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Updating the 238U(n,2n), 238U(n,3n), 238U(n,4n) and 238U(n,elastic) ENDL Cross Sections

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Updating the ^{238}U(n,2n),^{238}U(n,3n),^{238}U(n,4n) and ^{238}U(n,elastic) ENDL Cross Sections

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Our previous $^{238}\mathrm{U}(n,2n)$ cross section evaluation (Ref. [1]) contains two significant problems: 1) the threshold region does not have the right shape and 2) the peak is not high enough. In this note, we outline how we arrived at an improved cross section and what other changes are needed to the entire $^{238}\mathrm{U}(n,X)$ cross section set in ENDL99 to accomodate this fix. We also describe the processed data files we produced from this update.

Introduction

Our previous $^{238}\mathrm{U}(n,2n)$ cross section evaluation (Ref. [1]) contains two significant problems: 1) the threshold region does not have the right shape and 2) the peak is not high enough. Both points are illustrated in Fig. 1.

Looking carefully at this figure, one can see the rise from threshold is linear. This is no surprise since we fixed the slope of the cross section at threshold to be 0.15 barns/MeV, based on GNASH calculations of the same cross section. We did this to resolve problems caused by some of the data near threshold having too small uncertainties. In retrospect, this was not the best way to treat the threshold because one can show that the behavior of the cross section near threshold can be parameterized by [2]:

$$\sigma \approx (E - E_{\mathrm{thresh}})^2 \frac{\partial^2 \sigma(E_{\mathrm{thresh}})}{\partial^2 E} \tag{1}$$

The peak of our fit is also not quite correct. Here there are several datasets, each with relatively small uncertainties, that do not agree. When one blindly performs a least-square fit, one arrives at a value that somehow averages over the data in this region, but with unrealistically small uncertainties. We examined some of the dataset in this region,

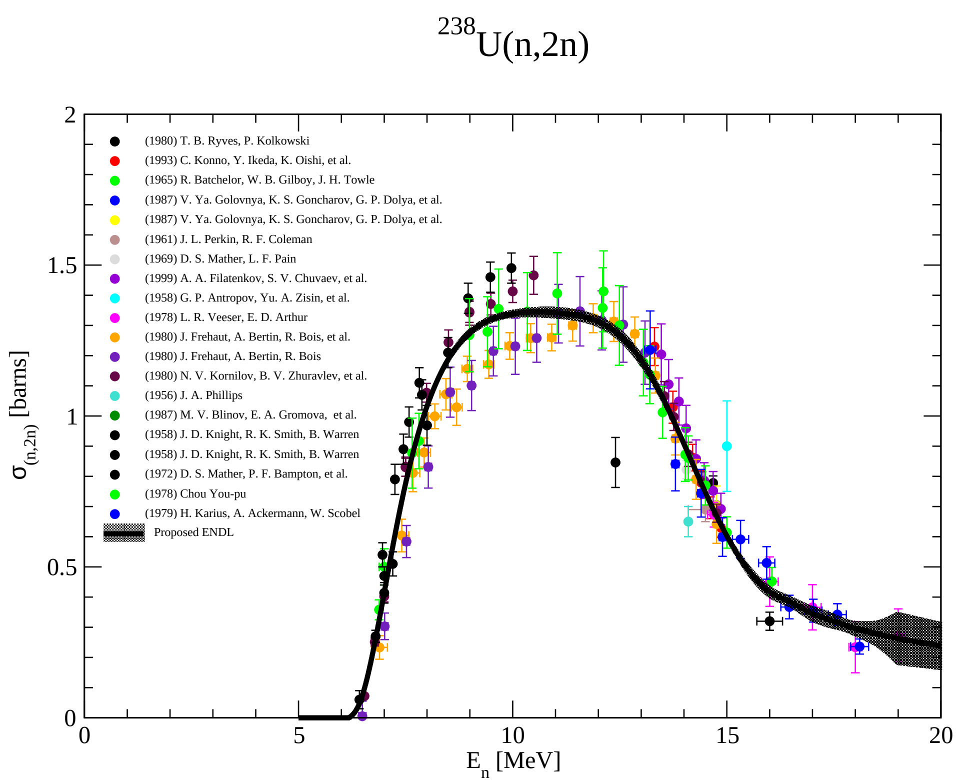

FIG. 1: Comparision of the $^{238}\mathrm{U}(n,2n)$ cross section from Ref. [1] with experimental data.

EXFOR Accession Number	Reference	Action taken
N/A	[5]	Discarded, we don't have data and is partial γ data.
N/A	[6]	Used, it is a systematics point averaging over mass range.
10376002 (set #2)	[10]	OK
10795004	[11]	OK
12459002	[12]	Replaced bad monitor with ^{238}U(n,f) evaluation in [7].
12459004	[12]	Discarded, don't understand point even after applying correction for bad monitor.
20416021	[13]	Replaced [8] ^{238}U(n,f) evaluation with that in [7] in rescaling.
20499002	[14]	OK
20794013	[15]	OK
20795012	[16]	Replaced bad monitor with ^{238}U(n,f) evaluation in [7], dropped last point.
21019025	[17]	OK
21208003	[18]	OK
21521003	[19]	OK
21568003	[20]	Replaced [8] ^{238}U(n,f) evaluation with that in [7] in rescaling.
21627008	[21]	OK
21976048	[22]	OK
22637090	[23]	OK
30537002	[24]	OK
30561002	[25]	OK
40411002	[26]	OK
40997002	[27]	OK
40997003	[27]	OK
41024002	[28]	Discarded, it is fission spectrum averaged with unknown spectrum.
41147007	[29]	Discarded, it is spectrum averaged with unknown spectrum.
41240070	[30]	OK
41298100	[31]	OK
V0021002	[24]	Discarded, it is an evaluation.
10376002 (set #1)	[32]	Discarded, it is same as 10376002 set#2.
30590002	[33]	Discarded, this data is superceeded by data in 30561002.
41068018	[34]	Discarded, is fast reactor neutron spectrum average data.

TABLE I: Expermental Database used in the fits and any treatment we needed to do to make them useful

and determined that many of them needed "repairs." These "repairs" are summarized in the list of measurements in Table I. Most of the "repairs" consisted of rescaling the data by a better estimate of the ^{238}U(n,f) cross section. In several cases, the authors made ratio measurements relative to ^{238}U(n,f), then folded their ratio measurement with an older ^{238}U(n,f) evaluation or measurement. In all cases I worked back with the original ratio data and folded them with JENDL-3.3's evaluation. This also allowed us to add in uncertainties in the evaluated ^{238}U(n,f) cross section. We also added the systematics point from Ref. [6], treating it as an independent measurement.

In this note, we first discribe our fitting procedure for determining the ^{238}U$(n,2n)$ cross section. Second, we list all of the changes we needed to make in addition to this one in order to maintain consistency with previously known total cross section. Finally we discuss the processed data files we produced from this work.

Refitting the ^{238}U$(n,2n)$ cross section

As we outlined in the introduction, we redid our least-square fit to the experimental data after applying the fixes outlined in Table I. Our fit used 3^{rd} degree Basis splines so it can in principal be converted to a cubic spline

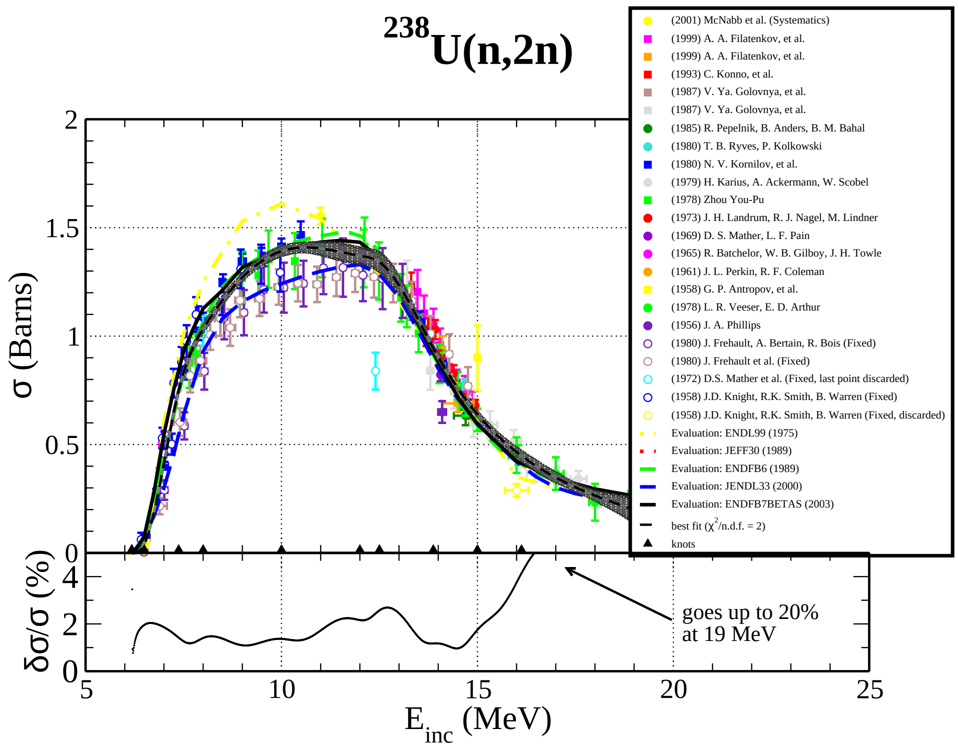

FIG. 2: Comparision of our ^{238}U$(n, 2n)$ cross section with other evaluations and experimental data.

analytically. In order to get a good knot density, we seeded our evaluation with an $(n, 2n)$ curve that came from the JENDL-3.3 $(n, 3n)$ cross section below 16 MeV and from the LANL ENDF/B-VII evaluation above. The seeding was a two step process. First, we determined all of the points in the evaluation with zero first, second or thrid derivative and chose this to be our list of collocation points. We then converted these points into knots using the prescription given in Ref. [9].

To further stabilize the fit near threshold, we applied three equality constraints: we fixed the cross section and its first deriviative to be zero at threshold and we fixed its second derivative to be 0.15 barns/MeV^2. The value for the second derivative was chosen to give a reasonable shape to the cross section. In principal could tune thie derivative to get lowest χ^2, but this makes no practical sense here. Since we do not treat the energy uncertainty properly, the computed χ^2 is not really correct. Furthermore, near threshold there are several points with energy uncertainty.

The final fit is shown in the Fig. 2. In this plot, we show the relative uncertainty in the lower panel. The relative uncertainty is around 2% for most energies but drops to 1% around 14 Mev, where there is a of data, then climbs to 20% at the edge of the plot. The overall χ^2 of the fit was 242.995 giving $\chi^2/ndf = 2.02496$. A good fit should have $\chi^2/ndf \approx 1$ so either the data uncertainties are underestimated or the data is correlated. We expect that there is probably some additional uncertainty due to systematic correlations between the datasets and this is not treated properly here. Either way we have no expedient way to remedy this other than to rescale the uncertianties of the fit via:

$$d\sigma \rightarrow \delta\sigma\sqrt{\chi^2/ndf}. \tag{2}$$

Both the original uncertainty and the enlarged uncertainties are shown in Table II. In Fig. 2, only the enlarged uncertainties are shown.

Treatment of other cross sections

When one updates one cross section, inevitably they must change other cross sections to maintain overall consistency across an entire isotope. Previously [1], we updated the ^{238}U(n, f) and ^{238}U(n, γ) cross sections and we still feel that they "optimal" so they are unchanged here. Further, we did not modify any outgoing distributions other than the inelastic outgoing neutron distributions. These had to change to maintain consistency with the (n, n') cross section changes summarized below.

Energy Range	(n,n')	$(n,2n)$	rescaled $(n,2n)$	$(n,3n)$	$(n,4n)$	Elastic	Total
(MeV)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
0.01 - 0.1	0.0	0.0	0.0	0.0	0.0	13.5	5.5
0.1 - 1.18	0.7	0.0	0.0	0.0	0.0	12.5	4.1
1.18 - 6.18	11.4	0.0	0.0	0.0	0.0	11.4	1.6
6.19 - 11.33	11.1	1.5*	2.1	0.0	0.0	11.1	1.0
11.33 - 17.9	11.1	2.9*	4.1	16.4	0.0	11.1	1.0
17.9 - 20.0	11.1	6.7*	9.5	16.4	19.8	11.1	1.0

TABLE II: Estimated average uncertainties in compiled cross sections. The asterisk in the $(n,2n)$ indicates that this result comes from the fit to the raw data and not from a calculation. We estimate a 14.3% uncertainty in the computed $(n,2n)$ cross section in the Hauser-Feshbach calculations.

We replaced ^{238}U$(n,3n)$, ^{238}U$(n,4n)$, ^{238}U(n,elas) with LANL's ENDF/B-VII evaluations. In all cases the ENDL99 cross sections were clearly dated. It makes sense to take all of these cross sections as a package since they were all computed within the same Hauser-Feshbach calculation with the same carefully tuned optical model potential. We made no comparisons to outgoing particle distribution data, even though this would bolster confidence in the elastic cross section evaluation in particular.

We also noticed that ENDL99's discrete ^{238}U(n,n') cross sections are seriously out of date – they are missing several levels and many of the level energies are wrong. We replaced them with LANL's ENDF/B-VII evaluation. To keep levels in sync between cross section and outgoing neutron distributions, we also replaced ENDL99's outgoing neutron distributions with LANL's ENDF/B-VII evaluation. While we could have done this within `fudge`, we found it to be expedient just to copy the relavent files into the ENDL99 formatted source from [1].

Since total cross section should remain fixed, we took cross section strength from the ^{238}U(n,n') continuum cross section to make up for increase in the ^{238}U$(n,2n)$ cross section over LANL's version. After these changes, we recomputed the total cross section given all of these changes to ensure overall consistency.

While producing these files, we also produced uncertainty estimates on all of the cross sections, using the method in Ref. [1]. They are summarized in Table II. Plots of the altered cross sections are given in Figs. 3, 4, 5, 6, and 7. We comment that the estimates for the elastic cross section are very rough. First, we assumed all of the uncertainty came from the Hauser-Feshbach modeling, which only accounts for the compound-elastic cross section, and did not fold in uncertainty from the shape-elastic cross section. Second, we only made a partial comparision to all the data and it may be that we could argue the data itself would support much smaller uncertainty.

Processed Data Files

In order that one can do sensitivity tests with these changes, we produced a second database that uses LANL's ^{238}U$(n,2n)$ cross section. LANL's cross section has a much different threshold region and both the peak region and high energy tail are different from our fits.

We have produced processed data files for both databases and placed them on the LC machines.

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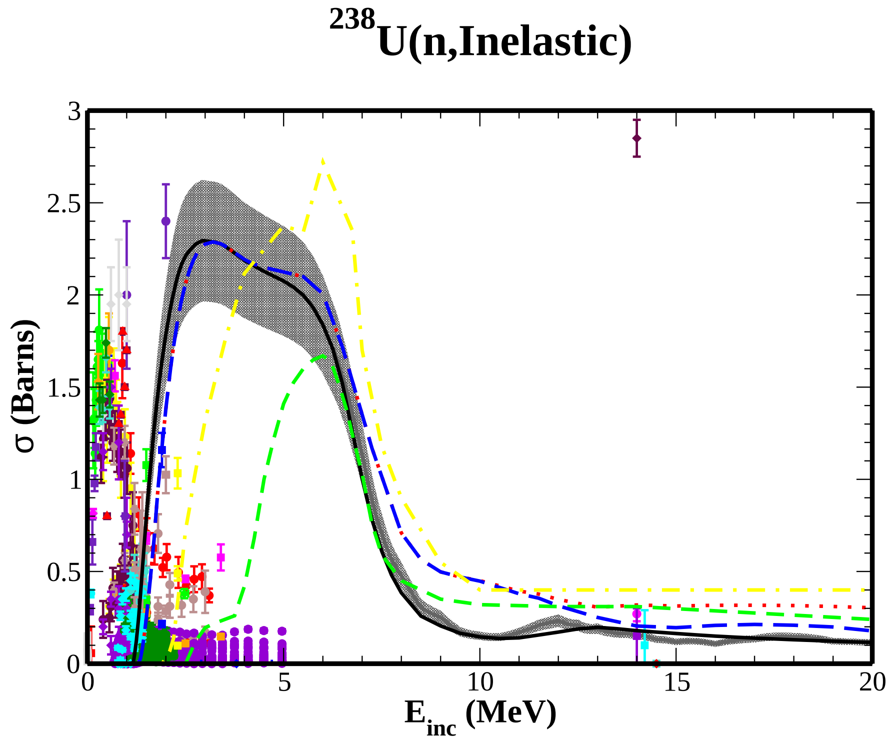

FIG. 3: Comparision of our $^{238}\mathrm{U}(n,n')$ cross section with other evaluations and experimental data. The grey curve and uncertainty band is our new evaluation. We have supressed the legend because of the large number of datasets and because these datasets all refer to different discrete excitations while the plotted $^{238}\mathrm{U}(n,n')$ evaluations are sums over all channels. The symbols for the evaluations are the same as in Fig. 2.

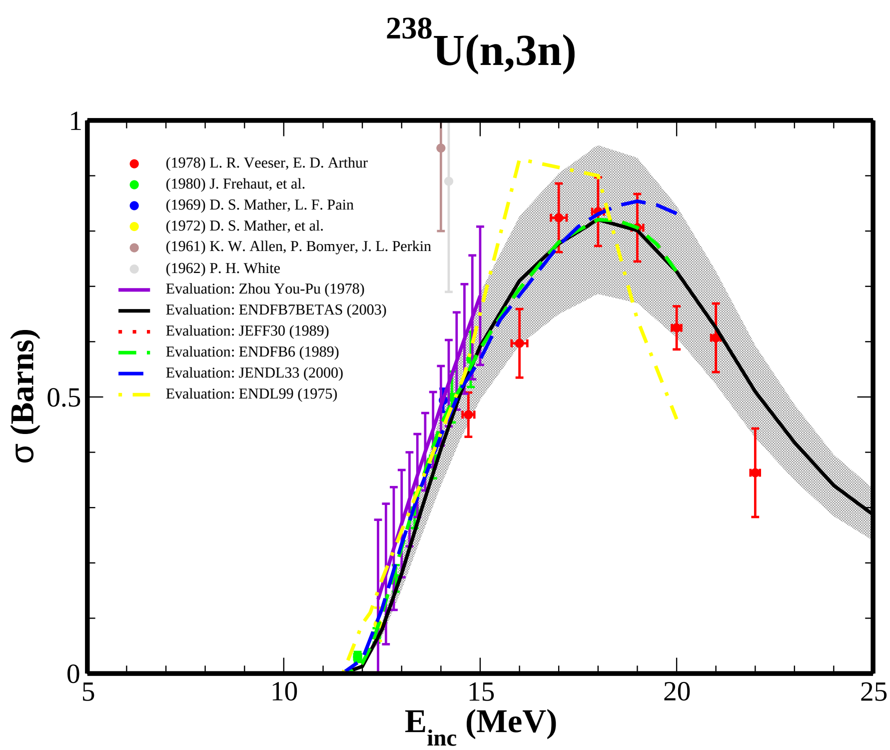

FIG. 4: Comparision of our $^{238}\mathrm{U}(n,3n)$ cross section with other evaluations and experimental data. We adopted the LANL cross section (labeled ENDFB7BETAS) here but affixed our own uncertainty estimate in the grey band.

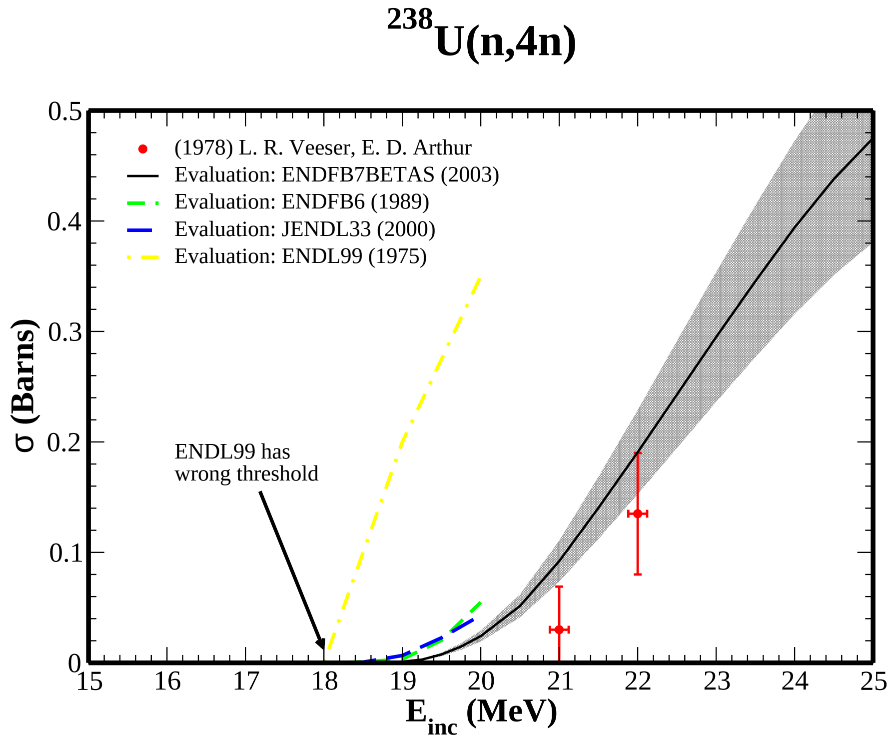

FIG. 5: Comparision of our ^{238}U$(n,4n)$ cross section with other evaluations and experimental data. We adopted the LANL cross section (labeled ENDFB7BETAS) here but affixed our own uncertainty estimate in the grey band.

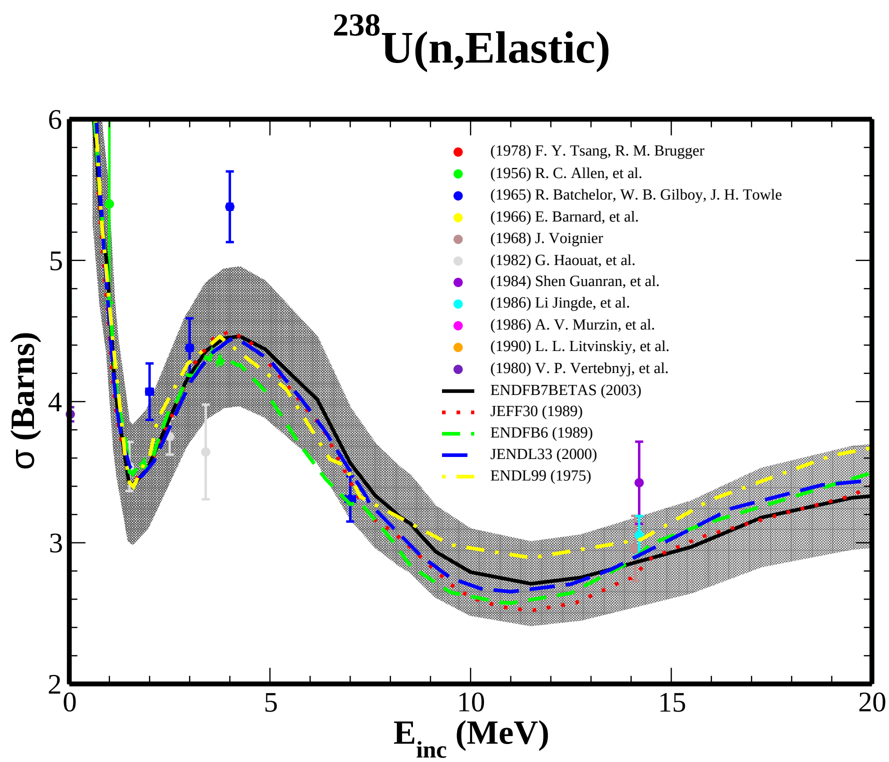

FIG. 6: Comparision of our ^{238}U(n,elas) cross section with other evaluations and experimental data. We adopted the LANL cross section (labeled ENDFB7BETAS) here but affixed our own uncertainty estimate in the grey band. Integrated differential data from EXFOR is not shown on this plot.

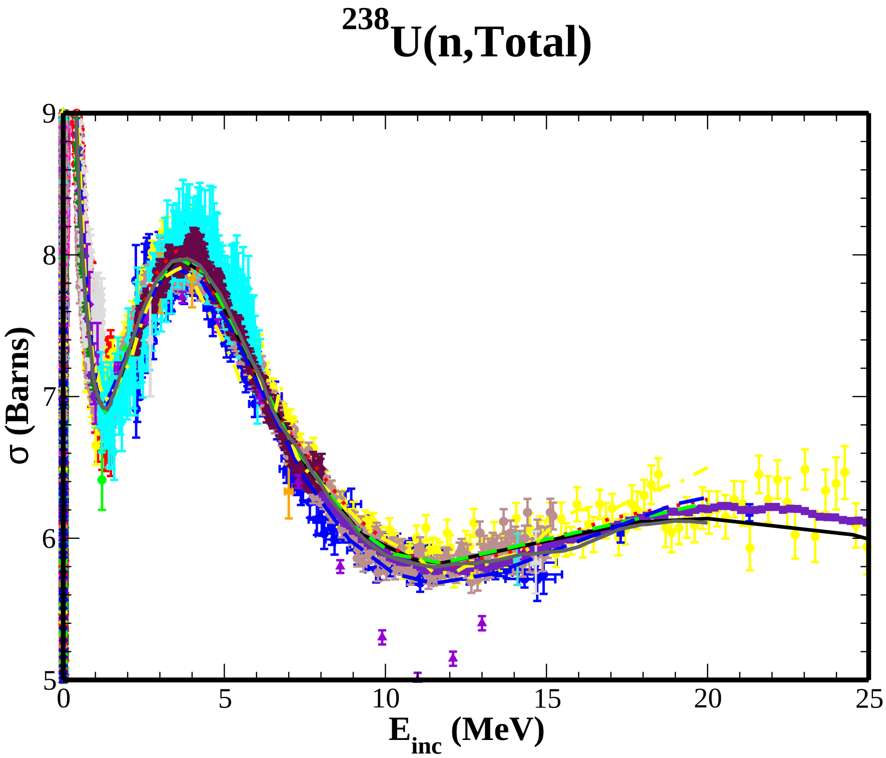

FIG. 7: Comparision of our ^{238}U(n, tot) cross section with other evaluations and experimental data. The grey curve and uncertainty band is our new evaluation. We have supressed the legend because of the large number of datasets. The symbols for the evaluations are the same as in Fig. 2.

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