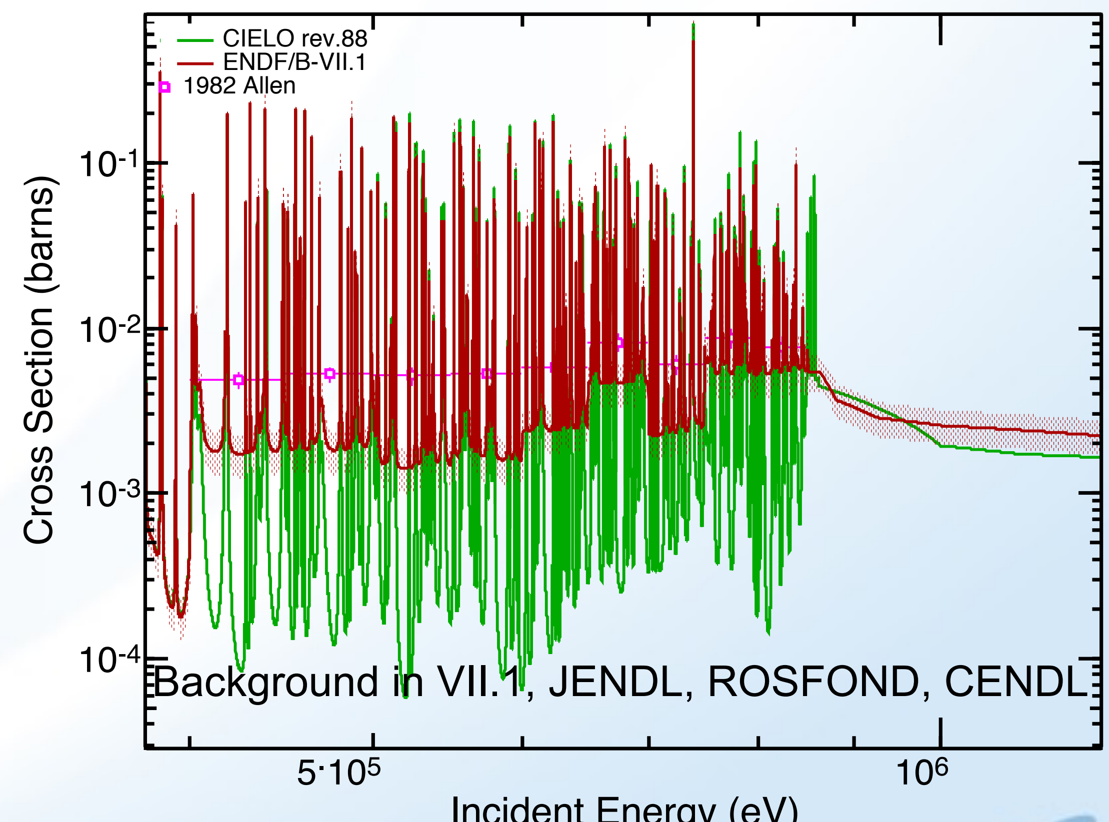


Capture in CIELO rev.88 & ENDF/B-VII.1



Capture in rev.88 lower than in ENDF/B-VII.1

Experimental data in the region do not constrain capture unambiguously



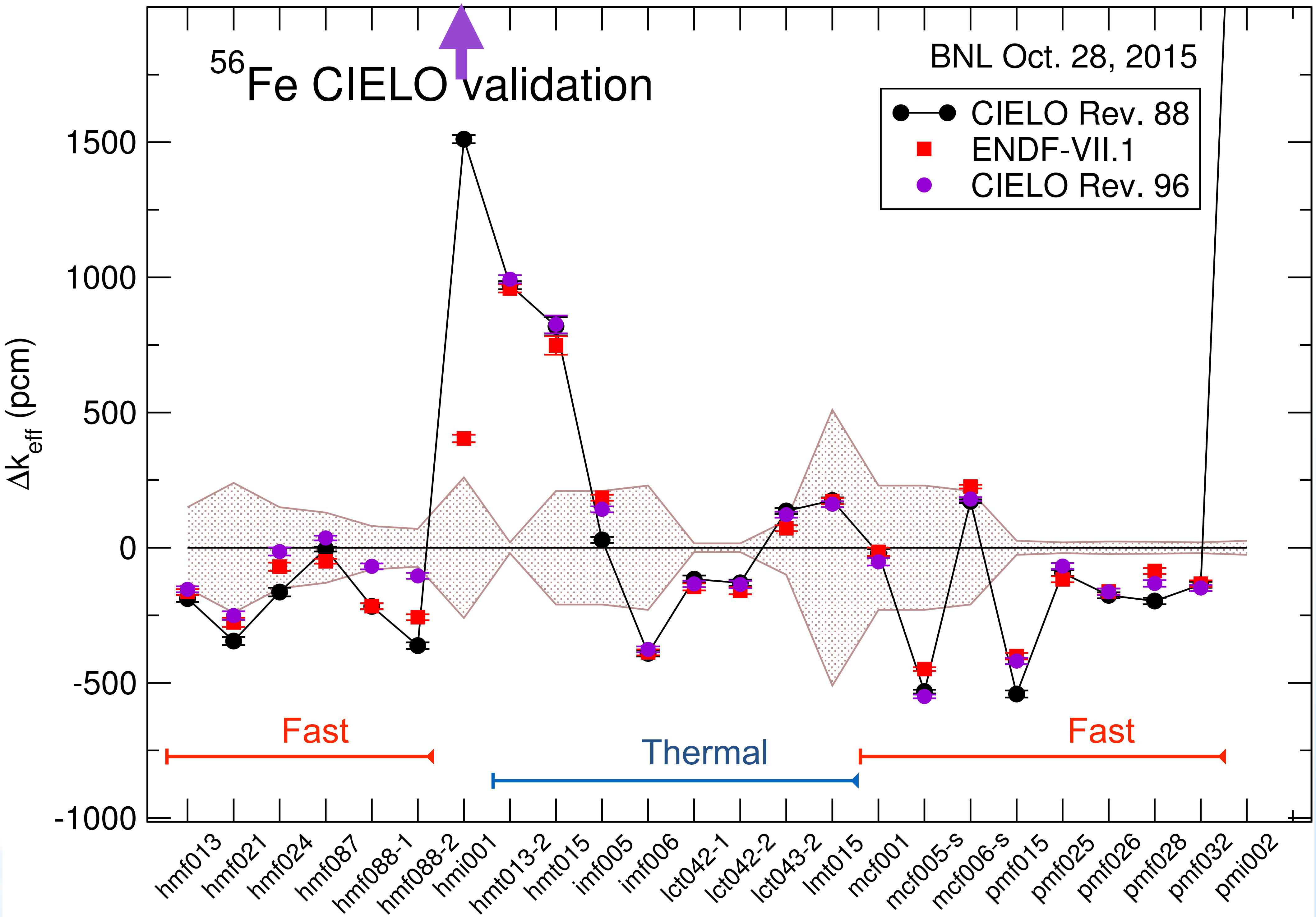
One could be tempted to revert to VII.1 but…

EGAF thermal

Atlas:	2.59(14)
EGAF:	**2.71**(4)
CIELO r88:	2.59067
ENDF/B-VII.1:	2.58936
ENDF/B-VII.0:	2.58933

After all, we need to know capture in CIELO ^{235}U

Rev.96 = rev.88 but RR from VII.1 **except** background



Conclusions – Next steps

- We've got fast neutron file that seems to fit differential data (subject to RPI validation though!)
- We still do not have clear picture in the RR:
  - how far to go (846 keV versus 2 MeV)?
  - although VII.1 RR wins 'beauty contest' in crits we can't use it
  - what elastic angular distributions to use?
    - constructed from resonance parameters (tempting but file is huge)
    - fit to Perey and Kinney data (JEFF-3.1.1) (not always the best choice)
    - JENDL-4.0, which seems to be smoothed results from resonance parameters (our choice in RR in rev.88)
    - OMP - increases reactivity for several fast crits (right direction) if applied in RR but irons out all fluctuations (rev.88 uses it above 846 keV)
- Elastic ang. distr. and capture can be used to improve agreement with benchmarks, however… we need to wait for the full CIELO library

Conclusions – Next steps

- Perform fine tuning to differential data (if needed) => ENDF/A
- Extend energy range to 150 MeV
- Extend evaluation to other isotopes in ^{Nat}Fe
- Validate new *set* of files
- Perform adjustment to the integral data (if needed) => ENDF/B ENDF/C