Resonance Region Evaluations of Minor Fe Isotopes

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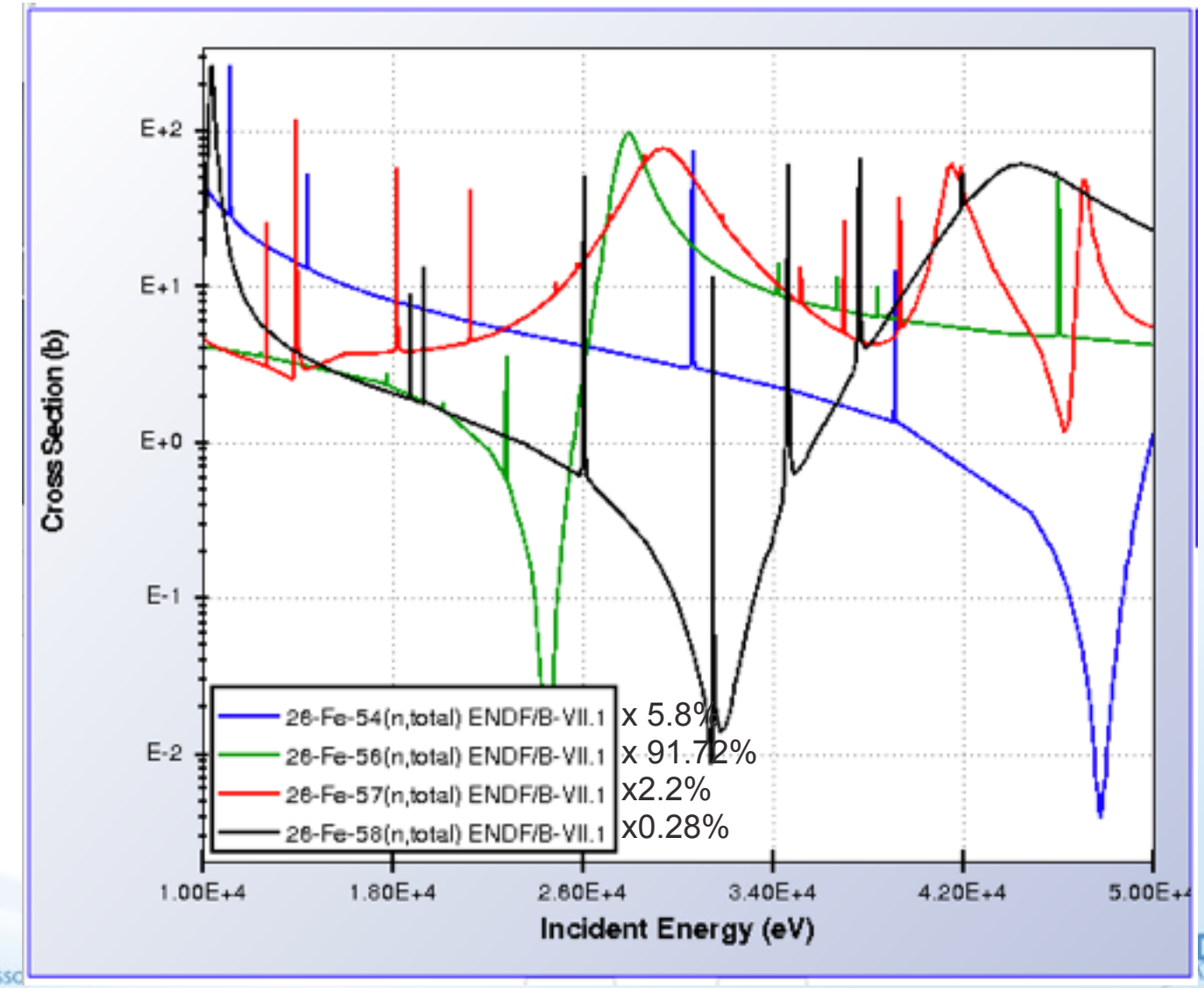
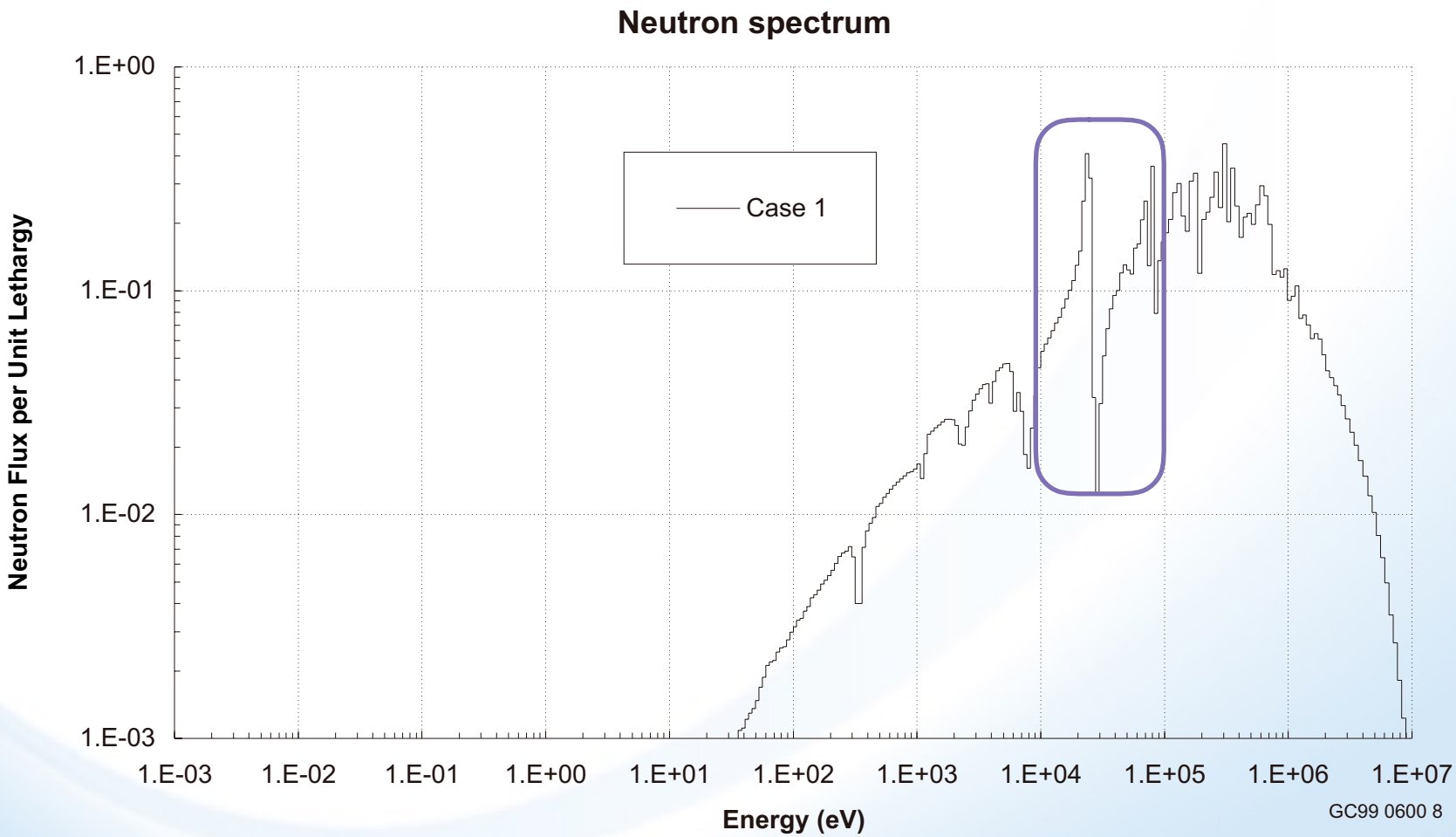
Minor Fe isotopes may play outsized role in some nuclear systems, especially systems used to validate 56Fe



HEU-MET-INTER-001 very sensitive to 10 - 50 keV part of cross section



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Major changes to RRR of minor Fe isotopes

- ^{54}Fe — modified from Atlas, converted to Reich-Moore
- ^{57}Fe — modified from Atlas, converted to Reich-Moore (LRF=7), including (n,n')
- ^{58}Fe — adopted JEFF-3.2 evaluation from Moxon
- not discussed — we may need to visit ^{52}Cr, the last untweaked component of stainless steel

Experimental results since last evaluation

The only new measurement of resonance parameters since 2005 is that of CERN which reported the capture Kernels at the ND13 conference in graphical form. The agreement of the CERN capture kernels with the ORNL and GEEL results is very good, showing that the resonance capture widths are well determined. As a result, the re-evaluation of the resonance parameters for the Fe isotopes received little or no change from values reported in the ATLAS.

— Said Mughabghab 3/2016

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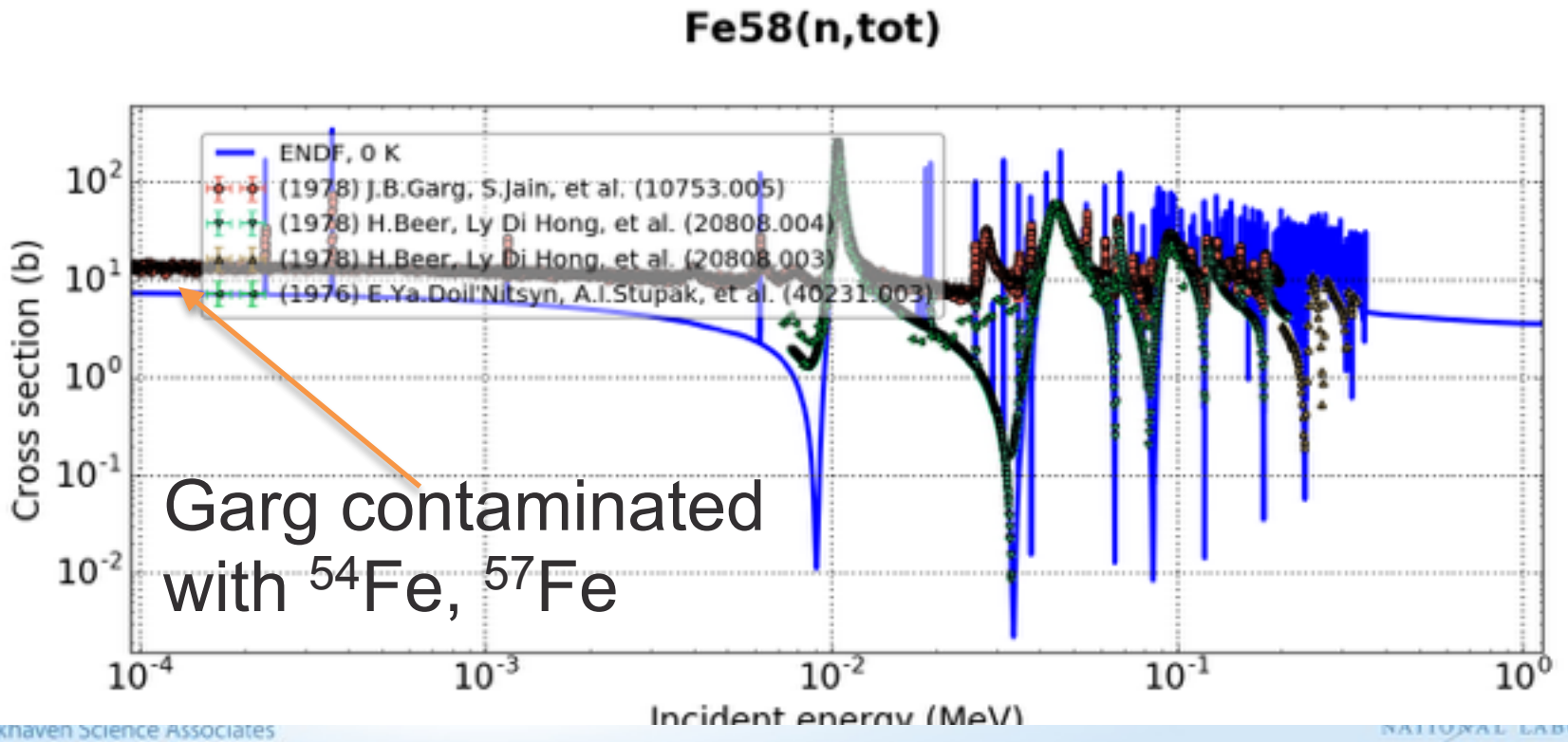
^{58}Fe: from Moxon

Moxon evaluation taken from JEFF-3.2. The unresolved region is for self-shielding only. All angular distributions, including RRR and URR, are calculated by EMPIRE.



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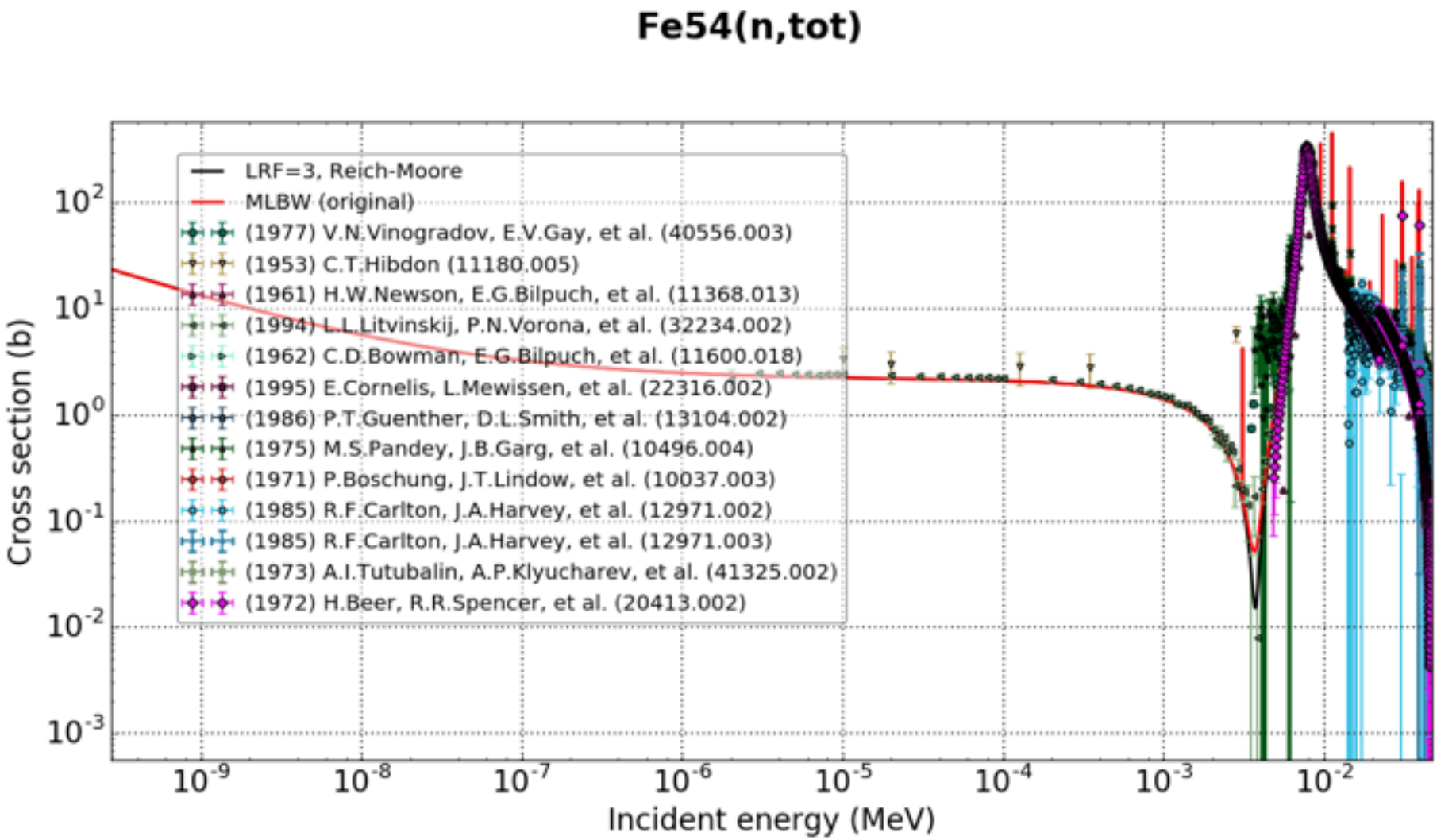
^{54}Fe: from new Atlas, but in RM

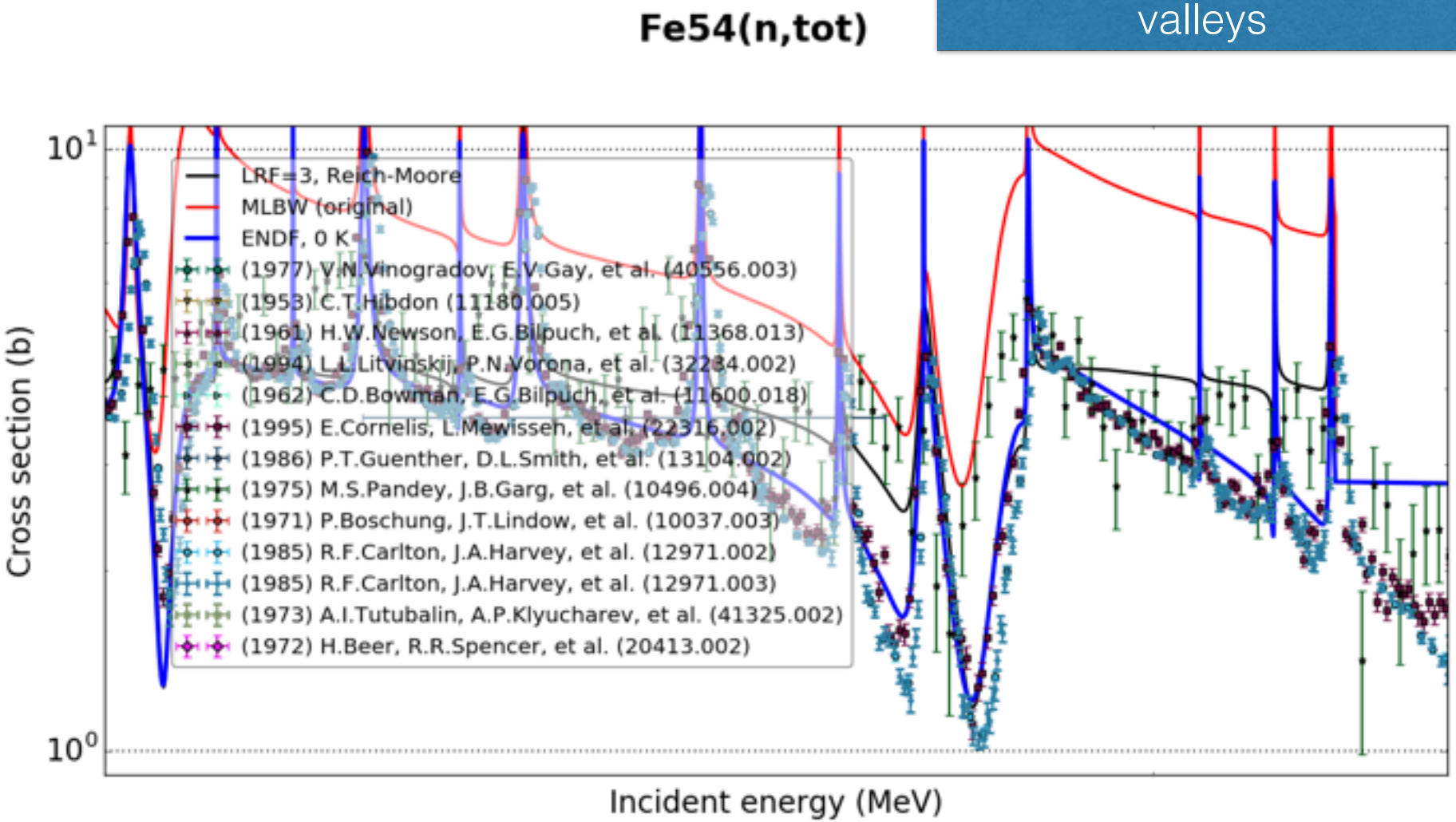
- **Convert MLBW (LRF=2) to Reich Moore (LRF=3)**
  - improved interference minima, but messed up thermal
- **Added/adjusted fictitious strong levels to fix thermal cross section**
- **Imposed fictitious strong levels above E_{max} to get better interference effects and improve agreement with total cross section data**

	Before				After		
E_R (keV)	L	J	Γ_γ (eV)	Γ_n (eV)	J	Γ_γ (eV)	Γ_n (eV)
-1223.3	**0**	n/a	n/a	n/a	**1/2**	**1.0**	**64,062**
-22.24 -> **-20.499**	0	1/2	1.55	8474	1/2	1.55	**6872**
740.56	2	**1/2**	0.96	386.5	**3/2**	0.96	386.5
741.44	2	**1/2**	0.96	424	**3/2**	0.96	424
814.627368	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**1508.68838**
815.801766	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**4148.82574**
824.106211	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**3848.05147**
833.931452	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**5844.58959**
847.326171	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**5565.40352**
1000	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**26,000**

Tweaks of bound levels get low energy part correct



Added a cluster of high energy S-wave resonances to interfere at the upper end and pull down the valleys



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^{57}Fe: from new Atlas, but converted to Reich-Moore (LRF=7)

- **Said's resonances given in MLBW formatted ENDF file with extra column containing (n,n') widths**
  - (n,tot), (n,el) and (n,g) widths based on Geel parameters, likely generated in Reich-Moore approximation
  - (n,n') resonances determined by subtracting capture resonances from (n,tot) where no (n,el) present
    - E_x = 14.410 keV
    - S wave only
    - Capture widths known only from area under resonance

- **MACS(30 keV)=42 mb, consistent with Bao's recommended value of 40 mb**
  - Switching to RM disturbs this result

- **Dave converted resonances into LRF=7 format and flipped the approximation flag to Reich-Moore, keeping resonance parameters (mostly) unchanged**

Summary of Said's work *on MLBW* parameters

For Fe-57, aside from the fictitious resonances, to achieve agreement with the measurements, the only significant change is an increase in the parameters of the 6.22 keV resonance from a scattering width of 380 eV (ATLAS value) to 400 eV. Because of this change, the parameters of the two postulated bound levels have to be adjusted to describe the thermal capture cross section as well as the coherent scattering amplitude.

— Said Mughabghab 3/2016

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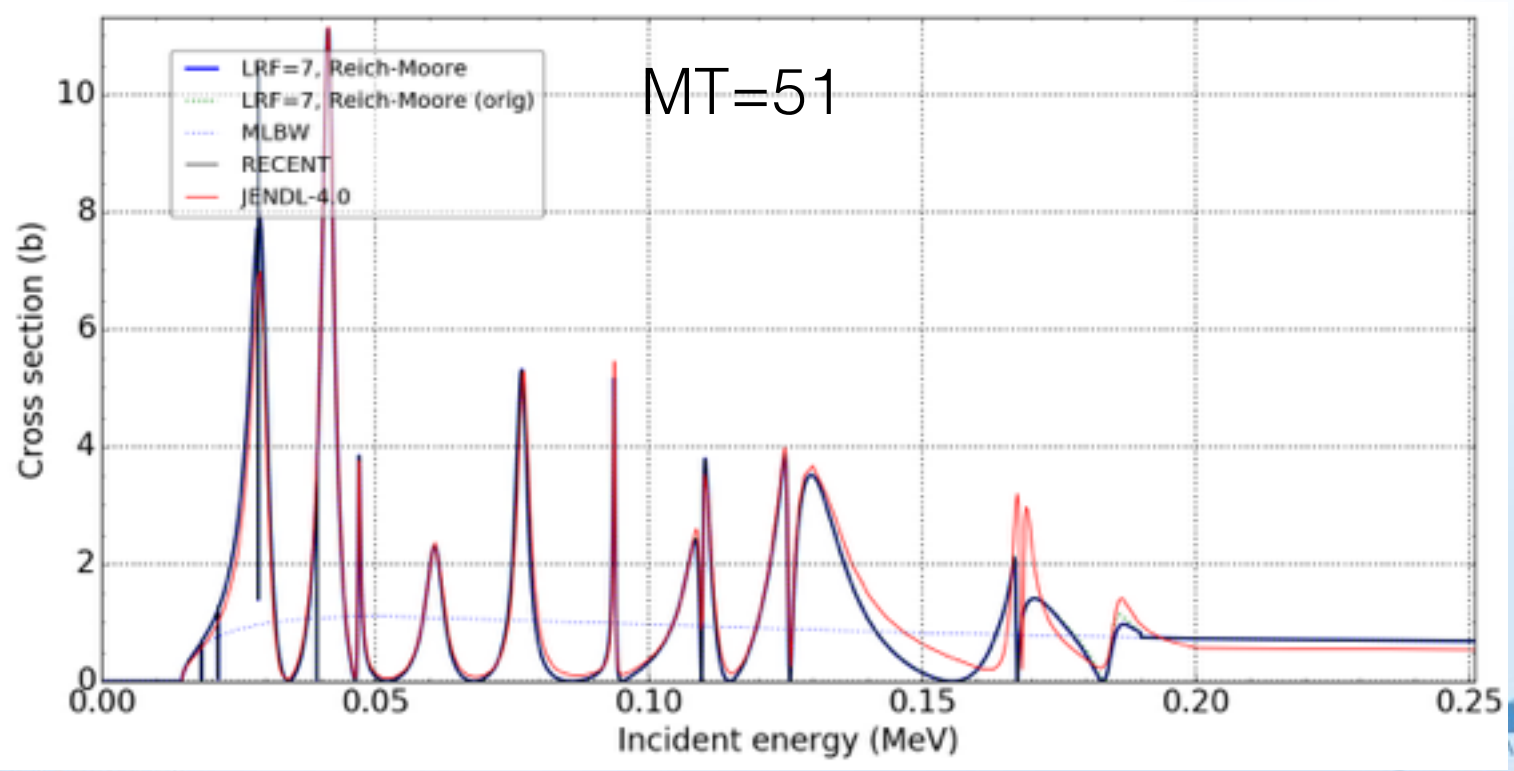
Therefore, peer review from Andrej Trkov and Red Cullen was essential

Red's major concerns

1. Have the background cross sections been correctly handled in all reactions?
2. Has potential scattering converged at the L specified in file?
3. Are there missing (L,J,S,MT) combinations from the channel specification?
4. Are there missing s- or p- wave resonances?
5. The valleys in the (n,tot) toward the upper end of the RRR are filled in in this evaluation
6. Do we match the MACS(30 keV) value for capture?

1. Have the background cross sections been correctly handled in all reactions?

Err… no. There was a bug in the assembly script that kept the MT=51 cross section from being zeroed. It is fixed now. The other reactions are OK.



2. Has potential scattering converged at the L specified in file?

- The potential scattering part of the total and elastic cross sections are expanded in terms of the orbital angular momentum of the incident neutron, L:

$$\sigma_{tot} = \sum_{L=0}^{\infty} \frac{2\pi}{k^2} g \left(1 - \Re S_L\right)$$

- The sum must be truncated at finite NL
- Added convergence test to FUDGE:

$$\sigma_{NL}/\sigma_0 < \text{tolerance}$$

- Q: Has the sum converged? A: No, but the scattering length has been tuned to get the potential scattering correct at the current NL (=1). Therefore, rather than refitting, keep the “unconverged” sum.

3. Are there missing (L,J,S,MT) combinations from the channel specification?

- RECENT has two tests to detect this:
  - Sum rule of statistical weights:

$$\sum_{L_c=L} g_{J_c} = \sum_{L_c=L} \frac{(2J_c+1)}{(2I_a+1)(2I_b+1)} = (2L+1)$$

  - “Brute force” loop through all allowed L,J,S
- FUDGE now has both of these tests:

```
WARNING: The spin statical weights for L=1 sums to 2.25, but should sum to 3.0.
         You have too few channels for reaction n + Fe57
WARNING: The spin statical weights for L=0 sums to 0.375, but should sum to 1.0.
         You have too few channels for reaction n + Fe57_e1
WARNING: The spin statical weights for L=1 sums to 1.125, but should sum to 3.0.
         You have too few channels for reaction n + Fe57_e1
WARNING: Missing a channel with angular momenta combination L = 0, J = 2.0 and S = 2.0 for "n + Fe57_e1"
WARNING: Missing a channel with angular momenta combination L = 1, J = 1.0 and S = 1.0 for "n + Fe57"
WARNING: Missing a channel with angular momenta combination L = 1, J = 1.0 and S = 2.0 for "n + Fe57_e1"
WARNING: Missing a channel with angular momenta combination L = 1, J = 2.0 and S = 2.0 for "n + Fe57_e1"
WARNING: Missing a channel with angular momenta combination L = 1, J = 3.0 and S = 2.0 for "n + Fe57_e1"
```

- Do we need these empty channels?
  - They are potential scattering only.
  - Evaluation apparently “pre-tuned” to match potential scattering without these channels
- None of ORNL LRF=7 evaluations have empty/pure potential scattering channels and in fact neither Luiz nor Vlad think they were needed

First attempt to fix: by adding more channels to get their potential scattering

spin group	J^{Π}	$\gamma+{}^{58}Fe$ (I=0+) L	$\gamma+{}^{58}Fe$ (I=0+) S	n+^{57}Fe (I=1/2-) L	n+^{57}Fe (I=1/2-) S	n'+^{57}Fe_e1 (I=3/2-) L	n'+^{57}Fe_e1 (I=3/2-) S	# res
0	**0+**	**0**	**1**	**0**	**0**			**~10**
1	**0-**	**1**	**1**	**1**	**1**	**1**	**1**	**6**
	0+					2	2	unused
2	**1+**	**0**	**1**	**0**	**1**	**0**	**1**	**~25**
4	**1-**	**1**	**1**	**1**	**0**	**1**	**1**	**~30**
	1-			1	1	1	2	unused
5	**1+**	**2**	**1**	**2**	**1**	**2**	**1**	**pot. only**
	1+					2	2	unused
	2+					0	2	unused
6	**2-**	**1**	**1**	**1**	**1**	**1**	**1**	**~40**
	2-					1	2	unused
7	**2+**	**2**	**1**	**2**	**0**	**2**	**1**	**pot. only**
	2+			2	1	2	2	unused
	2+					1	2	unused
	3-					1	2	unused
8	**3+**	**2**	**1**	**2**	**1**	**2**	**1**	**pot. only**
	3+					2	2	unused
	4+					2	2	unused

= spin ambiguity in MLBW

Despite the increased bookkeeping, it didn't change anything substantive

Have we blundered into a format failing?

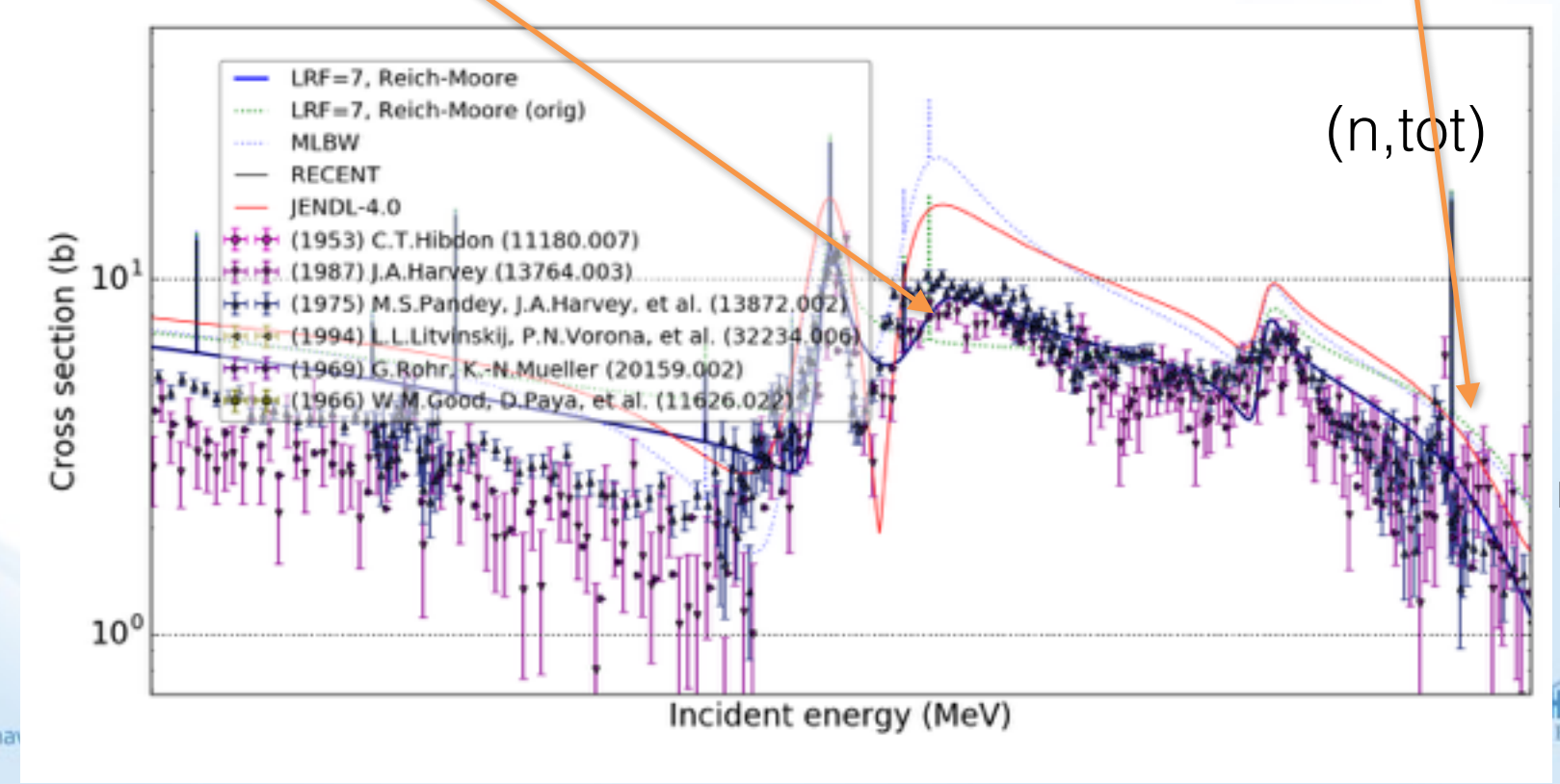
- LRF=7 groups resonances into spin groups with common J
- SAMMY and hence RECENT make some undocumented demands on spin groups:
  - All spin groups apparently are required to have MT=102 and MT=2 channels
  - Resonances in a spin group must be ordered by MT=102, then MT=2, then rest of channels in order of increasing mass (?)
- Does NJOY make these same demands?
- In 57Fe, not all channels could fit in spin groups that satisfy these requirements

4. Are there missing s- or p- wave resonances?

- Probably. The correct diagnosis is to look at the staircase plot for anomalous plateaus.
- This affects the angular distributions in a big way, less so for the cross sections after Doppler broadening.
- However, this evaluation is so low priority (no one will be transporting moles of neutrons though slabs of pure 57Fe) that its not clear if this passes the cost/benefit test.

5. The valleys in the (n,tot) toward the upper end of the RRR are filled in in this evaluation

- Reworked near Ehi
  - add 4 s-wave above Ehi to get tails
  - add 1 s-wave at 169.31 keV to get interference
- tweak 3 resonances near 185 keV to get interference better



log scale on too coarse a grid, sorry!

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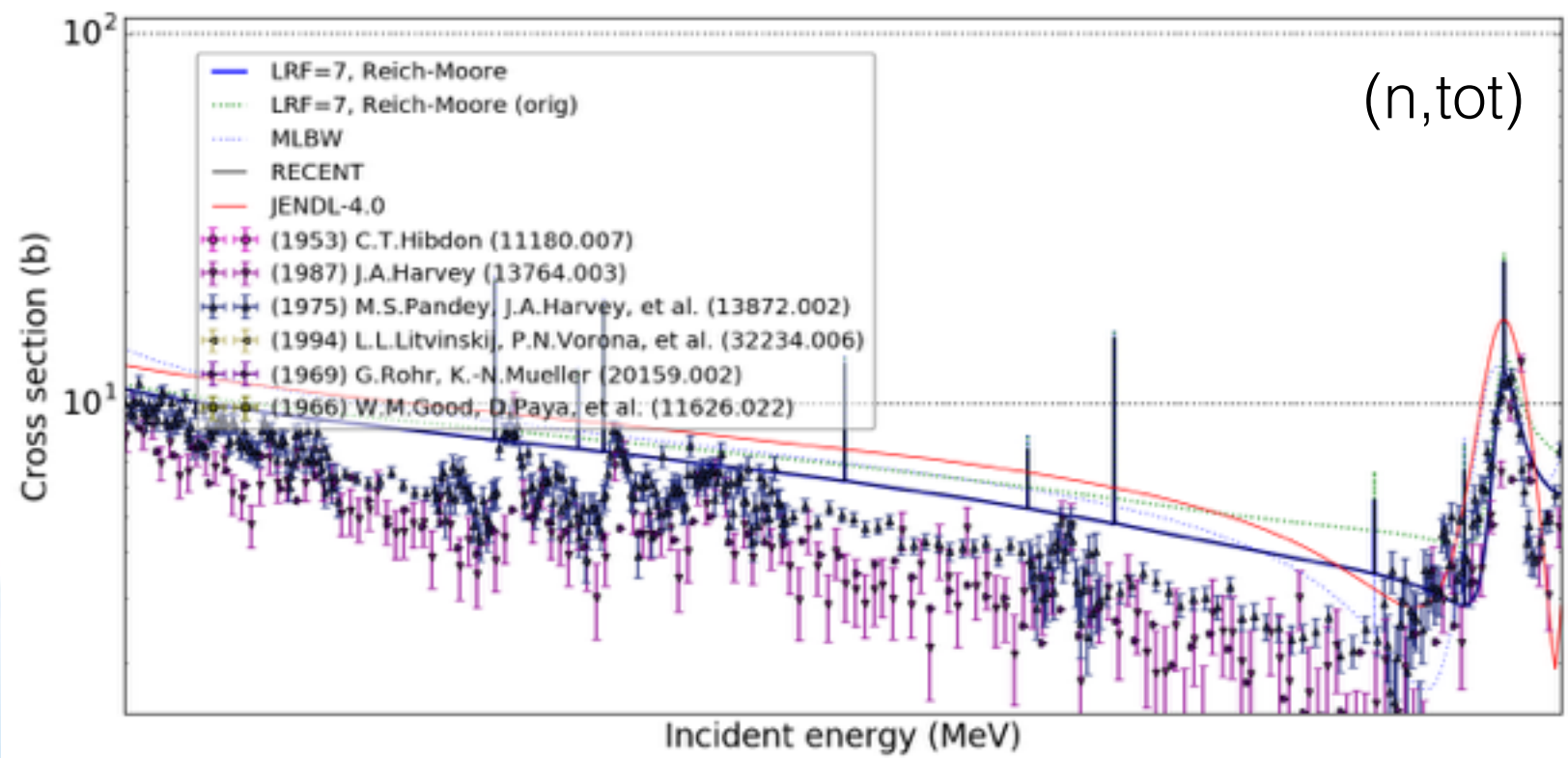
- In range 140 to 165 keV still too high



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		Before			After		
E_R (kev)	J	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)
169.31	0				1801.38	1800	1.38
176.30	0	701.20	700.00	1.20	501.20	500	1.20
185.00	1	3903.00	3500.00	3.00	5203.00	4800	3.00
189.50	0	3201.50	3200.00	1.50	4201.50	4200	1.50
194.25	0				703.55	700	3.55
197.30	0				702.57	700	2.57
198.90	0				701.18	700	1.18
200.10	0				700.99	700	0.99

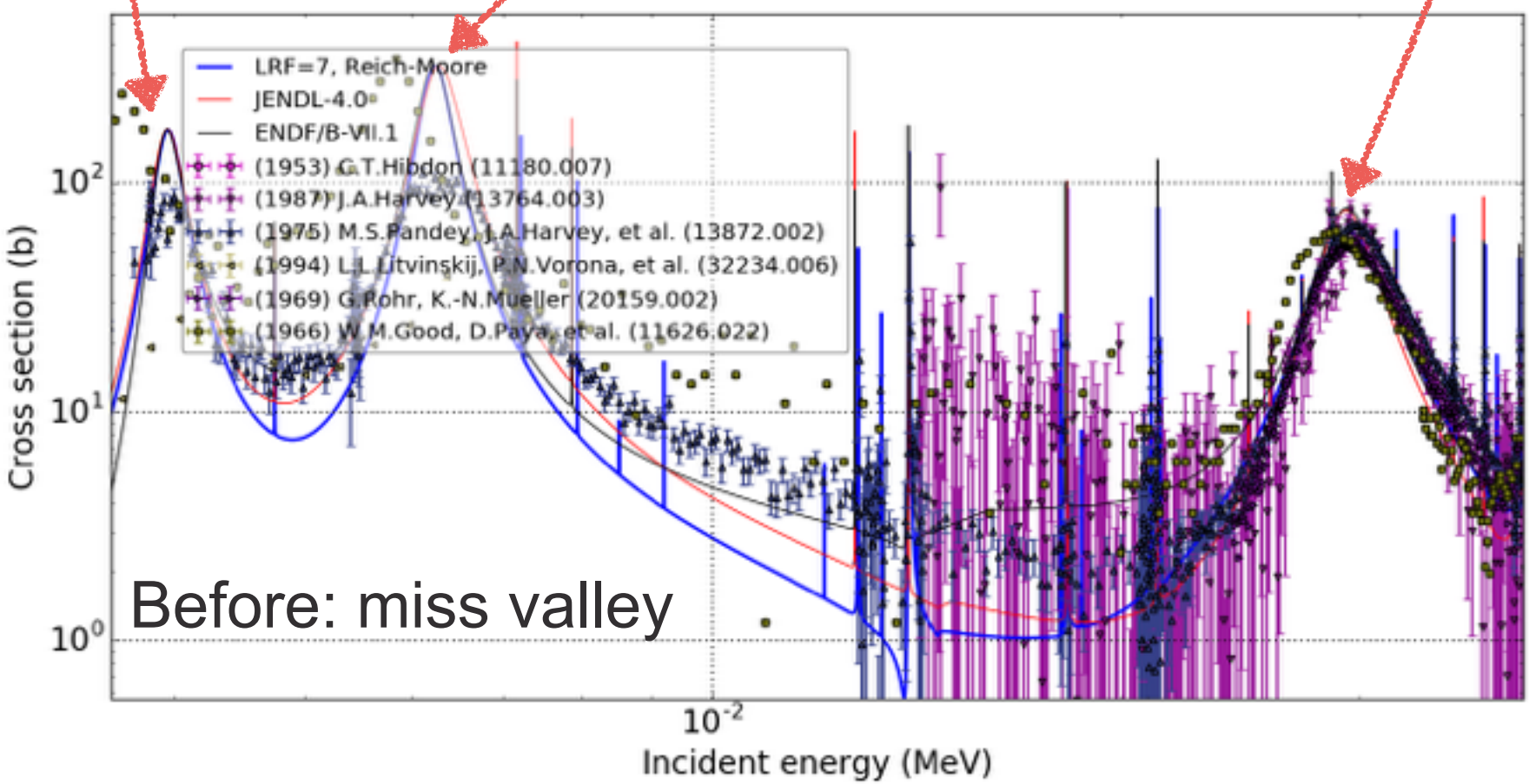
1) E_{hi}=190 keV; 2) Γ_γ determined from $g\Gamma_n\Gamma_\gamma/\Gamma$ assuming $g\Gamma_n/\Gamma$=0.253;
3) E_R=185 keV has MT51 resonance with $\Gamma_{n'}$=400 eV;
4) new resonances from Atlas with tuned Γ_n

5. The valleys in the (n,tot) near 25 keV live in “window” of 56Fe resonances

J^{Pi}=0+
L=0
E_0=3.955 keV
G_n=0.214 keV

J^{Pi}=1+
L=0
E_0=6.220 keV
G_n=0.380 keV

J^{Pi}=1+
L=0
E_0=29.05 keV
G_n=3.45 keV

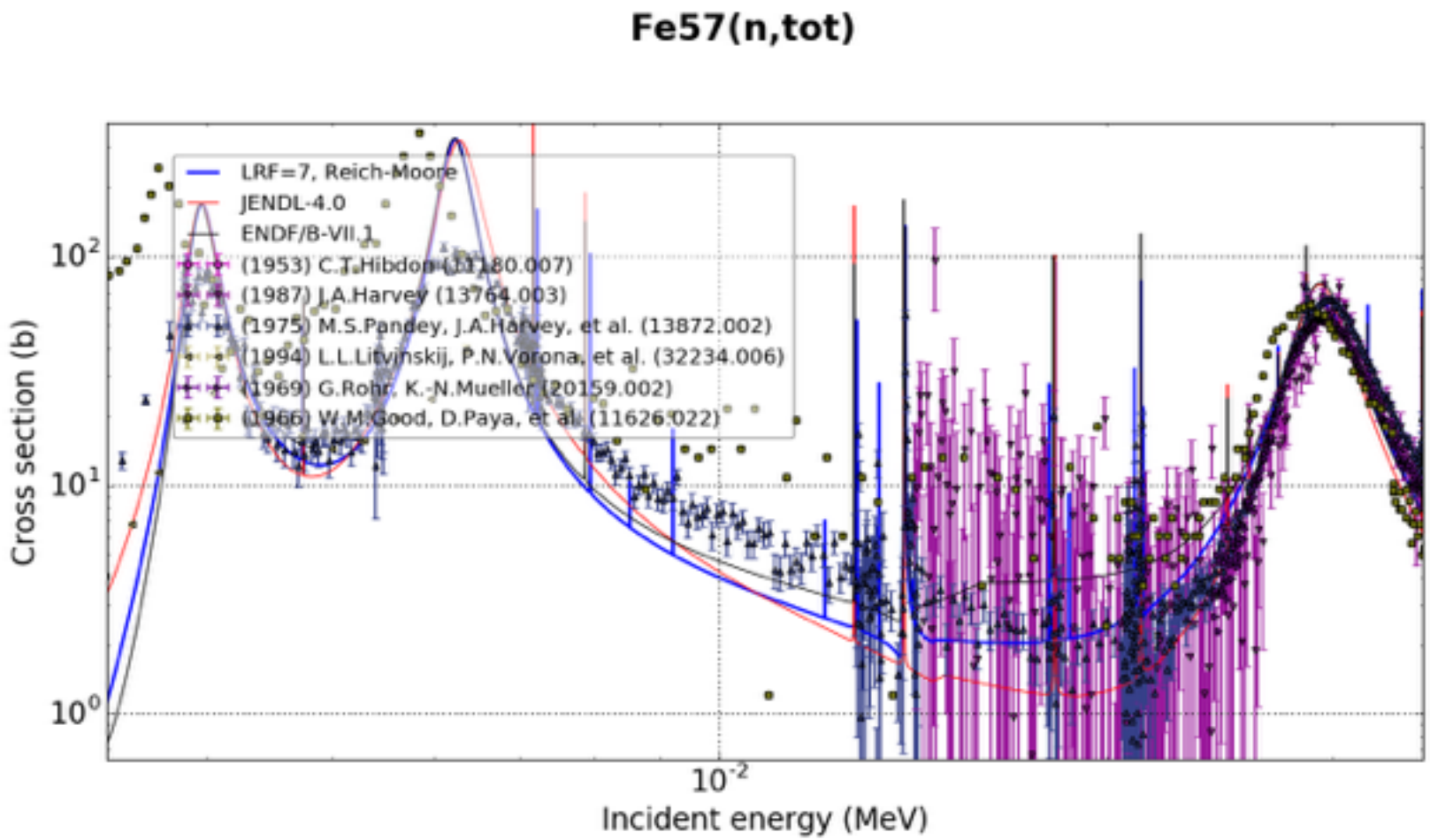


Tweaked bound levels and resonance at 6.22 keV

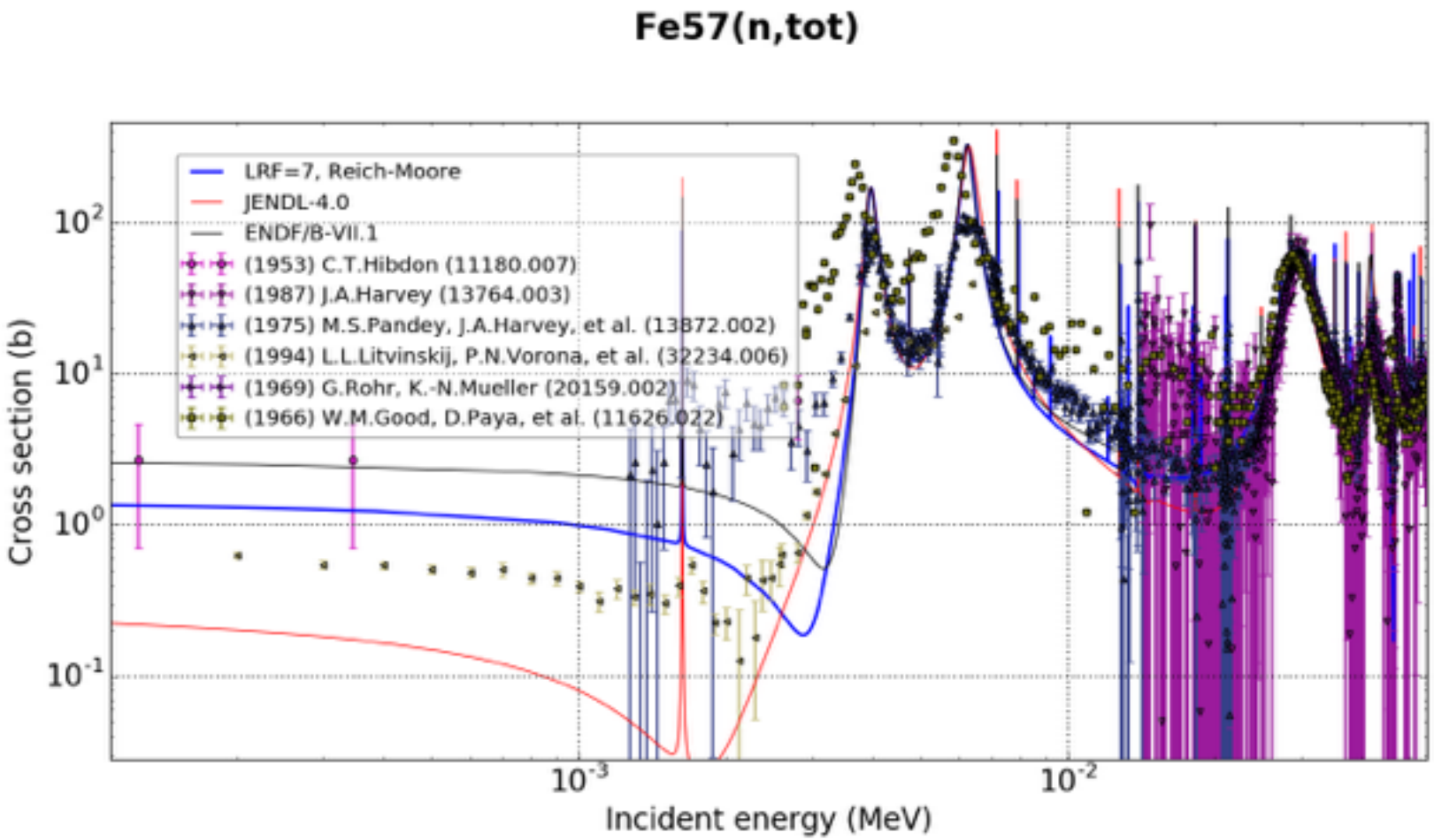
		Before			After		
E_R (kev)	J	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)
-55.00	0				27,000.8	27,000.0	0.8
-2.33	1	66.62	64.89	1.73			
-1.22	1				11.51	9.51	2.00
6.22	1	381.15	380.00	1.15	401.15	400.00	1.15

Also, remember R' = 6.3 -> 5.9 fm

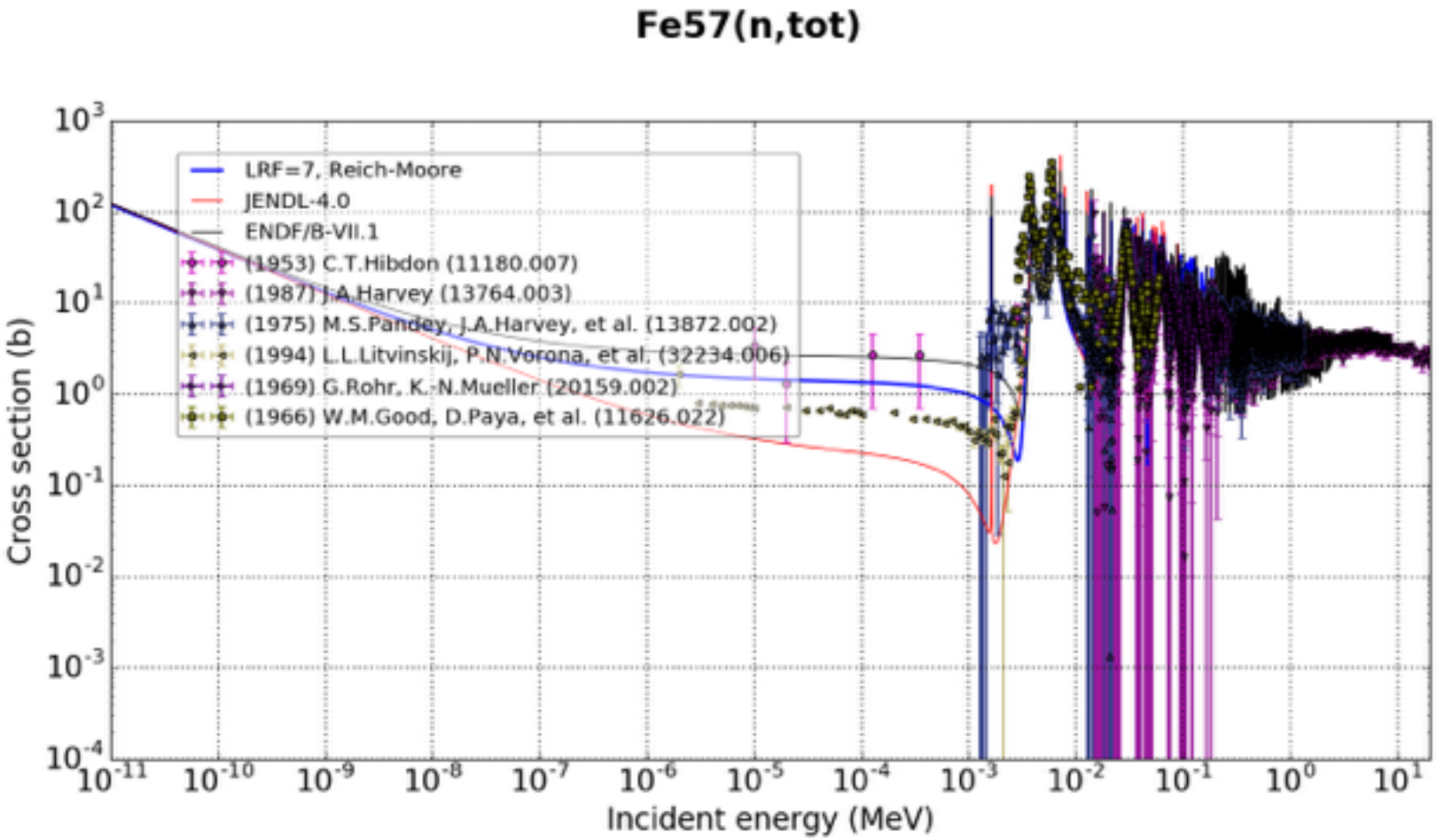
After: Nail valley



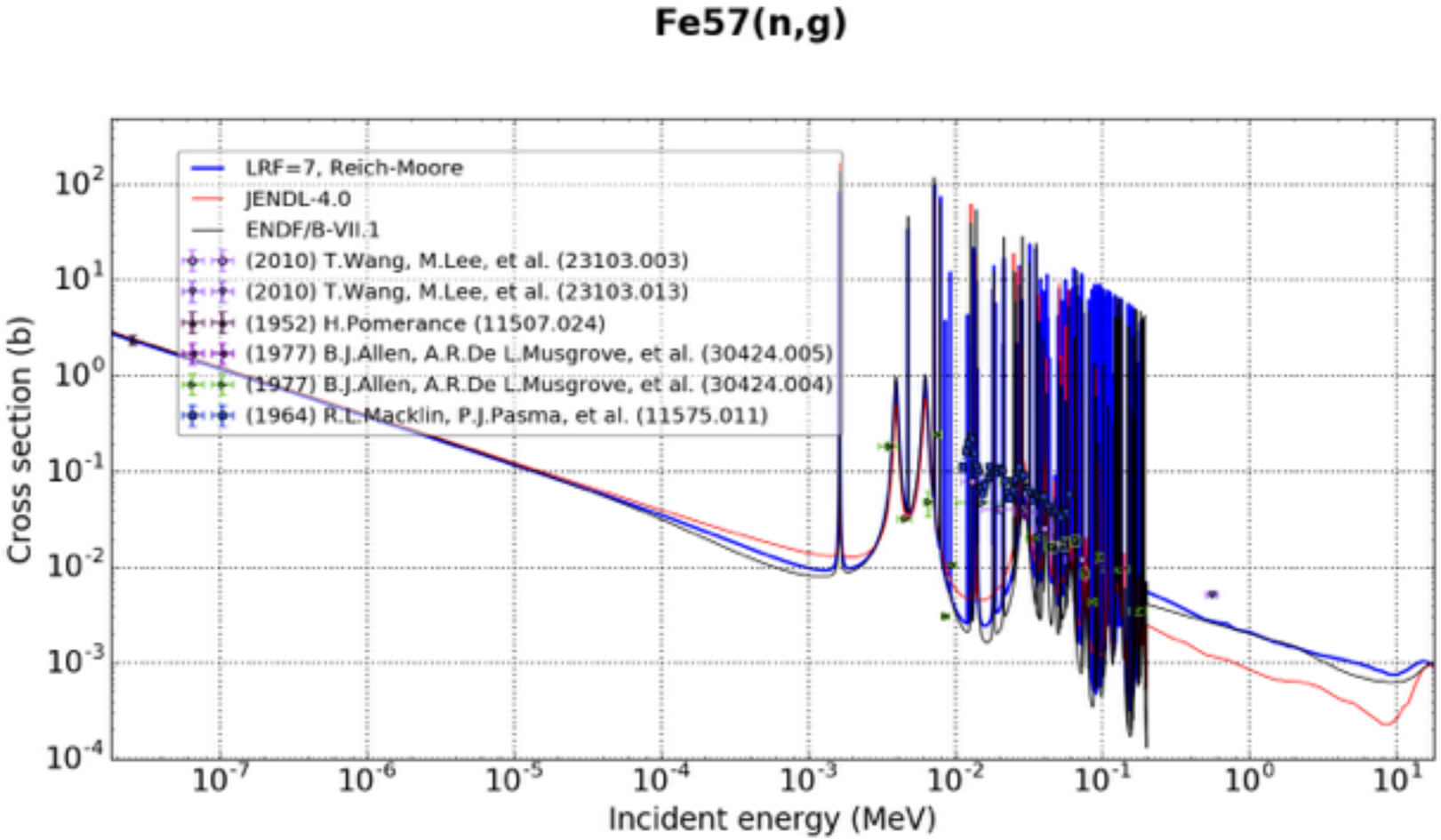
Don’t trust Hibdon or Litvinskij



ok here


Fe57(n,tot)
LRF=7, Reich-Moore
JENDL-4.0
ENDF/B-VII.1
(1953) C.T.Hibdon (11180.007)
(1987) J.A.Harvey (13764.003)
(1975) M.S.Pandey, J.A.Harvey, et al. (13872.002)
(1994) L.L.Litvinskij, P.N.Vorona, et al. (32234.006)
(1969) G.Rohr, K.-N.Mueller (20159.002)
(1966) W.M.Good, D.Paya, et al. (11626.022)
Cross section (b)
Incident energy (MeV)

get thermal dead on (by design)



6. Do we still match the MACS(30 keV) value for capture?

- MACS(30 keV) very useful for quick-n-dirty data validation
- Bao et al. values are the experimental values compiled in Bao et al. At. Data & Nucl. Data Tables **76**, 70-154 (2000)
- Given the spread in experimental data, the LRF=7 values are probably good enough

Source	MACS(30 keV)
MLBW	41.38 mb
LRF=7	36.02 mb
Atlas (exp)	36.0 +/- 2.7 mb
Atlas (calc)	42.1 +/- 8.4 mb
Kadonis-0.3	32 mb
Bao et al. (1)	39.9 +/- 4 mb
Bao et al. (2)	36.0 +/- 2.3 mb
Bao et al. (3)	28 +/- 6 mb

Summary

- Developed RRR evaluations for $^{54,57,58}Fe$
- Converting ^{57}Fe from MLBW to LRF=7 revealed potential format problems (or just processing code problems?)
- Added several new tests to FUDGE which will undoubtably reveal in many many more ENDF file bugs
- We have not made covariances yet

MACS (30 keV)

	β0	KADONIS	ENDF/B-VII.1*	JENDL-4.0*
^{54}Fe	28.3±1.3	29.6±1.3	21.6±2.7	21.6
^{56}Fe	11.2±1.1	11.7±0.5	11.5±1.1	11.8
^{57}Fe	36.02	40.0±4.0	28.5±4.6	30.2
^{58}Fe	13.7±1.5	13.5±0.7	19.7	14.0

B. Pritychenko and S. F. Mughabghab, Nuclear Data Sheets 113, 3120 (2012)