

Progress Report on neutron-induced alpha-emission analysis

[EUROfusion WPBB-S.05.02-T007-D004:
Validation of the assessment of particular alpha-particle emission induced by fast
neutrons on structural materials around 10 MeV]

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Content

1. Introduction: WPBB-S.05.02-T007-D004: **31.12.2024**
2. Analysis of 2022 first data of $^{91}\text{Zr}(n,\alpha)^{88}\text{Sr}$ reaction + (GQR) + %EWSR [EFFDOC-1538(Apr.2024)]
[accuracy/uncertainty]: PLB **858**(2024)139078
3. EWSR systematics: (α,α') , (γ,α) , (n,α) **reactions**: PLB **858**(2024)139078
4. (n,α) ISGQR / EWSR vs. (a) Γ_{syst} (2001), and (b) Lorentzian ISGQR: PLB Suppl. material
5. Conclusions: 1. **Suitable (GQR+)+DR+PE+CN account of alpha-particle emission confirmed**
2. **EWSR systematics: 50-100% [(α,α')] vs. 100-10% [(x,α)], $x=\gamma,n$**

Task Specification (TS)



EUROfusion

[EFFDOC-1538(Apr.2024)]

TS Title:	Nuclear Data Evaluations - 2024		
TS Ref. Nr.:	BB-S.05.02-T007	Task coordinator:	Dieter Leichtle
Status:	In review	Date:	14-Feb-2024

D004: Technical Specification: Validation of the assessment of particular alpha-particle emission induced by fast-neutrons on structural materials around 10 MeV (IAP)

Further validation of the alpha-particle optical model potential (OMP) developed within F4E/EUROfusion deliverables, for a sound description of the alpha-emission in neutron-induced reactions, is needed due to most recent measurement and analysis of (n, α) reaction cross sections [e.g, Phys. Rev. C **106**, 064602 (2022) for ^{91}Zr target nucleus]. Measured data larger by $\sim 100\%$ than actual evaluations (TENDL-2021/2023) led firstly to changes of the above-mentioned OMP (also the actual default option of the code-system TALYS-2.0 used to provide TENDL), however at variance with other recent measurements by wide collaborations (e.g., arXiv:2402.01534 [nucl-ex], 2 Feb 2024). Thus it becomes necessary and is proposed an additional analysis of these data as well as eventual role of the alpha-emission decay of nuclei excited just at the isoscalar Giant Quadrupole Resonance (GQR) energies within (n, α) reactions below and around the incident energy of 14 MeV. Former EUROfusion/WPBB similar analyses [Eur. Phys. J. A **57**, 54 (2021), **58**, 189 (2022), Phys. Rev. C **107**, 034613 (2023)] should and will be completed in this respect also by comparison of the corresponding Energy Weighted Sum Rule (EWSR) data with the available systematics

PM: 3 PM (IAP)

ID	Title	Start Date	End Date	RU	Del. Owner	AWP2024
						PM 50% standard
BB-S.05.02-T007 - D004	Validation of the assessment of particular alpha-particle emission induced by fast-neutrons on structural materials around 10 MeV	01-Jan-24	31-Dec-24	IAP	Vlad Avrigeanu	3.000

2.1 α 's OMP[1994/2003-2010/2014-2023] / α -emission



[EFFDOC-1538(Apr.2024)]

PHYSICAL REVIEW C 90, 044612 (2014)

F4E-GRT-168.01-5.1

Further explorations of the α -particle optical model potential at low energies for the mass range $A \approx 45-209$

PHYSICAL REVIEW C 91, 064611 (2015)

F4E-GRT-168.02-8.1

Consistent optical potential for incident and emitted low-energy α particles

Zn(p, α)

YES!

PHYSICAL REVIEW C 94, 024621 (2016)

F4E-GRT-168.02-8.1

Analysis of uncertainties in α -particle optical-potential assessment below the Coulomb barrier

α -emission

PHYSICAL REVIEW C 96, 044610 (2017)

PPPT-WPMAT-5.7.1-T001-D001

Consistent optical potential for incident and emitted low-energy α particles. (II) α emission in fast-neutron-induced reactions on Zr isotopes

Zr(n, α)

NO!!

α -OMP setting/validation

PHYSICAL REVIEW C 99, 044613 (2019)

PPPT-WPMAT-7.1-T004-D001

Role of consistent parameter sets in an assessment of the α -particle optical potential below the Coulomb barrier

PHYSICAL REVIEW C 106, 024615 (2022)

WPBB-S.05.02-T001-D018

Charged-particle optical potentials tested by first direct measurement of the $^{59}\text{Cu}(p, \alpha)^{56}\text{Ni}$ reaction

PHYSICAL REVIEW C 107, 034613 (2023)

WPBB-S.05.02-T001-D005

Consistent optical potential for incident and emitted low-energy α particles. (III) Nonstatistical processes induced by neutrons on Zr, Nb, and Mo nuclei

$^{90,91,92}\text{Zr}(\alpha, \gamma)$, ^{96}Zr , $^{100}\text{Mo}(\alpha, n)$

frontiers | Frontiers in Physics

DOI 10.3389/fphy.2023.1247311

M. Avrigeanu and V. Avrigeanu

Constrained model assumptions using recent data of α -particle reactions on ^{144}Sm .

WPBB-S.05.02-T005-D007

$^{144}\text{Sm}(\alpha, \gamma)$

2.1 α 's OMP[1994/2003-2010/2014-2023/2021-on] / α -emission / GQR



Eur. Phys. J. A (2021) 57:54
<https://doi.org/10.1140/epja/s10050-020-00336-0>

THE EUROPEAN
 PHYSICAL JOURNAL A

WPPMI-7.4-T004-D002

Check for updates

Validation of an optical potential for incident and emitted low-energy α -particles in the $A \sim 60$ mass range

Fe,Co,Cu,Zn(n,α) , (p,α)

α -emission
 YES!!!
 +DR+GQR

Eur. Phys. J. A (2022) 58:189
<https://doi.org/10.1140/epja/s10050-022-00831-6>

THE EUROPEAN
 PHYSICAL JOURNAL A

WPPMI-7.4-T004-D004

Validation of an optical potential for incident and emitted low-energy α -particles in the $A \sim 60$ mass range **II.** Neutron-induced reactions on Ni isotopes

Ni(n,α)

PHYSICAL REVIEW C 107, 034613 (2023)

Consistent optical potential for incident and emitted low-energy α particles **III.** Nonstatistical processes induced by neutrons on Zr, Nb, and Mo nuclei

WPBB-S.05.02-T001-D005

Zr,Nb,Mo(n,α)

frontiers | Frontiers in Physics

DOI 10.3389/fphy.2023.1142436

Consistent assessment of neutron-induced activation of ^{93}Nb

WPBB-S.05.02-T005-D007

Nb(n,x)

Phys. Lett. B 858 (2024) 139078



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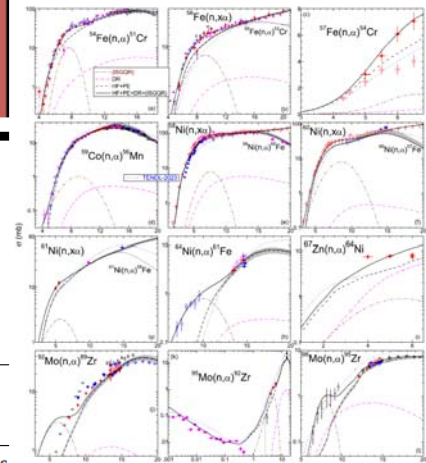
Physics Letters B

journal homepage: www.elsevier.com/locate/physletb



WPBB-S.05.02-T007-D004

$^{91}\text{Zr}(n,\alpha)^{88}\text{Sr}$ +



Letter

Giant quadrupole resonances within neutron-induced α -particle emission?

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ARTICLE INFO

ABSTRACT

Editor: A. Schwenk

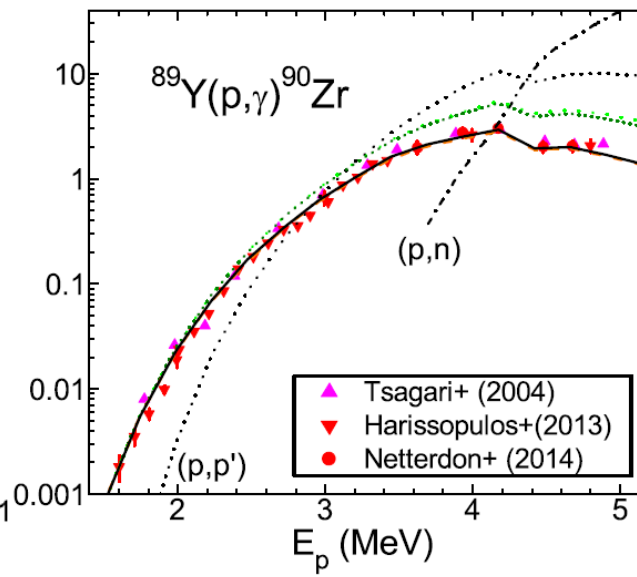
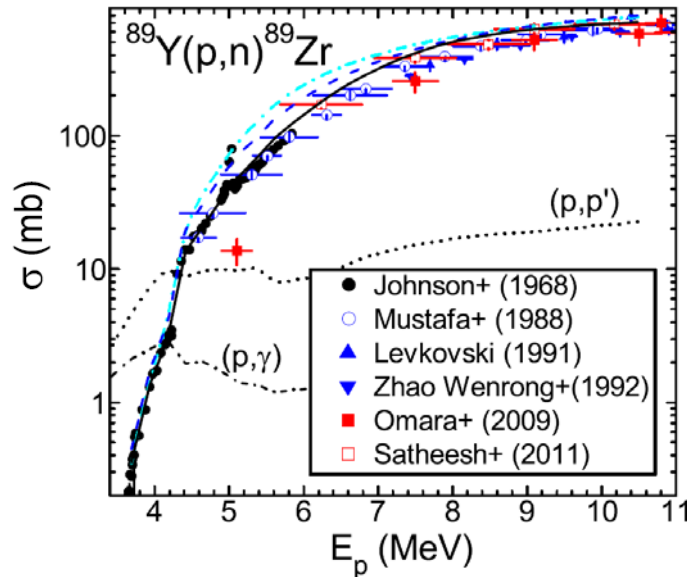
The particular conditions for the recent measurement of $^{91}\text{Zr}(n,\alpha)^{88}\text{Sr}$ reaction cross sections at incident energies

[E.D. Arthur – P.G. Young, LANL, '80]

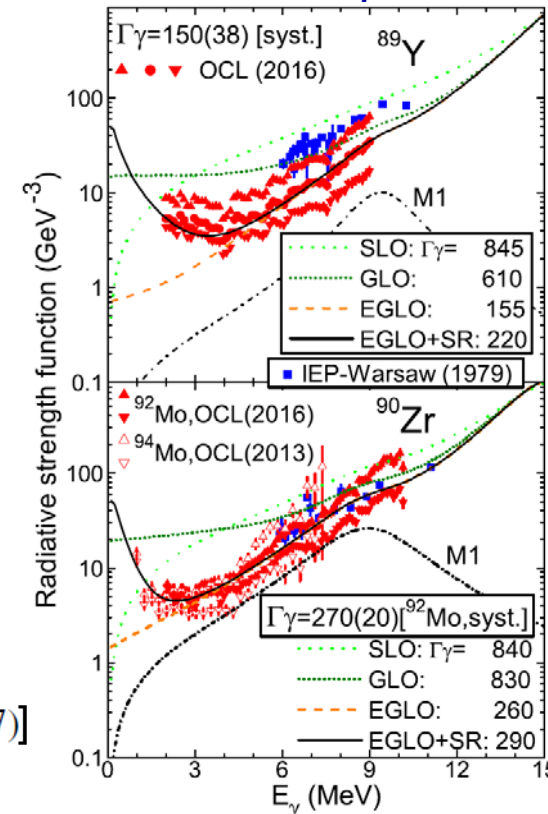
[EFFDOC-1518(Nov.2023)]+

YES

- i. unitary use of *common model parameters* for different mechanisms
- ii. use of *consistent sets of input parameters (IP)* validated by *analyses of various independent experimental data* (e.g., other than activation)
- iii. unitary account of whole body of related experimental data for isotope chains and *neighboring elements*



[PHYSICAL REVIEW C **96**, 044610 (2017)]



NO re-normalization or free parameters (**widely-used within ND libraries**)

OPTICAL MODEL: prime tool for all cross section calculations

- ❖ Phenomenological OMP (global parameter sets): still extensively used
- ❖ Microscopic OPs: reduced uncertainties (e.g., OM ambiguities)

▪ **Pure elastic scattering OP analysis**

SCAT2 [O. Bersillon]

- phenomenological OP
- + semi-microscopic (DF) OP →
(M. Avrigeanu - local version)

Phys. Rev. C **62** (2000) 017001
Nucl. Phys. A **693** (2001) 616
Eur. Phys. J. A **12** (2001) 399
Int. J. of Mod. Phys. E **11** (2002) 249
Nucl. Phys. A **723** (2003) 104
Nucl. Phys. A **759** (2005) 327
Nucl. Phys. A **764** (2006) 246

▪ **DWBA / Coupled Reaction Channel (CRC)**

FRESCO-2003 [I.J. Thompson]: **(n,α), (p,α) PICK-UP**

▪ **Composite system equilibration**

- **Geometry Dependent Hybrid (GDH)** preequilibrium-emission model
- **Hauser-Feshbach (HF)** statistical model

STAPRE-H95 [V. Avrigeanu, M. Avrigeanu] (updated)

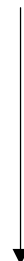
▪ **Giant Quadrupole Resonance (GQR)** [PLB **613**,128 (2005), NPA **764**, 246 (2006)]

- **Gaussian: $E_{0,GQR} = 64/A^{1/3}$ MeV** (phenomenologically: $\Gamma \sim 1$ MeV, $\sigma \sim 1$ mb)
[M.N. Harakeh and A. van der Woude, *Giant Resonances*, Oxford,2001]

LOCAL APPROACH:

STAPRE-H95 (updated-2020) [OM/PE/SM: SCAT2, GDH, HF]

- n/p- spherical OMP: Koning-Delaroche, Nucl.Phys. **A713**, 231 (2003)
- α - spherical OMP: V. Avrigeanu+, PRC **90**, 044612 (2014)
- Nuclear-level density ($E > E_d$ [ENSDF]): **BSFG**: [DOI: 10.1103/PhysRevC.107.034613]
 - + $E^* < S$: (a, Δ) by fit of **D0 (RIPL-3)** & **Nd (ENSDF, RIPL3)**
 - + $E^* > S$: $a(E^*)$ [A.R. Junghans+, NPA **629**, 635 (1998),
A.J. Koning+, PRC **56**, 970 (1997)]
 - + I/I_r : $1/2(gs)-3/4(S)-1(15 \text{ MeV})$
[V.Avrigeanu+, JNST **S2**, 746(2002);
M.Avrigeanu+, PRC **85**, 044618 (2012)]



Fitted level and resonance data									
Nucleus	N_d	E_d^* (MeV)	N_d	E_d^* (MeV)	$S + \frac{\Delta E}{2}$ (MeV)	I_0	$D_0^{\text{exp } a}$ (keV)	a (MeV $^{-1}$)	Δ (MeV)
^{88}Sr	47	4.801	47	4.801	11.113	9/2	0.29(8)	8.70	1.63
^{91}Zr	37	3.053	37	3.053	7.260	0	6.0(14)	9.77	0.40
^{92}Zr	42	3.500	54(2)	3.725	8.647	5/2	0.55(10)	9.67(27)(25)	0.79(9)(6)

^aRIPL-3 [22] if not otherwise mentioned.

- γ -ray strength functions: E1 [EGLO/OCL: NDS **163**, 109(2020), PRC **94**, 025804(2016)]
[IAEA CRP-photonuclear]; M1 [SLO + upbend, PRC **94**, 025804 (2016)]
- PE: Geometry Dependent Hybrid model [M. Blann+, PRC **28**, 1493 (1984)]
 - + J^π -conservation [Z.Phys. A **329**, 177(1988)]
 - + $g_p(u) \sim u$, $A_K(p, h)$, $f_K(p, h, E, F_1(I, E_i))$ [Phys. Rev. C **58**, 295 (1998)], $F=40 \text{ MeV}$
 - + α -emission: [Milano approach, ZPA **329**, 177 (1988)] replaced by $g_\alpha = (6/\pi^2)a$

2.2. Analysis of 2022 first (n,α) data/question (91Zr)

(1/2)



[EFFDOC-1518 (Nov.2023)]

Cross sections of the $^{91}\text{Zr}(n, \alpha)^{88}\text{Sr}$ reaction in the 3.9–5.3 MeV neutron energy region

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(Received 20 July 2022; accepted 17 November 2022; published 8 December 2022)

Cross sections of the $^{91}\text{Zr}(n, \alpha)^{88}\text{Sr}$ reaction were measured at four incident neutron energies in the range of 3.9 to 5.3 MeV. The experiment was carried out on the Van de Graaff accelerator EG-100 at the Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia. Fast neutrons were produced by the $^2\text{H}(d, n)^3\text{He}$ reaction with a deuterium gas target. A twin gridded ionization chamber (GIC) charged particle detector, in which ^{91}Zr back-to-back samples on a tantalum backing were placed as cathode and anode. The relative and absolute neutron fluxes were measured using two $^{238}\text{U}_3\text{O}_8$ samples. Cross-section data obtained in this measurement were compared with those in existing data and theoretical calculations using TALYS code. The present data for the $^{91}\text{Zr}(n, \alpha)^{88}\text{Sr}$ reaction show **clarifying the discrepancies in various published nuclear evaluation data**. An alpha clustering factor was determined using the statistical model and knock-on mechanism.

(n,α₀) - cross sections measured

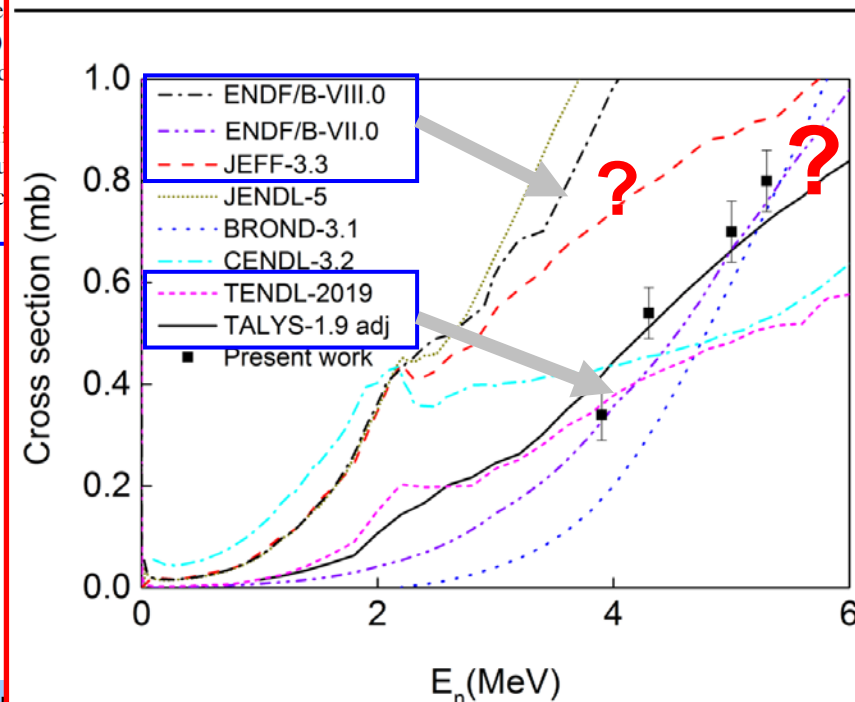
(n,α₁) - cross sections by TALYS

(n,α_{0,1}) – c.s. deduced

At variance with:

- PRC **107**, 034613 (2023): $^{90-92,94,96}\text{Zr}(n,x)$
Avrighanu+ (submitted: 21 Oct. 2022)
- PRC **34**, 2065 (1986): $^{90,91}\text{Zr}(n,\alpha)$, $d\sigma/dE$
Gadioli+, $E_n=14.3, 18.15$ MeV,
pick-up support !

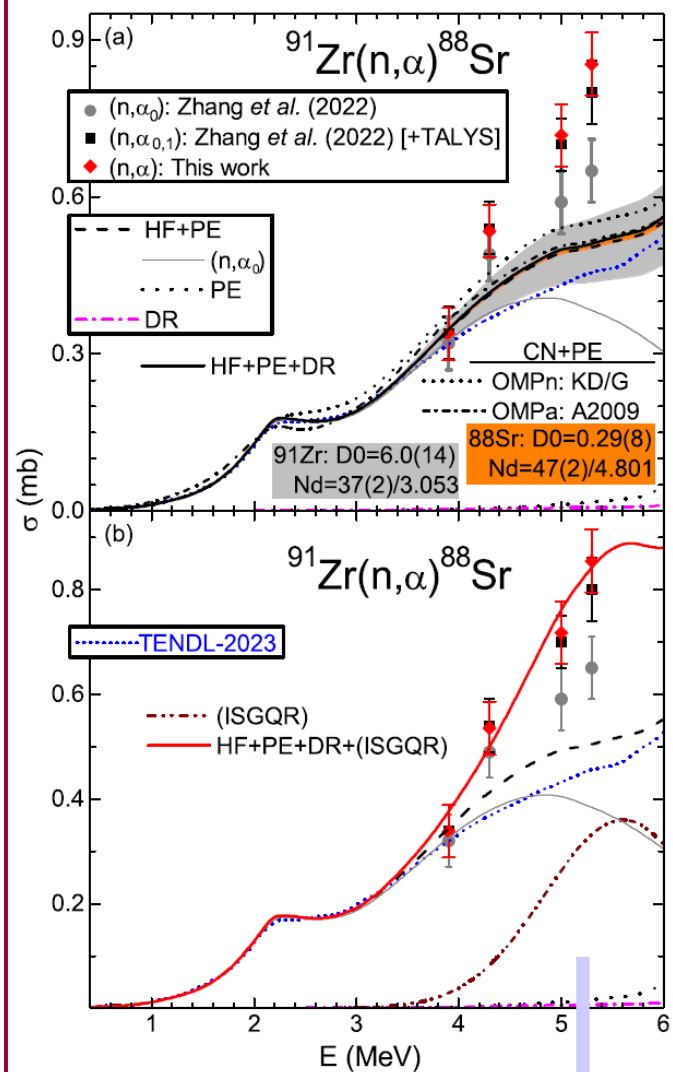
GUOHUI ZHANG *et al.*



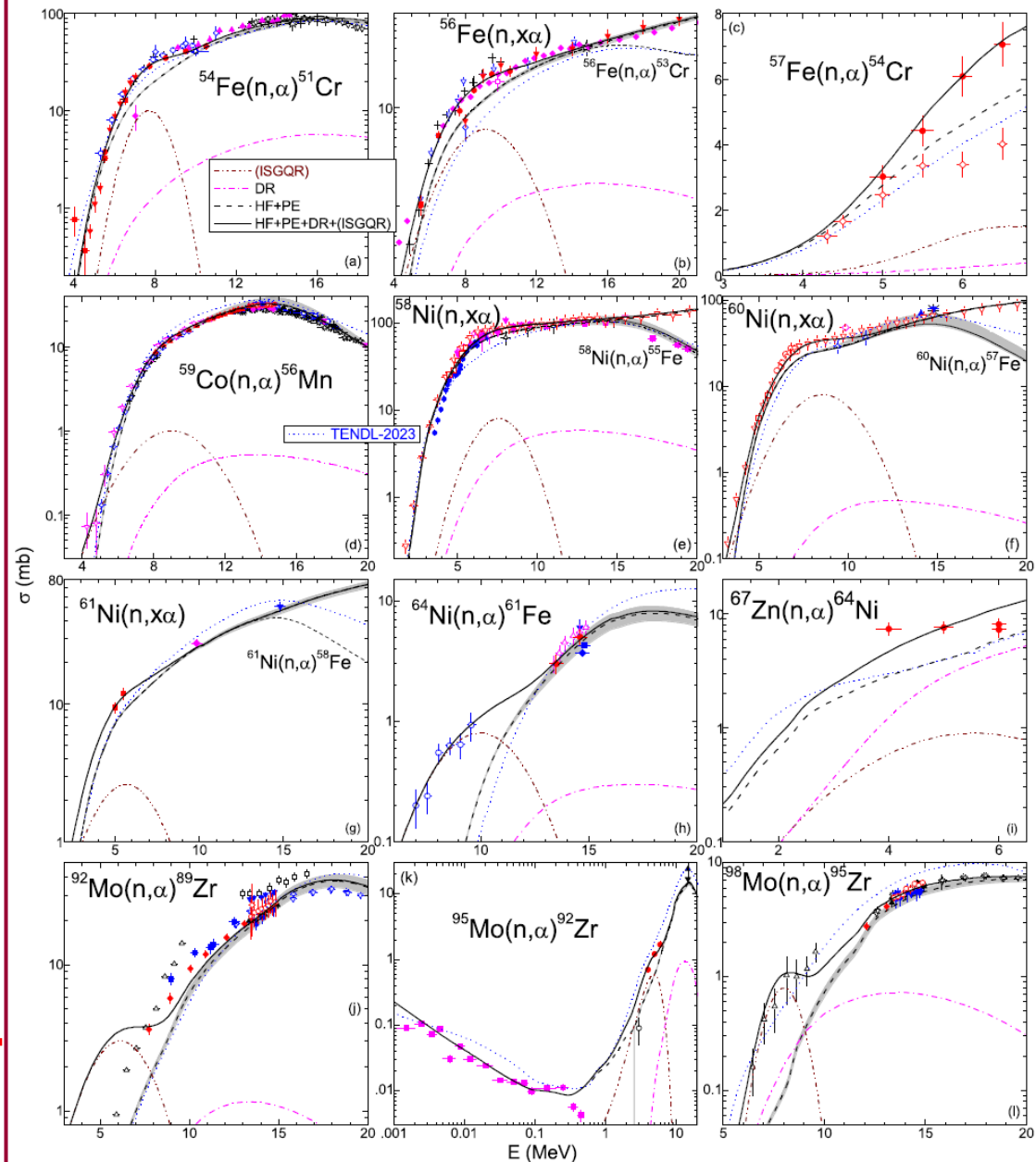
Physics Letters B 858 (2024) 139078

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4.3(24) %EWSR !!!



3. EWSR systematics: (α,α') , (γ,α) , (n,α) reactions

(1/2)



[EFFDOC-1538(Apr.2024)]

ISGQR:

$$S_{-2}^{E2} = \int \sigma^{GQR} dE / E^2 = (1/E_0^2) \int \sigma^{GQR} dE$$

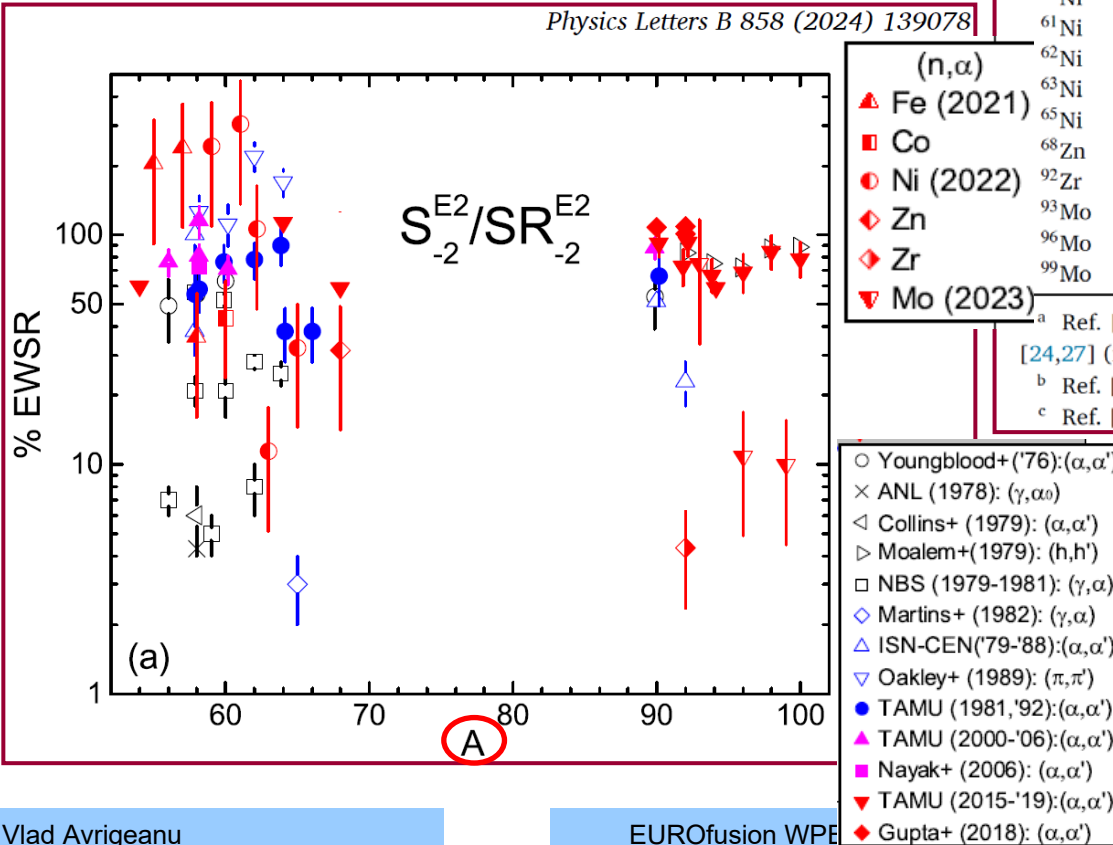
K. Raghunathan, L. L. Rutledge, R. E. Segel, and L. Meyer-Schützmeister. Phys. Rev. C **22**, 2409 (1980).

EWSR (energy weighted sum rule):

$$SR_{-2}^{E2} = 0.22 Z^2 A^{-1/3} \mu b / \text{MeV}$$

E. Kuhlmann, E. Ventura, J. R. Calarco, D. G. Mavis, and S. S. Hanna, Phys. Rev. C **11**, 1525 (1975),

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M. Avrigeanu and V. Avrigeanu

Table 1

The ISGQR energies [24] and the ISGQR-like peak cross sections and FWHM for neutron-induced α -emission (given in this work if not otherwise mentioned) and ISGQR Gaussian distribution, the corresponding integrated yields and ISGQR strength functions S_{-2}^{E2} as well as their EWSR fractions SR_{-2}^{E2} .

Excited nucleus	E_0 [24] (MeV)	σ_0 (mb)	Γ (MeV)	$\int \sigma^{GQR} dE$ (mb MeV)	S_{-2}^{E2} ($\mu b / \text{MeV}$)	SR_{-2}^{E2} (%)
^{55}Fe	16.829	10^a	2.1^a	22.6	79.7	204
^{57}Fe	16.630	6^a	4^a	25.6	92.5	239
^{58}Fe	16.534	1.5^a	2.4^a	3.76	13.8	35.8
^{60}Co	16.348	1	4.5	4.8	17.8	43.5
^{59}Ni	16.440	8^b	3.4^b	29.1	108	243
^{61}Ni	16.258	8^b	4.1^b	35.1	133	303
^{62}Ni	16.170	2.6^b	4.4^b	12.1	46.1	106
^{63}Ni	16.084	0.3^b	4^b	1.28	4.9	11.4
^{65}Ni	15.918	0.8^b	4.1^b	3.51	13.9	32.3
^{68}Zn	15.680	0.9	3.9	3.76	15.3	31.5
^{92}Zr	14.177	0.36	1.8	0.68	3.4	4.3
^{93}Mo	14.126	3^c	4^c	12.8	64.1	74.8
^{96}Mo	13.977	0.6^c	2.8^c	1.81	9.2	10.9
^{99}Mo	13.835	0.8^c	1.9^c	1.6	8.4	10

^a Ref. [13], with eventual minor changes due to slightly different ISGQR energies [24,27] (including an improved account for the excited nucleus ^{57}Fe).

^b Ref. [14], as above.

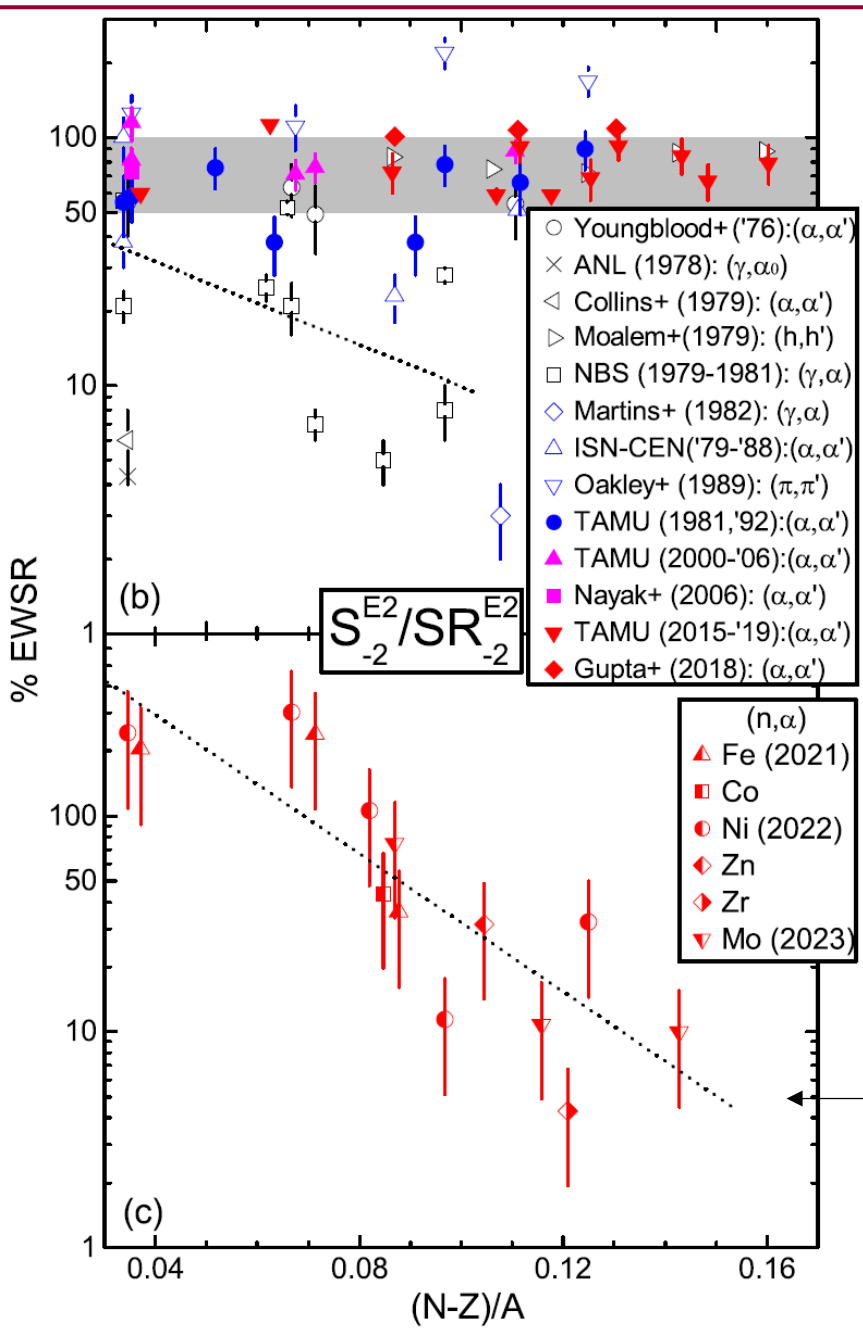
^c Ref. [8], as above.

3. EWSR systematics: (α, α') , (γ, α) , (n, α) reactions

(2/2)



[EFFDOC-1538(Apr.2024)]



ISGQR: 50-100% of EWSR ($\pm 25\%$)

[M. N. Harakeh and A. van der Woude, *Giant Resonances Fundamental High-Frequency Modes of Nuclear Excitation* (Oxford University Press, New York, 2001) , p. 184]

Fig. 3. Comparison of EWSR fractions of ISGQR-like strength functions for neutron-induced α -emission on target nuclei with $54 \leq A \leq 98$ (Table 1), and ISGQR strength functions measured by inelastic scattering of ^3He and α -particles, and (γ, α) reaction [9,26,31,36–53], vs. (a) mass number A and (b,c) the $(N - Z)/A$ asymmetry parameter. There are included (b) the band of systematic values between 50–100% for the latter data, and a linear fit (dotted line) of the (γ, α) measurements [39,40,42], and (c) a linear fit (dotted line) of the neutron-induced α -emission results.

'effective' Q-value effect

[(n,p), (n,α) reactions "isotope effect":

D.G. Gardner: NP **29**, 73 (1962);

H.L. Pai et al., NPA **164**, 526 (1971): $Q'_{(a,b)} = Q_{(a,b)} + \Delta_A - \Delta_B$

N.I. Molla, S.M. Qaim: NPA **283**, 269 (1977)]

4. (n,α) ISGQR / EWSR systematics vs. G_{sys} (2001) and Lorentzian ISGQR (1/4)



[PLB 858 (2024) 139078 Suppl. Material: <https://www.sciencedirect.com/science/article/pii/S0370269324006361#ec0010>:

The ISGQR systematics' widths and Lorentzian shapes use within neutron-induced α-emission analysis

Table 1

The ISGQR energies [24] and the ISGQR-like peak cross sections given in this work (if not previously^{a,b,c}) for neutron-induced α-emission, corresponding to ISGQR Gaussian distribution with either the average FWHM value of $(16.0 \pm 1.8)/A^{1/3}$ MeV [24] or its lower limit^d $14.2/A^{1/3}$ MeV, the corresponding integrated yields and ISGQR strength functions $S_{-2}^{E_2}$ as well as their EWSR fractions $SR_{-2}^{E_2}$.

Excited nucleus	E_0 [24] (MeV)	σ_0 (mb)	Γ (MeV)	$\int \sigma^{GQR} dE$ (mb MeV)	$S_{-2}^{E_2}$ (μb/MeV)	$S_{-2}^{E_2}$ (% $SR_{-2}^{E_2}$)
⁵⁵ Fe	16.829	4	3.73 ^d	15.9	56.1	144
⁵⁷ Fe	16.630	6 ^a	4.16	26.6	96.0	248
⁵⁸ Fe	16.534	0.8	3.67 ^d	3.12	11.4	29.7
⁶⁰ Co	16.348	1	4.09	4.35	16.3	39.7
⁵⁹ Ni	16.440	8 ^b	3.65 ^d	31.1	115	259
⁶¹ Ni	16.258	8 ^b	4.07	34.6	131	299
⁶² Ni	16.170	2.6 ^b	4.04	11.2	42.8	98.2
⁶³ Ni	16.084	0.3 ^b	4.02	1.28	5.0	11.5
⁶⁵ Ni	15.918	0.8 ^b	3.98	3.39	13.4	31.2
⁶⁸ Zn	15.680	0.9	3.92	3.76	15.3	31.5
⁹² Zr	14.177	0.24	3.15 ^d	0.804	4.0	5.1
⁹³ Mo	14.126	3 ^c	3.53	11.3	56.5	66.0
⁹⁶ Mo	13.977	0.6 ^c	3.10 ^d	1.98	10.1	12.0
⁹⁹ Mo	13.835	0.5	3.07 ^d	1.63	8.5	10.2

^aRef. [13], with eventual minor changes due to slightly different ISGQR energies [24,27].

^bRef. [14], as above.

^cRef. [8], as above.

[24] M. N. Harakeh and A. van der Woude, *Giant Resonances Fundamental High-Frequency Modes of Nuclear Excitation* (Oxford University Press, New York, 2001).

Table 2

The ISGQR energies and lower limit $14.2/A^{1/3}$ MeV of the average FWHM values [24], and the ISGQR-like peak cross sections given in this work (if not previously^{a,b,c}) for neutron-induced α-emission and ISGQR Lorentzian distribution, the corresponding integrated yields and ISGQR strength functions $S_{-2}^{E_2}$ as well as their EWSR fractions $SR_{-2}^{E_2}$.

Excited nucleus	E_0 [24] (MeV)	σ_0 (mb)	Γ (MeV)	$\int \sigma^{GQR} dE$ (mb MeV)	$S_{-2}^{E_2}$ (μb/MeV)	$S_{-2}^{E_2}$ (% $SR_{-2}^{E_2}$)
⁵⁵ Fe	16.829	4	3.73	23.5	82.8	212
⁵⁷ Fe	16.630	6 ^a	3.71	34.8	126	325
⁵⁸ Fe	16.534	0.8	3.67	4.61	16.9	43.9
⁶⁰ Co	16.348	1	3.63	5.70	21.3	52.0
⁵⁹ Ni	16.440	8 ^b	3.65	45.8	170	383
⁶¹ Ni	16.258	8 ^b	3.61	45.3	172	391
⁶² Ni	16.170	2.6 ^b	3.59	14.7	56.0	129
⁶³ Ni	16.084	0.3 ^b	3.57	1.68	6.5	15.0
⁶⁵ Ni	15.918	0.8 ^b	3.53	4.44	17.5	40.8
⁶⁸ Zn	15.680	0.9	3.48	4.92	20.0	41.2
⁹² Zr	14.177	0.24	3.15	1.19	5.9	7.6
⁹³ Mo	14.126	3 ^c	3.13	14.8	74.0	86.4
⁹⁶ Mo	13.977	0.6 ^c	3.10	2.92	15.0	17.7
⁹⁹ Mo	13.835	0.5	3.07	2.41	12.6	15.0

^aRef. [13], with eventual minor changes due to slightly different ISGQR energies [24,27].

First of all, it should be noted that the ISGQR-like widths for five of the fourteen nuclei in Table 1 (⁵⁵Fe, ^{61,63,65}Ni, ⁶⁸Zn) agree within 4% with the average value $\Gamma = (16.0 \pm 1.8)/A^{1/3}$ MeV [24]. Additionally, the widths are even higher by 9%–13% for three other nuclei (⁶⁰Co, ⁶²Ni, ⁹³Mo) in this table, but roughly lower for the remaining ones (^{55,58}Fe, ⁵⁹Ni, ⁹²Zr, ^{96,99}Mo). Despite

4. (n,α) ISGQR / EWSR systematics vs. G_{sys} (2001) and Lorentzian ISGQR (2/4)



[PLB 858 (2024) 139078 Suppl. Material: <https://www.sciencedirect.com/science/article/pii/S0370269324006361#ec0010>]

The ISGQR systematics' widths and Lorentzian shapes use within neutron-induced α -emission analysis

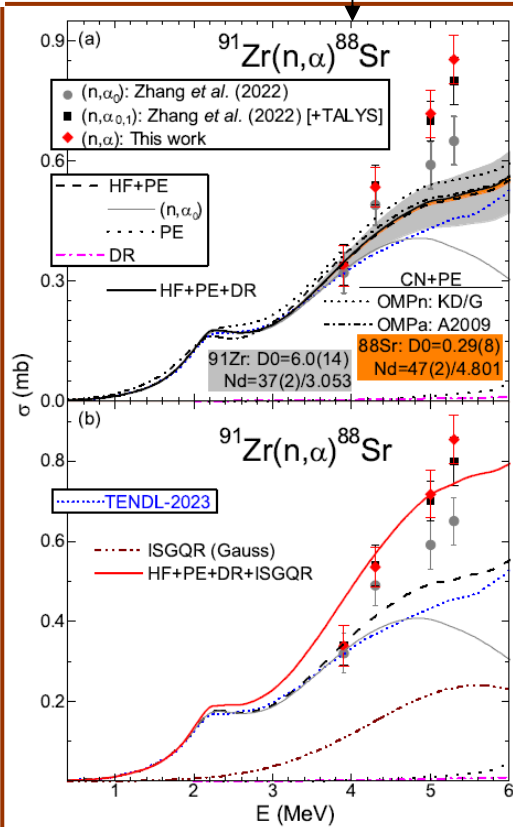


Fig. 1. (Color online) Comparison of cross sections measured [1] (symbols with error-bars) with model calculations (solid and dashed curves). Panels show measured data for $^{91}\text{Zr}(n,\alpha_0)^{88}\text{Sr}$ reaction (circles) and deduced for $(n,\alpha_{0,1})$ reaction [1] (squares) and (n,α) reaction (diamonds), and compare them to calculated values for (n,α) reaction DR (dash-dotted), PE (dotted), and HF+PE (dashed) components. In particular, we show (a) HF+PE+DR sum (solid), HF+PE uncertainty bands related to the error bars of fitted N_d and D_0^{exp} by level densities of target ^{91}Zr (gray) and residual nucleus ^{88}Sr (orange), and HF+PE results using other OMPs for α -particles [22] (short-dash-dotted) or neutrons [23] (short-dashed), and (b) the ISGQR component corresponding to a Gaussian distribution for the extra-yield beyond the DR+PE+CN calculated cross sections (dash-dot-dotted), and HF+PE+DR+ISGQR sum (solid).

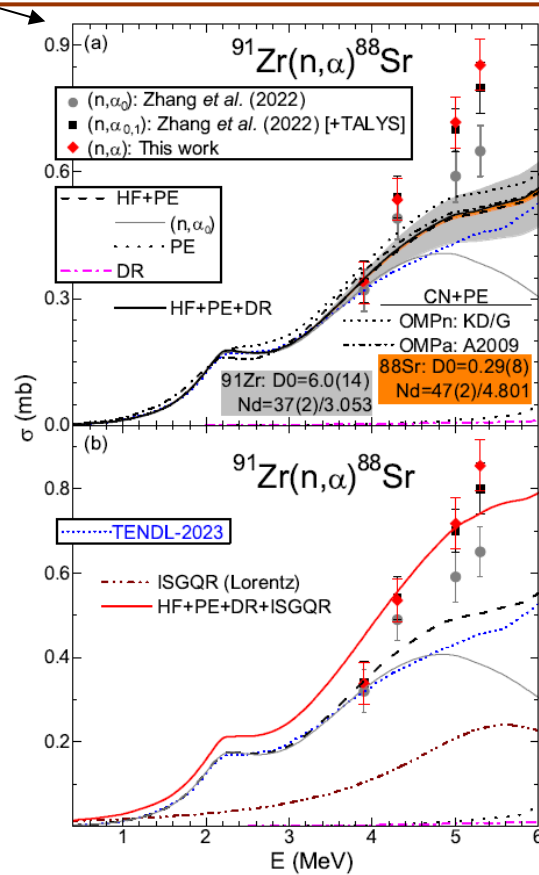


Fig. 4. (Color online) As Fig. 1 but for assumption of a Lorentzian distribution for the extra-yield beyond the DR+PE+CN calculated cross sections (dash-dot-dotted).

4. (n,α) ISGQR / EWSR systematics vs. G_{sys} (2001) and Lorentzian ISGQR (3/4)



[PLB 858 (2024) 139078 Suppl. Material: <https://www.sciencedirect.com/science/article/pii/S0370269324006361#ec0010>:

The ISGQR systematics' widths and Lorentzian shapes use within neutron-induced α-emission analysis

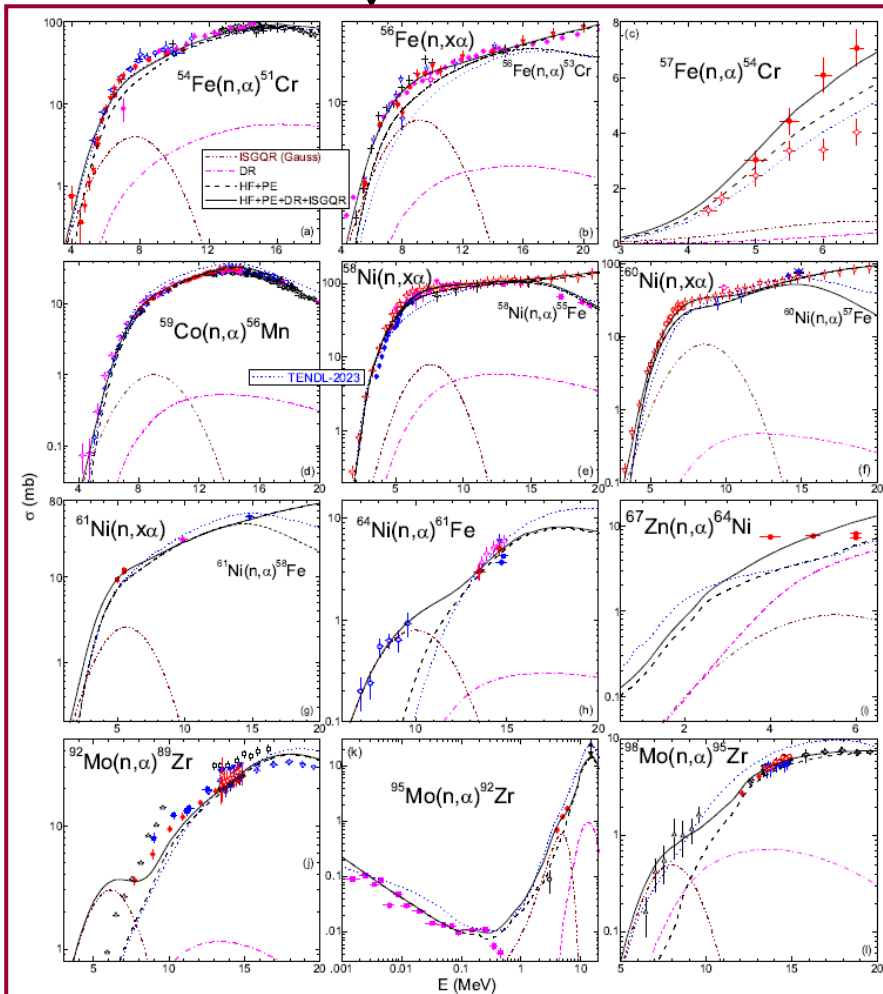


Fig. 2. (Color online) Comparison of measured [15] and calculated neutron-induced α -emission cross sections (solid curves) for $^{54,56,57}\text{Fe}$, ^{59}Co , $^{58,60,61,62,64}\text{Ni}$, ^{67}Zn , and $^{92,95,98}\text{Mo}$ target nuclei, including the ISGQR (dash-dot-dotted), DR (dashed), and HF+PE (dashed) components, and HF+PE uncertainty bands for the residual-nuclei level densities [8,13,14]. The ISGQR components correspond to a Gaussian distribution (Table 1) for the extra-yield beyond the DR+PE+CN calculated cross sections.

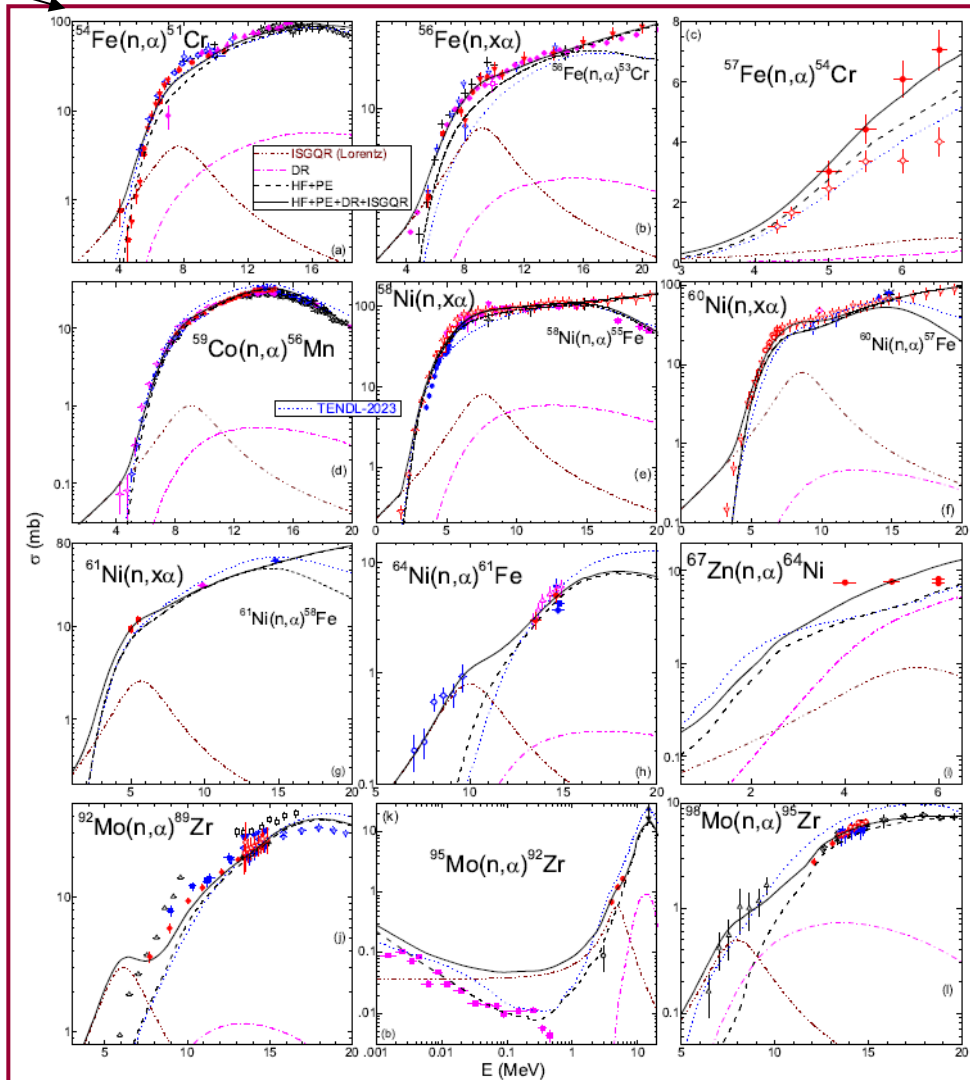


Fig. 5. (Color online) As Fig. 2 but for ISGQR components corresponding to the assumption of a Lorentzian distribution (Table 2) for the extra-yield beyond the DR+PE+CN calculated cross sections.

4. (n,α) ISGQR / EWSR systematics vs. G_{sys} (2001) and Lorentzian ISGQR (4/4)



[PLB 858 (2024) 139078 Suppl. Material: <https://www.sciencedirect.com/science/article/pii/S0370269324006361#ec0010>:

The ISGQR systematics' widths and Lorentzian shapes use within neutron-induced α-emission analysis

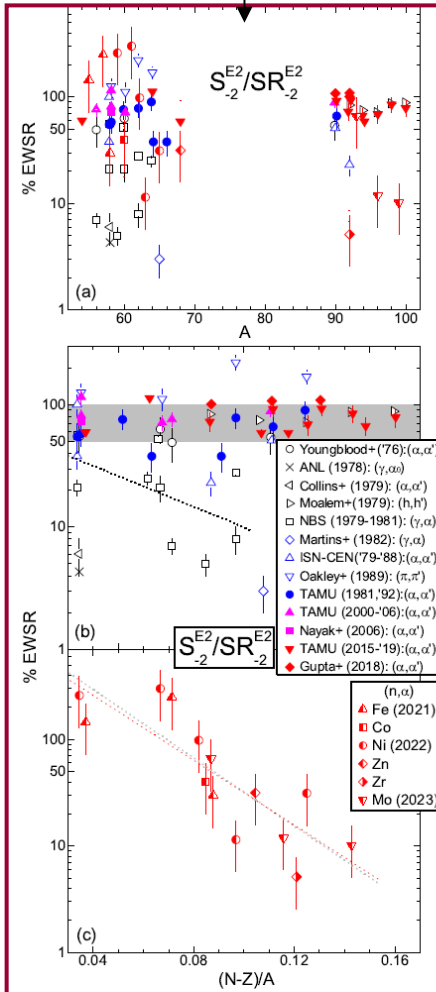


Fig. 3. (Color online) Comparison of EWSR fractions of ISGQR strength functions for neutron-induced α-emission on target nuclei with $54 \leq A \leq 98$ (Table 1), and ISGQR strength functions measured by inelastic scattering of ^3He and α-particles, and (γ, α) reaction [9,26,31,36–53], vs. (a) mass number A and (b,c) the $(N - Z)/A$ asymmetry parameter. There are included (b) the band of systematic values between 50–100% for the latter data, and a linear fit (dotted line) of the (γ, α) measurements [39,40,42], and (c) a linear fit (dotted line) of the neutron-induced α-emission results.

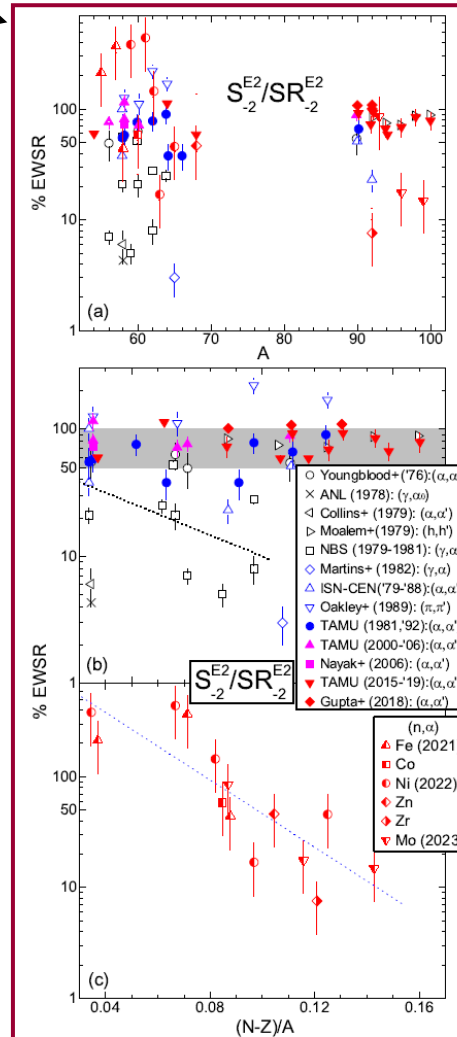


Fig. 6. (Color online) As Fig. 3 but for ISGQR components corresponding to the assumption of a Lorentzian distribution (Table 2) for the extra-yield beyond the DR+PE+CN calculated cross sections.

4. Conclusions



Latest results concerning alpha-particle emission (confirmed):

- α -OMP A+(2014): suitable description [NO fit/normalization] + DI + (ISGQR)
- NO emitted α -particle OMP parameters
- (n,α) / (p,α) reaction systematical analysis
- ISGQR EWSR systematics: 50-100% [(α,α')] vs. 100-10% [(x,α)], $x=\gamma,n$
- Further, next to <https://conferences.iaea.org/event/368/contributions/31753/> poster at Compound Nuclear Reactions and Related Topics (CNR*24), July 8-12, 2024, Vienna, IAEA
 - ❖ Possible microscopic path: - H. Sasaki *et al.* (LANL), CNR*24, 31760
- P. Stevenson (Univ. Surrey), CNR*24, 31769
 - ❖ Preliminary new experimental data (Peking Univ., Beijing): $^{64,66,67}\text{Zn}(n,\alpha)$

Availability for (n,x) , (p,x) activation evaluation

[Fe, Co, Cu, Ni, Zn, Zr, Nb, Mo (2021-2023)
- available data analysis/description
- additional calculations on request]

Thank you for your attention !



PNIII-P4-PCE-2021-0642

UE fisci di



EUROfusion

WPBB-S.05.02-T007-D005

JEFF NDW, Session Fusion, Nov. 2024, EFFDOC-1546
(EUROfusion WPBB-S.05.02-T007 Monitoring meeting)

[https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1546.pdf]

Progress Report on deuteron-induced reaction analysis

[EUROfusion WPBB-S.05.02-T007-D005:
Advanced analysis of isomeric cross sections of deuteron-
induced reactions on A=90-100 nuclei]

Marilena Avrigeanu and Vlad Avrigeanu

Horia Hulubei National Institute for Physics & Nuclear Engineering, (IFIN-HH), Bucharest, Romania

Content

1. Introduction: **WPBB-S.05.02-T007-D005**
2. Comparative analysis of the CN and PE spin distribution options on
A=90-100 target nuclei
 - preeqspin 1
 - preeqspin 3
 - preeqspin 4
4. Conclusions

Task Specification (TS)

TS Title:	Nuclear Data Evaluations - 2024		
TS Ref. Nr.:	BB-S.05.02-T007	Task coordinator:	Dieter Leichtle
Status:	In review	Date:	14-Feb-2024

D005: Technical Specification: Advanced analysis of isomeric cross sections of deuteron-induced reactions on A=90-100 nuclei (IAP)

A suitable account of the measured ground and isomeric state excitation functions of deuteron-induced reactions on Zr and Mo stable isotopes and natural elements has been obtained within actual state-of-art TALYS calculations by amending the nuclear-level density (NLD) spin distribution cut-off parameter by a factor of 0.25 [EUROFUSION WPBB-PR(24) 36171]. Actually these results are in line with the most recent compilation of isomeric ratios of light particle induced reactions [At. Data Nucl.Data Tables **153**, 101583 (2023)]. On the other hand, a large amount of measured isomeric cross sections of reactions induced by deuterons on Nb [Phys. Rev. C **88**, 014612 (2013)] as well as neutrons on Mo [Phys. Rev. C **71**, 044617(2005)] was already well described using no spin cut-off adjustment but an advanced particle-hole state density [Comp. Phys. Comm. **112**, 191 (1998)] including a PE spin cut-off [Nucl. Sci. Eng. **92**, 440 (1986)]. These results agree with the previous conclusion that reduced values of the spin cut-off parameter, obtained from isomeric cross-section analysis, were artificial and resulted from the use of an improper pre-equilibrium (PE) spin distribution, namely the compound-nucleus (CN) spin distribution [Phys. Rev. C **80**, 044612 (2009)]. Therefore, an advanced analysis of isomeric cross sections of deuteron-induced reactions on A=90-100 nuclei is aimed in this work, next to the proper account of the contributions of all involved reaction mechanisms as the breakup, stripping, pick-up, PE and CN processes, with the results provided in the TALYS code format. At the same time it will be taken the advantage of becoming available similar data just measured at Ganil on Mo up to 40 MeV.

PM: 3 PM (IAP)	ID	Title	Start Date	End Date	RU	Del. Owner	AWP2024
							PM 50% standard
	BB-S.05.02-T007 - D005	Advanced analysis of isomeric cross sections of deuteron-induced reactions on A=90-100 nuclei	01-Jan-24	31-Dec-24	IAP	Marilena Avrigeanu	3.000

Dedicated projects to IFMIF and ITER: EURATOM, F4E, EUROfusion

PHYSICAL REVIEW C **79**, 044610 (2009)

Low and medium energy deuteron-induced reactions on ^{27}Al

PHYSICAL REVIEW C **84**, 014605 (2011)

Low and medium energy deuteron-induced reactions on $^{63,65}\text{Cu}$ nuclei

PHYSICAL REVIEW C **88**, 014612 (2013)

Low-energy deuteron-induced reactions on ^{93}Nb

PHYSICAL REVIEW C **89**, 044613 (2014)

Low energy deuteron-induced reactions on Fe isotopes

PHYSICAL REVIEW C **94**, 014606 (2016)

Deuteron-induced reactions on Ni isotopes

PHYSICAL REVIEW C **100**, 014607 (2018)

Consistent accounting of deuteron-induced reactions on ^{nat}Cr up to 60 MeV

PHYSICAL REVIEW C **101**, 024605 (2020)

Deuteron-induced reactions on manganese at low energies

PHYSICAL REVIEW C **104**, 044615 (2021)

Deuteron-induced reactions on ^{nat}Zr up to 60 MeV

Journal of Fusion Energy (2024) **43**:15

Modeling of Deuteron-Induced Reactions on Molybdenum at Low Energies

EURATOM

**d+Al,
d+Cu,
d+Nb**

**GRT 4 for
Low Energy (F4E)**

**d+Fe
d+Ni**

 **EUROfusion**
**d+Cr
d+Mn**

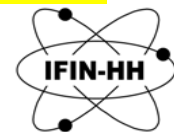
SPIRAL 2

d+Zr

 **EUROfusion**
d+Mo

Priority list of IFMIF-DONES candidate materials

Deuteron-nucleus interaction analysis



Motivation: Nuclear Data Needs: ITER, IFMIF, SPIRAL2, SARAF, Medical Installations

DEUTERONS BEAM

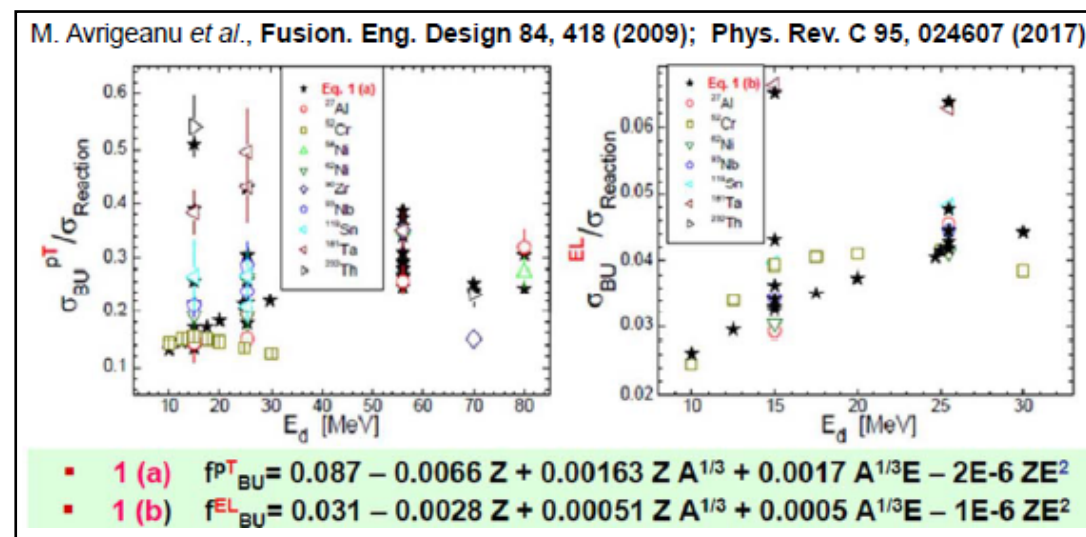
Associated Research Projects: New data & Updated theory
FENDL, EURATOM, F4E, EUROfusion

❑ **Breakup** – in **TALYS-1.96**, option **breakupmodel 2**: M. Avrigeanu *et al.*, Eur. Phys. J. A (2022) 58:3

BREAKUP [M. Avrigeanu, V. Avrigeanu]

- parametrization of total BU protons & elastic-breakup c.s.:

- inelastic breakup enhancement brought by breakup-nucleons reactions



❑ **Direct reactions**

FRESCO (Version **FRES 2.9**) [I.J. Thompson]

- **stripping & pick-up, DWBA** : (d,p), (d,n), (³He,d), (d,t), (d,α), (d,³He)

❑ **Composite system equilibration for both deuteron and breakup-nucleon reactions**

STAPRE-H95 [V. Avrigeanu, M. Avrigeanu] (updated)

- **OMP:SCAT2000**; preequilibrium (PE): **GDH / EXCITON**; evaporation: **Hauser-Feshbach**

TALYS - 1.0 - 1.97 [A. Koning, S. Hilaire, S. Goriely]

- **OMP:ECIS'97**; breakup, preequilibrium (PE): **MSD / EXCITON**; evaporation: **Hauser-Feshbach**

TALYS-2.0

Simulation of nuclear reactions

Arjan Koning, Stephane Hilaire, Stephane Goriely

$$\sigma^2 = \sigma_{\parallel}^2 = \sigma_F^2(E_x) = I_0 \frac{a}{\bar{a}} t,$$

with $\bar{a}$ from Eq. (8.13) and

$$I_0 = \frac{\frac{2}{5} m_0 R^2 A}{(\hbar c)^2}, \quad \text{moment of inertia of the nucleus } I_0 \quad (8.24)$$

thermodynamic temperature t ,

$$t = \sqrt{\frac{U}{a}}. \quad (8.22)$$

$$\sigma_F^2(E_x) = 0.01389 \frac{A^{5/3}}{\bar{a}} \sqrt{aU}. \quad (8.25)$$

On average, the $\sqrt{aU}/\bar{a}$ has the same energy- and mass-dependent behaviour as the temperature $\sqrt{U/a}$. The differences occur in the regions with large shell effects. Eq. (8.25) can be altered by

means of **Rspincut** = I/I_0 :

Range

$$0. \leq \text{Rspincut} \leq 10.$$

Default

Rspincut 1.

Fermi gas spin distribution

$$R_F(E_x, J) = \frac{2J+1}{2\sigma^2} \exp \left[-\frac{(J + \frac{1}{2})^2}{2\sigma^2} \right]$$

(8.23)

preeqspin

Flag to use the pre-equilibrium or compound nucleus spin distribution for the pre-equilibrium population of the residual nuclides. For backward-compatibility with earlier versions of TALYS, the following options are now possible:

Examples

preeqspin n or **preeqspin 1**: the pre-equilibrium spin distribution is made equal to the relative spin-dependent population after compound nucleus emission

preeqspin 2: the spin distribution from total level densities is adopted

preeqspin y or **preeqspin 3**: the pre-equilibrium spin distribution is based on particle-hole state densities

Range

y or n, or $1 \leq \text{preeqspin} \leq 3$.

Default

preeqspin n

12.3 Pre-equilibrium spin distribution

The function $R_n(J)$ represents the spin distribution of the states in the continuum. It is given by

$$R_n(J) = \frac{2J+1}{\pi^{1/2} n^{3/2} \sigma^3} \exp \left[-\frac{(J + \frac{1}{2})^2}{n \sigma^2} \right], \quad (12.59)$$

The used expression for the spin cut-off parameter σ is that by Gruppelaar et al. [108],

$$\sigma^2 = 0.24 n A^{\frac{1}{3}}. \quad (12.61)$$

Options 12.3.1 With **preeqspin y** (p. 596) Eq. (12.61) is invoked. Another option is the more a microscopic-based QRPA expression from Dupuis et al. [109].

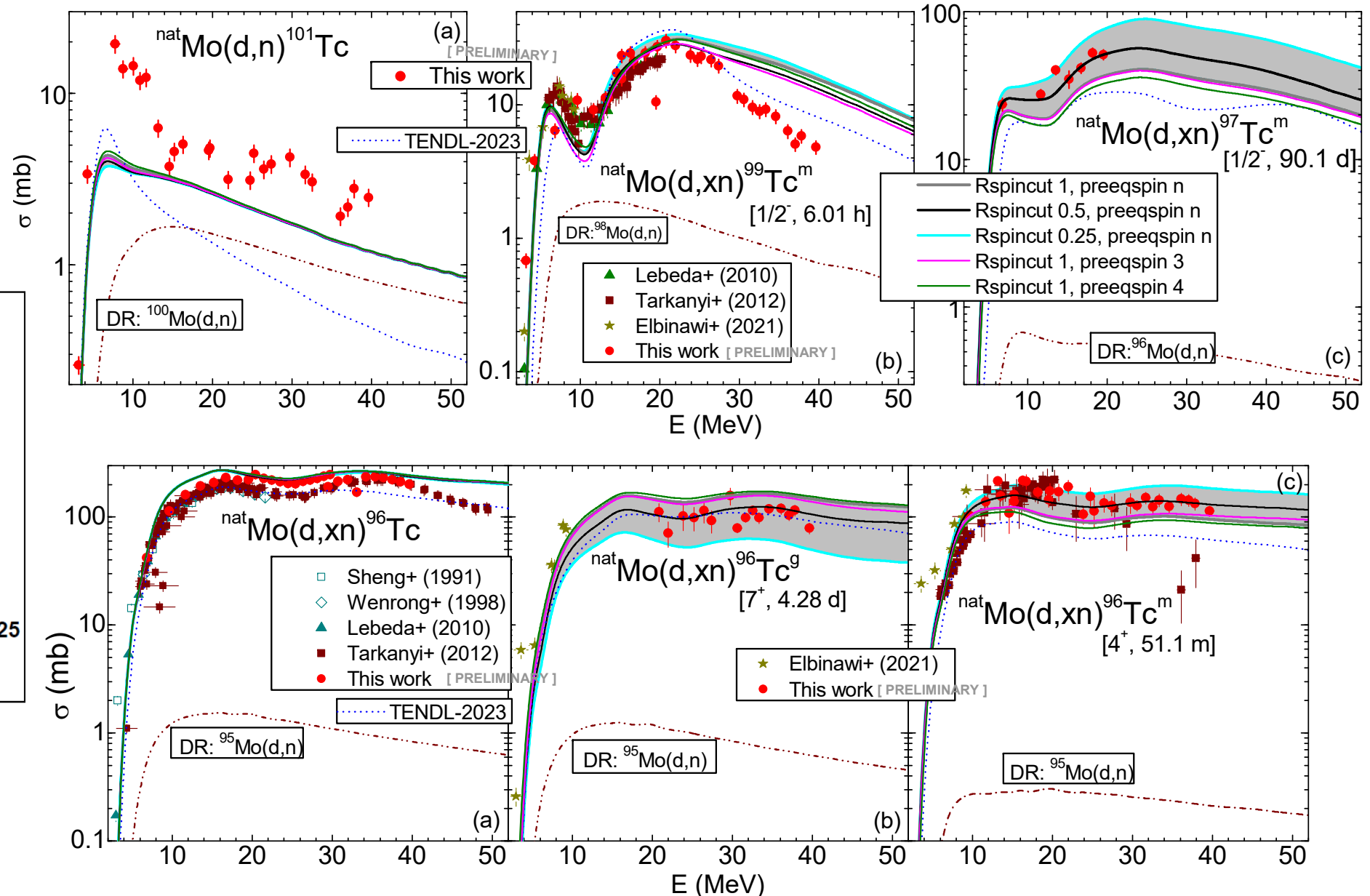
rspincutpreeq

- December 7, 2022

$$\sigma_n^2 = 0.04 n A^{2/3}$$

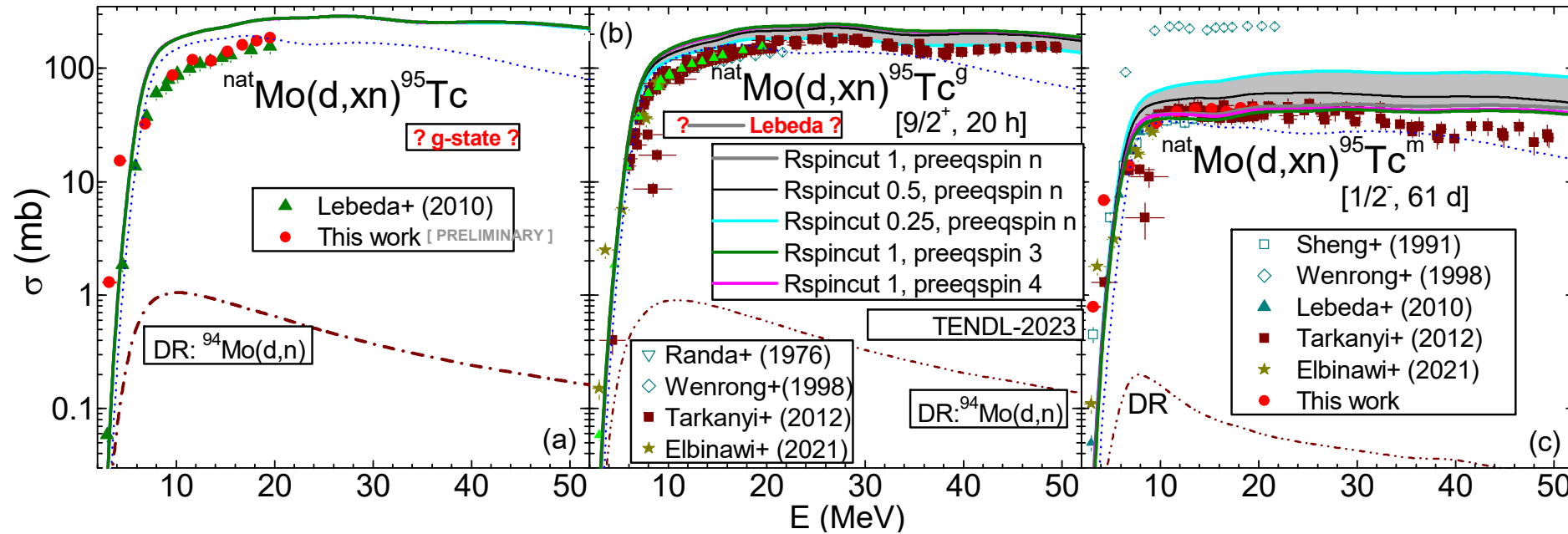
Added pre-equilibrium spin distribution model 'preeqspin 4' from Marc Dupuis inferred from JLM/QRPA calculations. Also added keyword 'Rspincutpreeq' to adjust pre-equilibrium spin cutoff parameter.

Effects of various options for level density spin distribution on $d + Mo$ (d, xn)



* decreasing I/I_0 ratio, Rspincut, or Rspincutpreeq (preeqspin 4), increases low spin isomeric states population

Effects of various options for level density spin distribution on $d + \text{Mo}$ (d, xn)-2

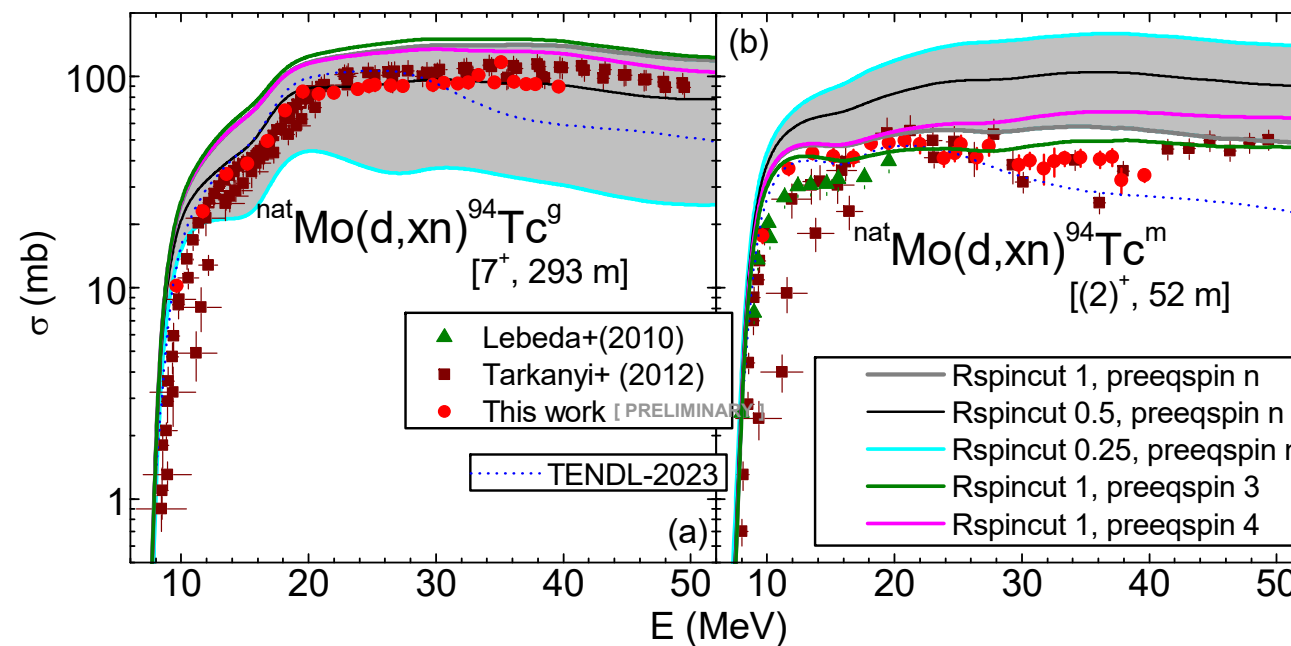


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energy energies
popeps 1.e-12
partable y

bins 100
breakupmodel 2
deuteronomp 2

Preeqspin 1/y/4
Rspincut 1.; 0.5; 0.25

filetotal y



Effects of various options for level density spin distribution on $d + Mo$ (d,xn)-3

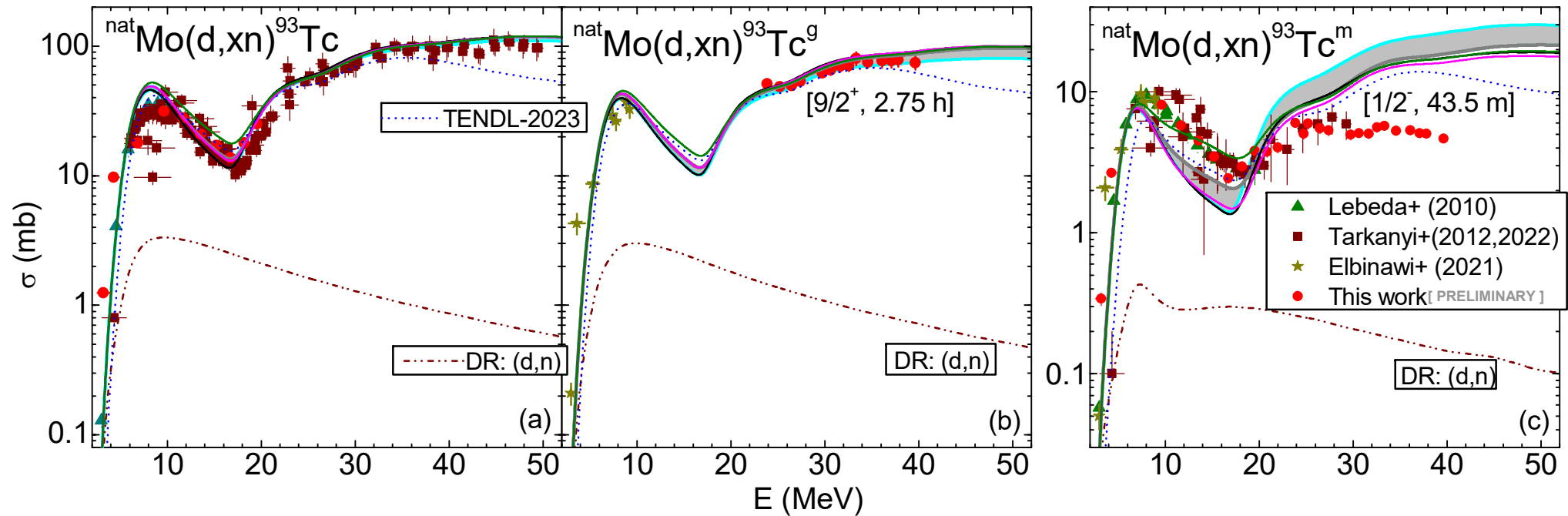
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mass 0
energy energies
popeps 1.e-12
partable y

bins 100
breakupmodel 2
deuteronomp 2

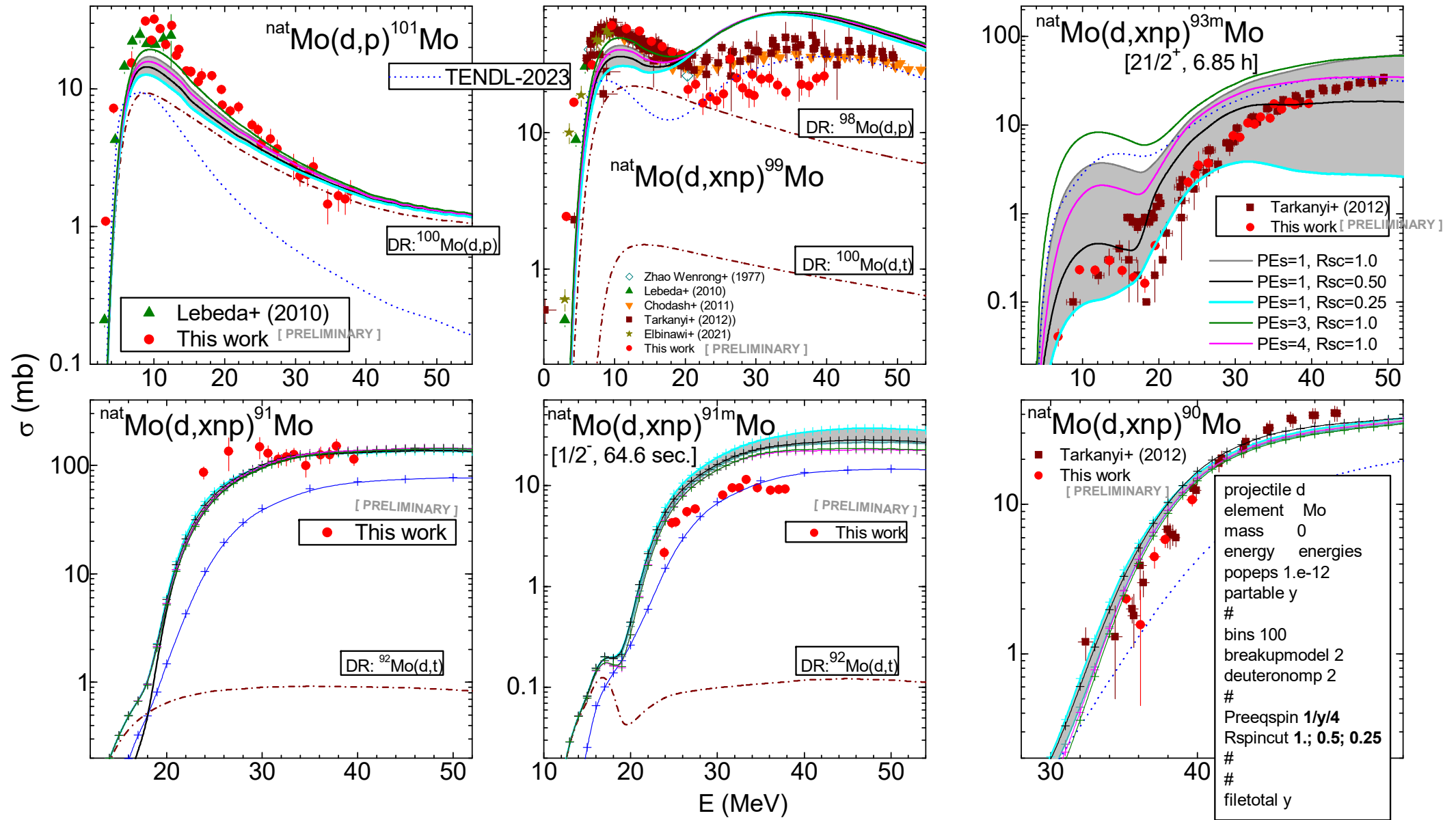
Preeqspin 1/y/4
Rspincut 1.; 0.5; 0.25

filetotal y

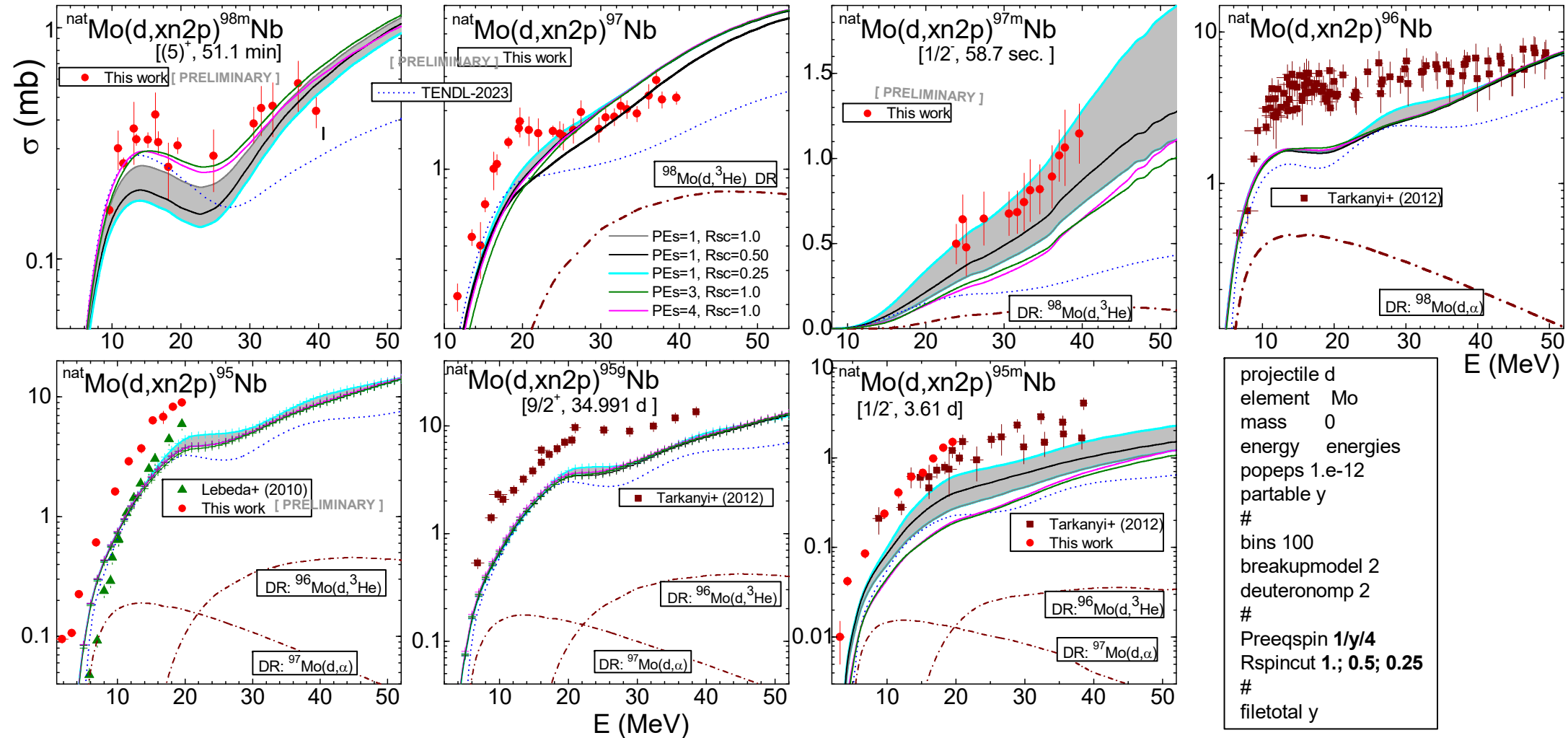
— Rspincut 1, preeqspin n
— Rspincut 0.5, preeqspin n
— Rspincut 0.25, preeqspin n
— Rspincut 1, preeqspin 3
— Rspincut 1, preeqspin 4



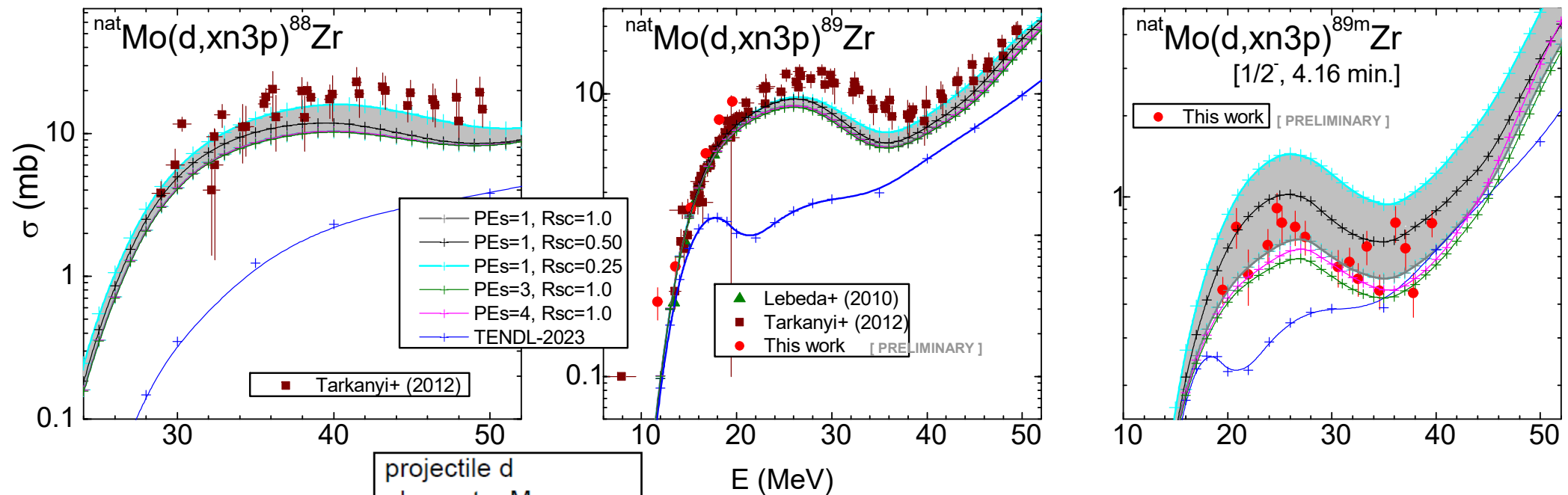
Effects of various options for level density spin distribution on $d + \text{Mo}$ (d, xnp)



Effects of various options for level density spin distribution on $d + \text{Mo}$ ($d, xn2p$)

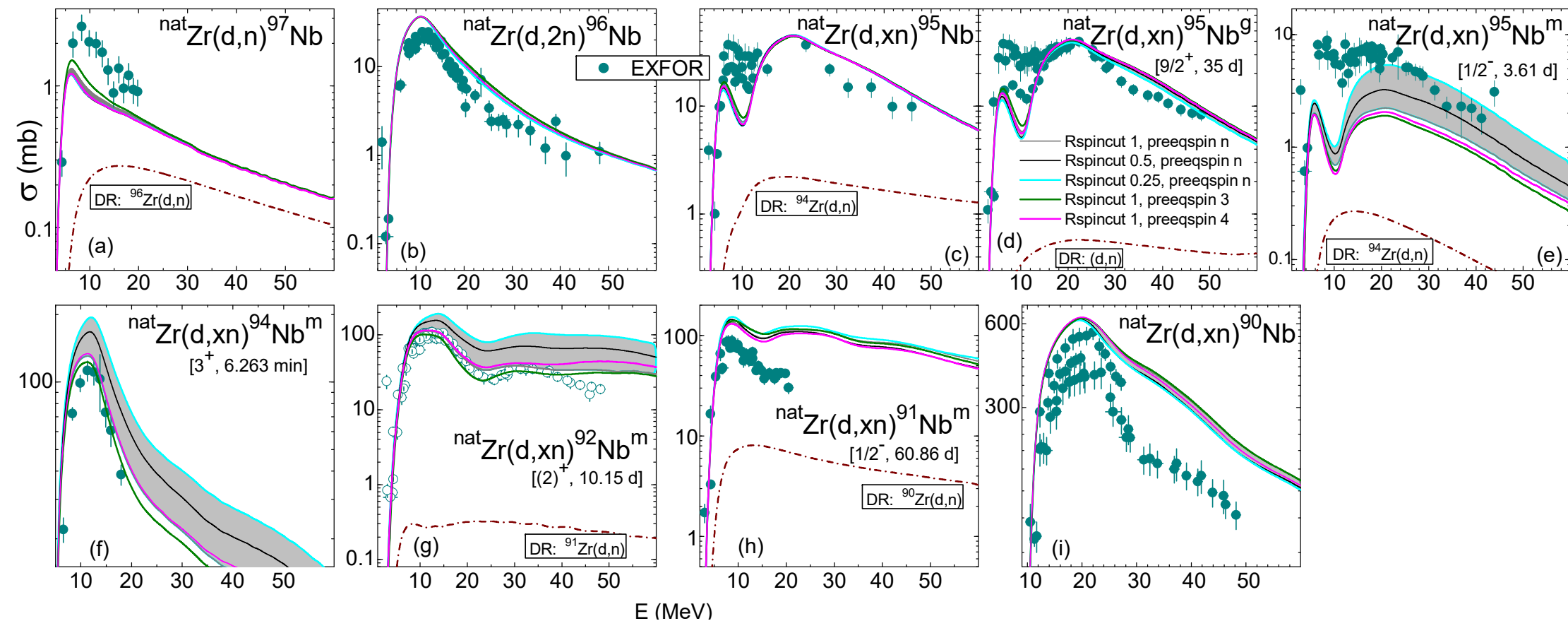


Effects of various options for level density spin distribution on $d + \text{Mo}$ ($d, xn3p$)

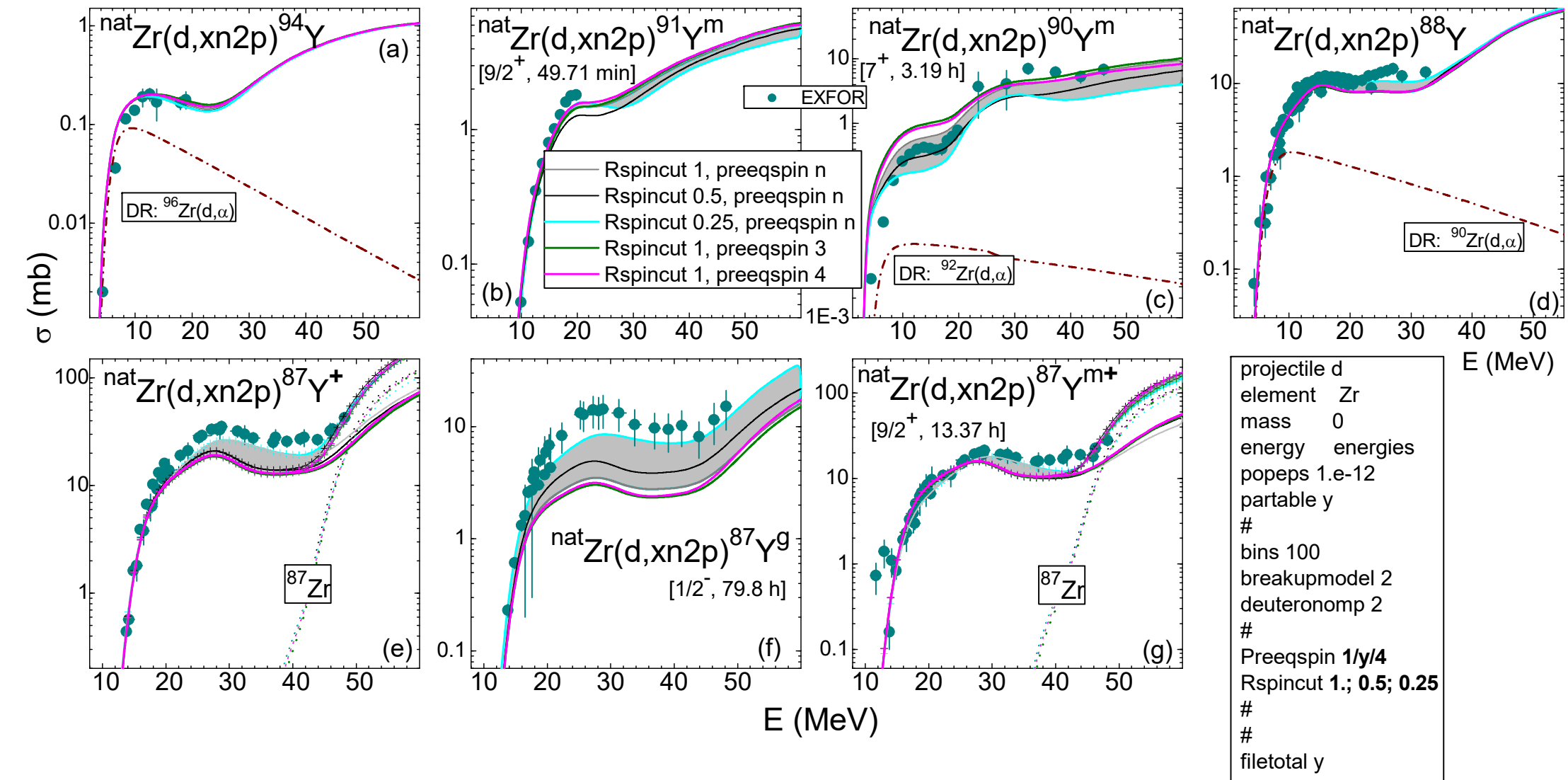


projectile d
 element Mo
 mass 0
 energy energies
 popeps 1.e-12
 partable y
 #
 bins 100
 breakupmodel 2
 deuteronomp 2
 #
 Preeqspin 1/y/4
 Rspincut 1.; 0.5; 0.25
 #
 filetotal y

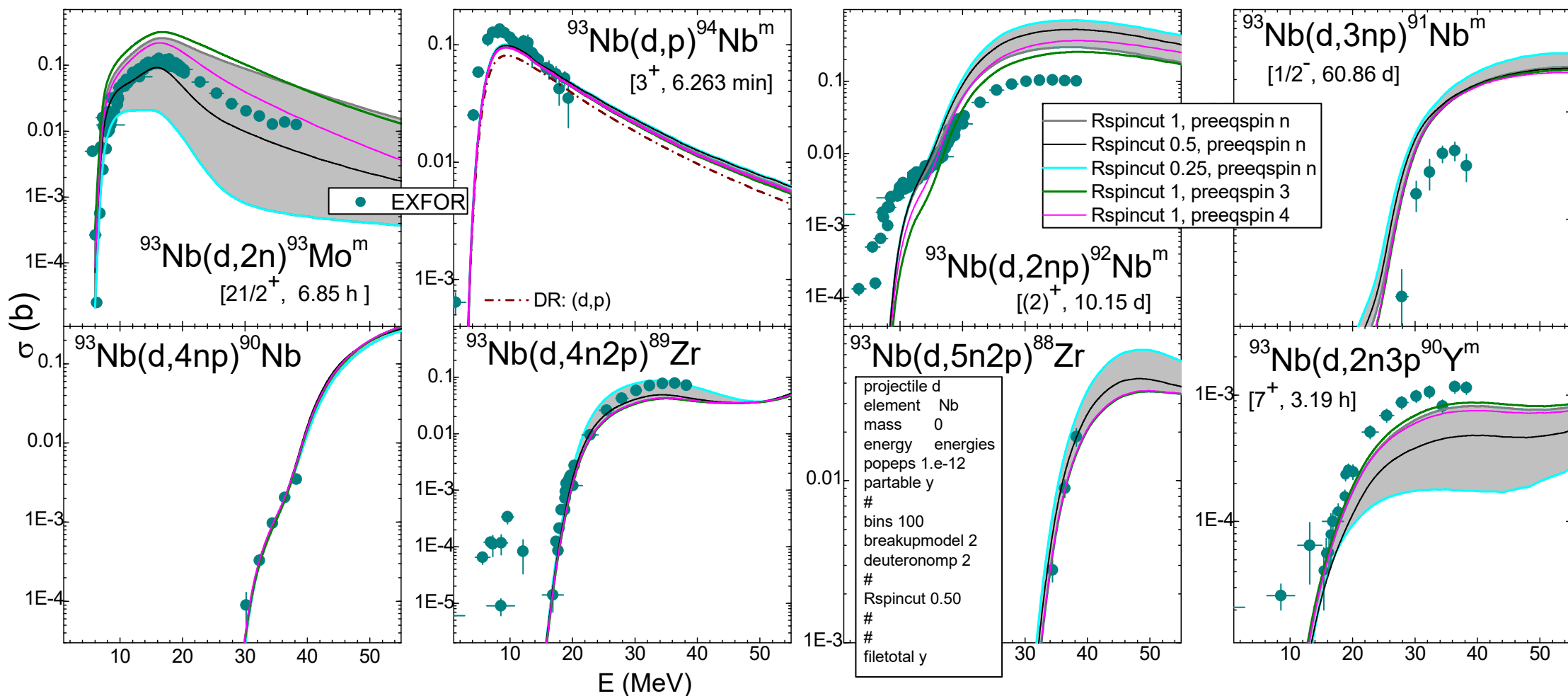
Effects of various options for level density spin distribution on $d + \text{Zr}$ (d, xn)



Effects of various options for level density spin distribution on $d + \text{Zr}$ ($d, xn2p$)



Effects of various options for level density spin distribution on $d + \text{Nb}$



CONCLUSIONS

Thank you!

Effects of various options for specific level density spin distribution:

□ preeqspin 1 (def)

- ✓ Rspincut 1. (def)
- ✓ Rspincut 0.50
- ✓ Rspincut 0.25

□ preeqspin 3

- ✓ Rspincut 1.; Rspincutpreeq 1.

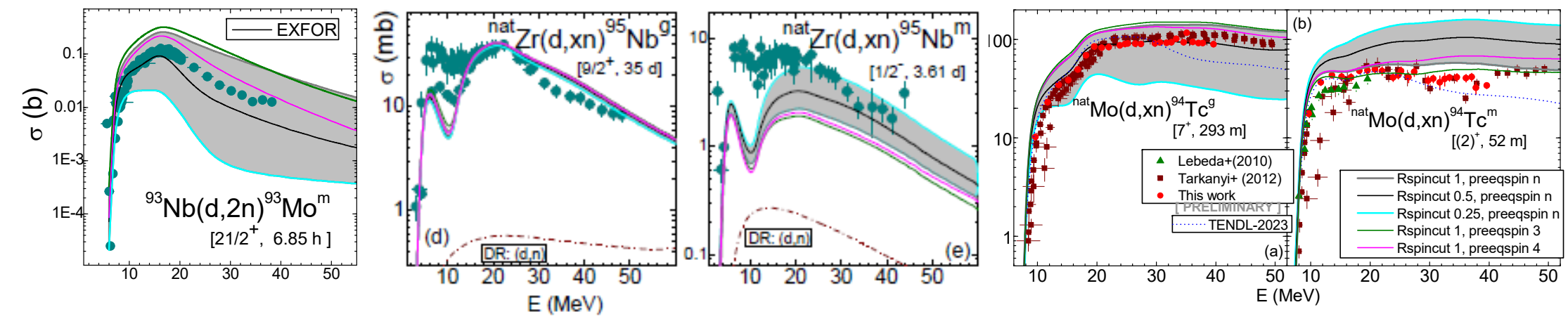
□ preeqspin 4 [corresponding to Rspinpreeq 0.17]

- ✓ Rspincut 1.

- Rspincut 1, preeqspin n
- Rspincut 0.5, preeqspin n
- Rspincut 0.25, preeqspin n
- Rspincut 1, preeqspin 3
- Rspincut 1, preeqspin 4

```
projectile d
element Nb/Zr/Mo
mass 0
energy energies
popeps 1.e-12
partable y
#
bins 100
breakupmodel 2
deuteronomp 2
#
Preeqspin 1/3/4
Rspincut 1./ 0.5/ 0.25
#
#
filetotal y
```

analyzed through the comparison of the experimental and TALYS-1.97 activation excitation functions corresponding to **Nb(d,x)**, **^{nat}Zr(d,x)**, **^{nat}Mo(d,x)**



Decreasing I/I_0 ratio, Rspincut, or Rspincutpreeq (preeqspin 4), increases low spin isomeric states population