

Building better optical-model potentials

FRIB Achievement Award for Early Career Researchers Presentation (Theory)

Low-Energy Community Meeting 2025
Texas A&M University

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Acknowledgments



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Bob Charity



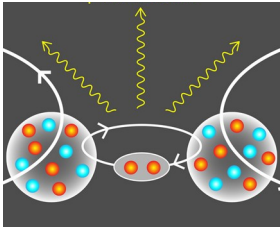
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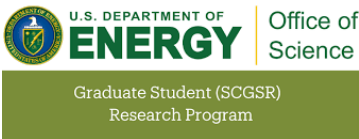
Oliver Gorton
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Simone Perrotta
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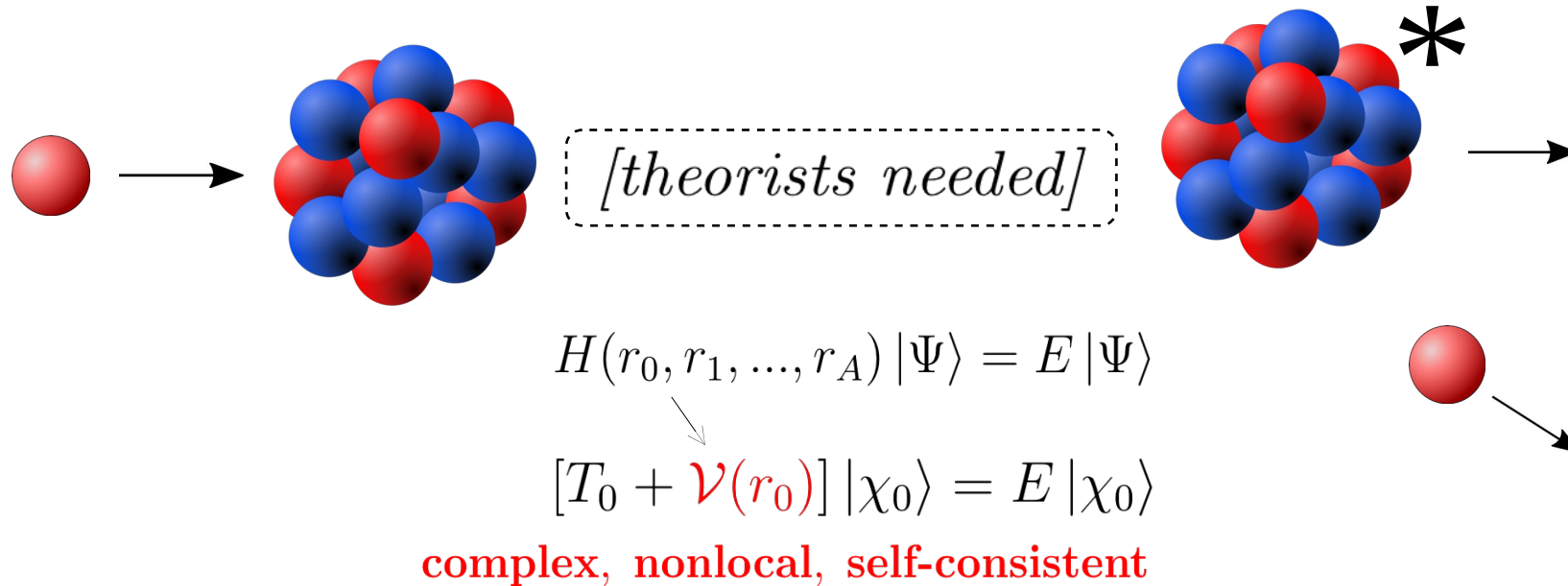
Filomena Nunes



“No one trusts a model except the one who wrote it; everyone trusts an observation, except the one who made it.”

Harlow Shapley (1885-1972)

Optical-model potentials (OMPs): an effective interaction for nuclear reactions

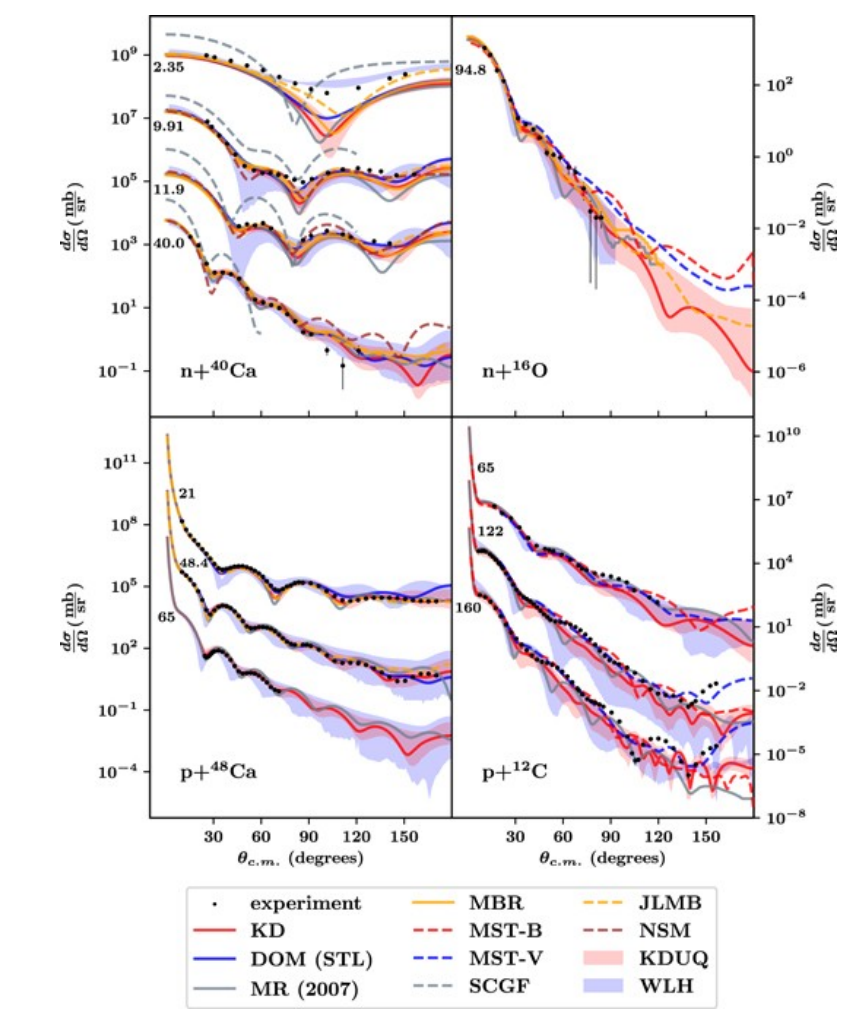


fully ab initio treatment is (usually) too hard... instead use **optical potential**

$$\mathcal{V}(r_0) \rightarrow U_{opt}(r_0)$$

Most empirical OMPs are substantially the same as they were in 1960:
A glorified particle-in-a-box (Woods-Saxon) with energy-dependent real and imaginary depths

Many OMPs are available, but most lack uncertainty estimates and agreement is spotty



	Mass	Energy	D.	Mic.	UQ	Bib	section
KD	$24 \leq A \leq 209$	$1 \text{ keV} \leq E \leq 200 \text{ MeV}$	×	×	×	[14]	3.1.1
KDUQ	$24 \leq A \leq 209$	$1 \text{ keV} \leq E \leq 200 \text{ MeV}$	×	×	✓	[185]	3.1.1
DOM	C, O, Ca, Ni,	$-\infty < E < 200 \text{ MeV}$	✓	×	✓	[172]	3.1.2
(STL)	Sn, Pb isotopes					[176]	
MR	$12 < Z < 83$	$E < 200 \text{ MeV}$	✓	×	×	[99]	3.1.2
MBR	$12 < Z < 83$	$E < 200 \text{ MeV}$	✓	×	×		3.1.2
NSM	$^{40}\text{Ca}, ^{48}\text{Ca}, ^{208}\text{Pb}$	$E < 40 \text{ MeV}$	✓	✓	×	[204]	3.2.1
SCGF	O, Ca, Ni isotopes	$E < 100 \text{ MeV}$	✓	✓	×	[249]	3.2.2
MST-B	$A \leq 20$	$E \geq 70 \text{ MeV}$	×	✓	×	[295]	3.2.3
MST-V	$4 \leq A \leq 16$	$E \geq 60 \text{ MeV}$	×	✓	×	[292]	3.2.3
						[285]	
WLH	$12 \leq A \leq 242$	$0 \leq E \leq 150 \text{ MeV}$	×	✓	✓	[326]	3.2.4
JLMB	$A > 30$	$1 \text{ keV} < E < 340 \text{ MeV}$	×	✓	×	[96]	3.2.4
						[98]	

- Only 3 potentials from a recent OMP survey even attempted UQ (via MCMC, bootstrapping, and Gaussian approximation over models, respectively)
- Essentially no substantive UQ efforts until the last 5 years
- Mediocre model agreement even on the “easy stuff” (elastic scattering on magic systems up to 50 MeV)

J. Phys G. 50 060601 (2023) C. Hebborn et al.

Building better phenomenological OMPs

- Improving methodology
 - Parameter inference: classical methods vs. MCMC and beyond
 - Outliers, correlations, and underestimated experimental error
 - Empirical coverage over common data sets
- Improving traditional OMPs
 - What is the “wiggle room” (parameter uncertainty) in widely used OMPs like CH89 and KD?
 - What is the impact on downstream observables?
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 - Linking structure and reactions with the Dispersive Optical Model
 - Does OMP uncertainty matter for reactions on unstable systems?

PRC **95**, 024611 (2017) A. E. Lovell et al.
PRC **102**, 034601 (2020) C. D. Pruitt et al.
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PRC **112**, 014302 (2025) O. C. Gorton, K. Kravvaris

PRC **107**, 014602 (2023) C. D. Pruitt, J. Escher, R. Rahman
PRL **131**, 212503 (2023) C. Hebborn, F. M. Nunes, A. E. Lovell
PRL **133**, 042501 (2024) Z. Y. Xu et al.
PRC **110**, 034602 (2024) A. J. Smith et al.
PRC **112**, 024604 (2025) K. A. Beyer et al.

PRL **119**, 222503 (2017) M. H. Mahzoon et al.
PRC **101**, 044303 (2020) M. C. Atkinson et al.
PRL **125**, 102501 (2020) C. D. Pruitt et al.
EPJ Web of Conf. **322**, 05001 (2025) C. D. Pruitt et al.

We use OMPs throughout nuclear physics and nuclear data:
how much should we trust them, where, and why?

Training a phenomenological OMP involves computing cross sections via a scattering formalism (the calculable R-matrix)

KD OMP
46 parameters

$$\begin{aligned}
 W_V(E) &= w_1^p \frac{(E - E_f^p)^2}{(E - E_f^p)^2 + (w_2^p)^2}, \\
 r_V &= 1.3039 - 0.4054 A^{-1/3}, \\
 a_V &= 0.6778 - 1.487 \times 10^{-4} A, \\
 W_D(E) &= d_1^p \frac{(E - E_f^p)^2}{(E - E_f^p)^2 + (d_2^p)^2} \exp[-d_3^p (E - E_f^p)], \\
 r_D &= 1.3424 - 0.01585 A^{1/3}, \\
 a_D &= 0.5446 - 1.656 \times 10^{-4} A, \\
 V_{SO}(E) &= v_{so1} \exp[-v_{so2} (E - E_f^p)], \\
 W_{SO}(E) &= w_{so1} \frac{(E - E_f^p)^2}{(E - E_f^p)^2 + (w_{so2}^p)^2}, \\
 r_{SO} &= 1.1854 - 0.647 A^{-1/3}, \\
 a_{SO} &= 0.59, \\
 V_V(E) &= v_1^p [1 - v_2^p (E - E_f^p) + v_3^p (E - E_f^p)^2 - v_4^p (E - E_f^p)^3] \\
 &\quad + \bar{V}_C v_1^p [v_2^p - 2v_3^p (E - E_f^p) + 3v_4^p (E - E_f^p)^2], \\
 W_V(E) &= w_1^p \frac{(E - E_f^p)^2}{(E - E_f^p)^2 + (w_2^p)^2}, \\
 r_V &= 1.3039 - 0.4054 A^{-1/3}, \\
 a_V &= 0.6778 - 1.487 \times 10^{-4} A, \\
 W_D(E) &= d_1^p \frac{(E - E_f^p)^2}{(E - E_f^p)^2 + (d_2^p)^2} \exp[-d_3^p (E - E_f^p)], \\
 r_D &= 1.3424 - 0.01585 A^{1/3}, \\
 a_D &= 0.5187 + 5.205 \times 10^{-4} A, \\
 V_{SO}(E) &= v_{so1} \exp[-v_{so2} (E - E_f^p)], \\
 W_{SO}(E) &= w_{so1} \frac{(E - E_f^p)^2}{(E - E_f^p)^2 + (w_{so2}^p)^2}, \\
 r_{SO} &= 1.1854 - 0.647 A^{-1/3}, \\
 a_{SO} &= 0.59, \\
 r_C &= 1.198 + 0.697 A^{-2/3} + 12.994 A^{-5/3}, \\
 V_V(r, E) &= V_V(E) f(r, R_V, a_V), \\
 W_V(r, E) &= W_V(E) f(r, R_V, a_V), \\
 W_D(r, E) &= -4a_D W_D(E) \frac{d}{dr} f(r, R_D, a_D), \\
 V_{SO}(r, E) &= V_{SO}(E) \left(\frac{\hbar}{m\pi c} \right)^2 \frac{1}{r} \frac{d}{dr} f(r, R_{SO}, a_{SO}), \\
 W_{SO}(r, E) &= W_{SO}(E) \left(\frac{\hbar}{m\pi c} \right)^2 \frac{1}{r} \frac{d}{dr} f(r, R_{SO}, a_{SO}).
 \end{aligned}
 \tag{2}$$

As usual, the form factor $f(r, R_i, a_i)$ is a Woods-Saxon shape

$$f(r, R_i, a_i) = (1 + \exp[(r - R_i)/a_i])^{-1},
 \tag{3}$$

where, with A being the atomic mass number, the geometry parameters are the radius $R_i = r_i A^{1/3}$ and the diffuseness parameters a_i . For charged projectiles, the Coulomb term V_C , as usual, is given by that of a uniformly charged sphere

$$V_C(r) = \begin{cases} \frac{Zz e^2}{2R_C} \left(3 - \frac{r^2}{R_C^2} \right), & \text{for } r \leq R_C, \\ \frac{Zz e^2}{r}, & \text{for } r \geq R_C, \end{cases}
 \tag{4}$$

with $Z(z)$ the charge of the target (projectile), and $R_C = r_C A^{1/3}$ the Coulomb radius.

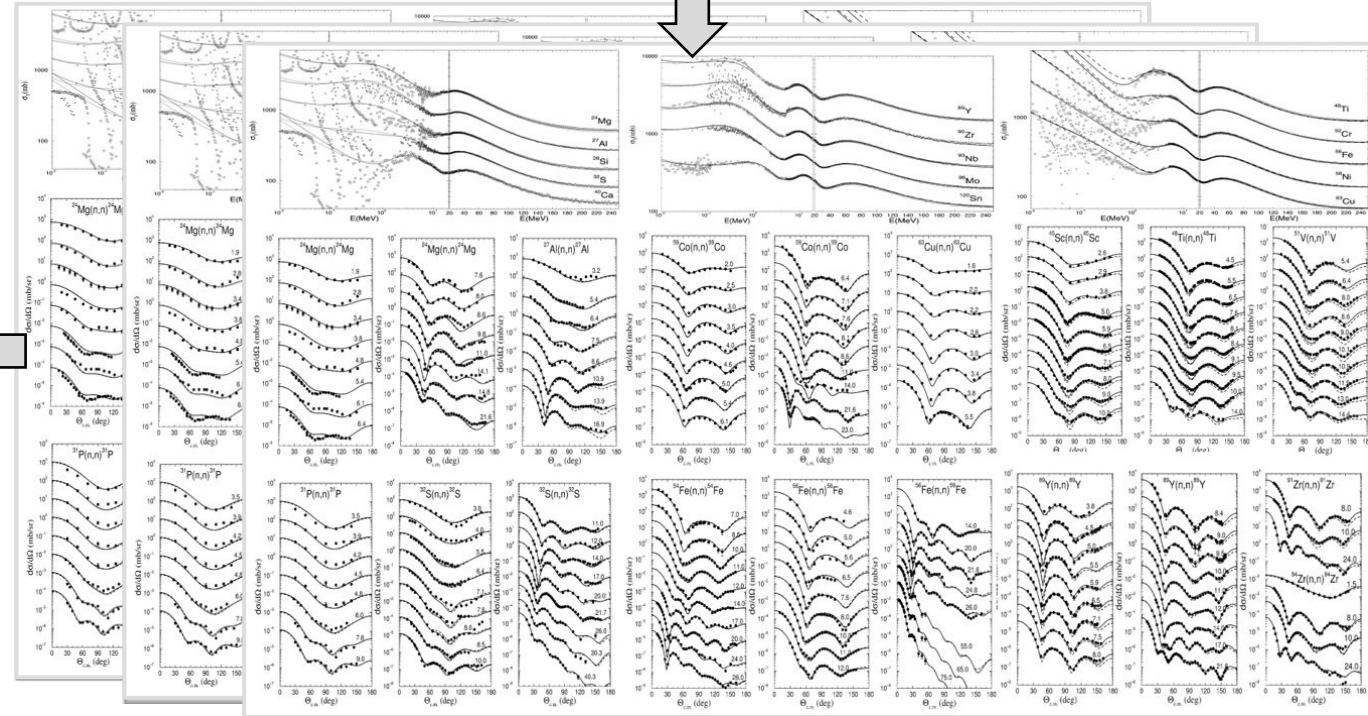
Nucl. Phys. A 713 (2003) 231-310

N, Z
t, E

$$\frac{d^2 u_{\ell,s}(r)}{dr^2} - \left[\frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2} U_{opt}(r, \ell, s) - k^2 \right] u_{\ell,s}(r) = 0$$

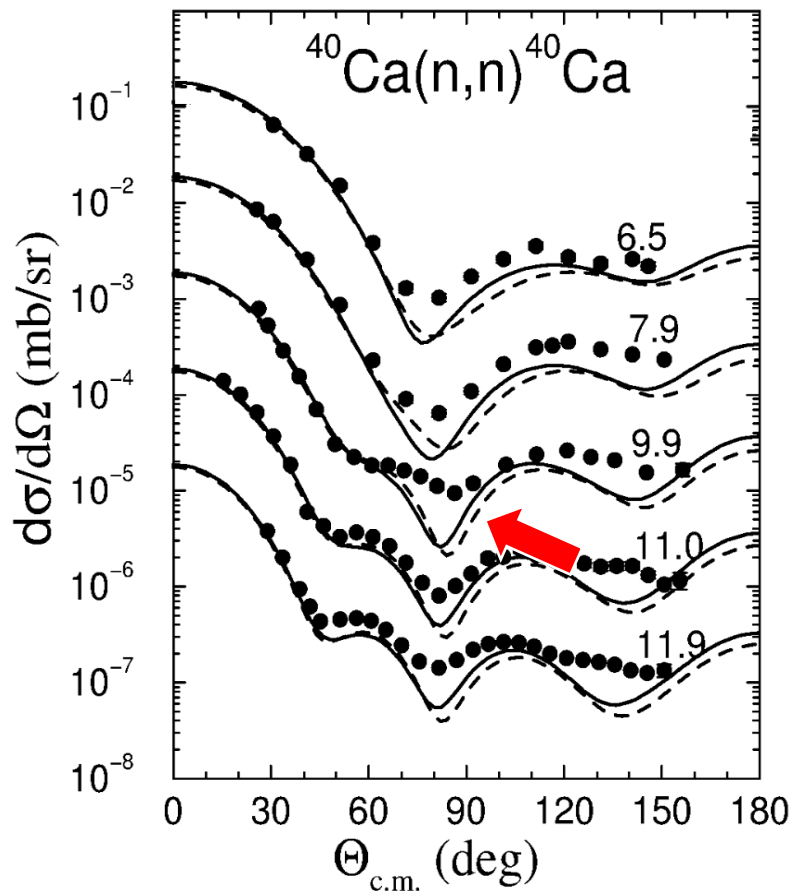
$$\sigma_{rxn} = \sum_{l=0}^{\infty} \frac{\pi}{k^2} [(2\ell+1) - (\ell+1)|e^{2i\delta_{\ell+}} - \ell|e^{2i\delta_{\ell-}}|^2]$$

Highly nonlinear
spherical model



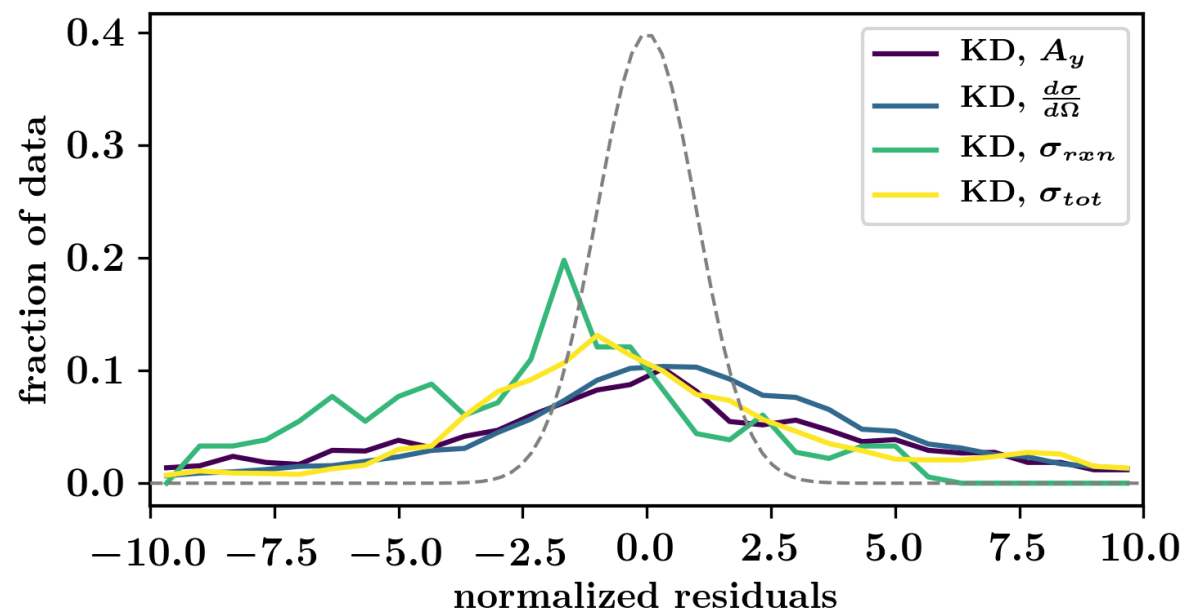
KD corpus:
6 data types
~70 nuclei
~1000 data sets
~25000 points

Even state-of-the-art phenomenological OMPs are several-sigma discrepant with their training data



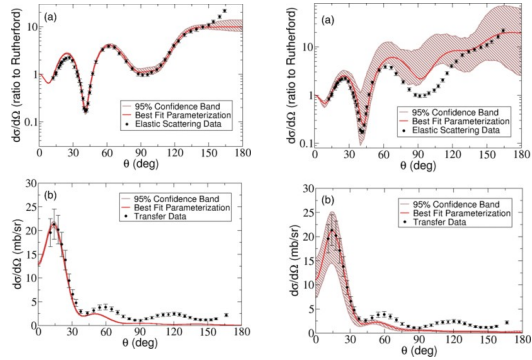
Nucl. Phys. A 713 (2003) 231-310

OMP	A	$E \text{ (MeV)}$	χ^2_{ad}/N	χ^2_{ad}/N (this)	χ^2_{tot}/N	χ^2_{tot}/N (this)
Wilmore–Hodgson [57]	40–208	0–15	11.2	7.4	9.2	6.7
Rapaport et al. [47]	40–208	7–26	10.0	7.0	4.1	1.8
Varner et al. [4]	40–208	7–26	8.3	7.0	4.7	1.8
Walter–Guss [58]	53–208	10–80	6.3	6.1	2.3	1.3
Madland [59]	40–208	50–200	8.6	4.5	6.9	1.2



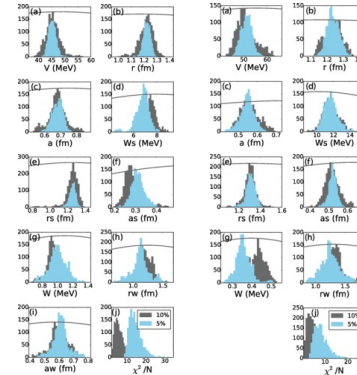
An abbreviated timeline of reaction-model UQ methodology

Training models to correlated data



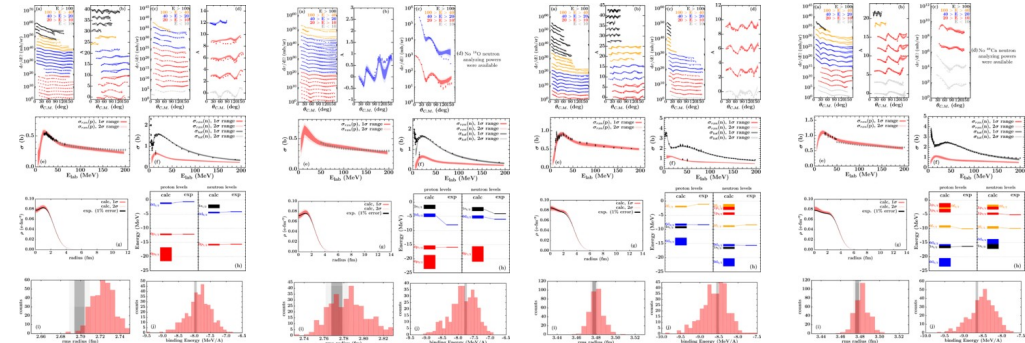
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MCMC (Metropolis-Hastings)



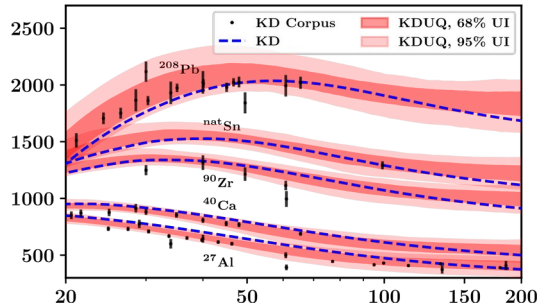
PRC **97**, 064612 (2017) A. E. Lovell and F. M. Nunes

Fixed unaccounted-for uncertainties (UAUs), MCMC (stretch move)



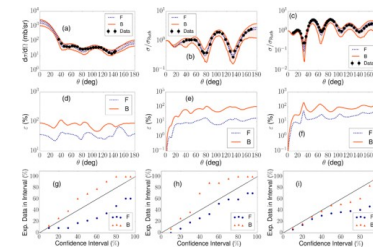
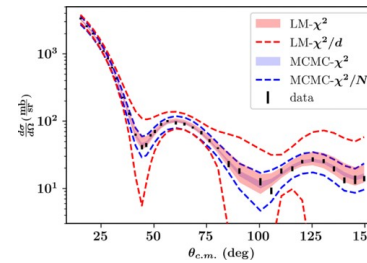
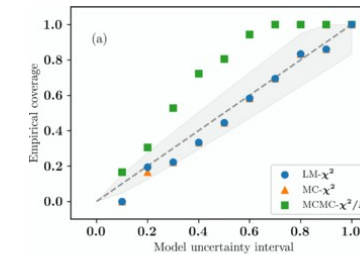
PRC **102**, 034601 (2020) C. D. Pruitt et al.

Dynamic UAUs, outlier rejection



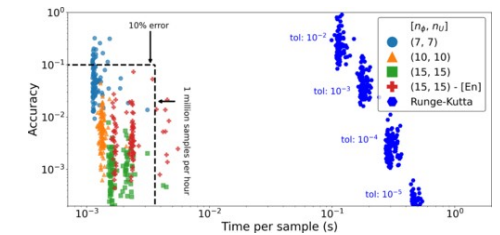
PRC **107** 014602 (2023) C. D. Pruitt, J. Escher, R. Rahman

Gradient descent vs. MCMC comparison and empirical coverage



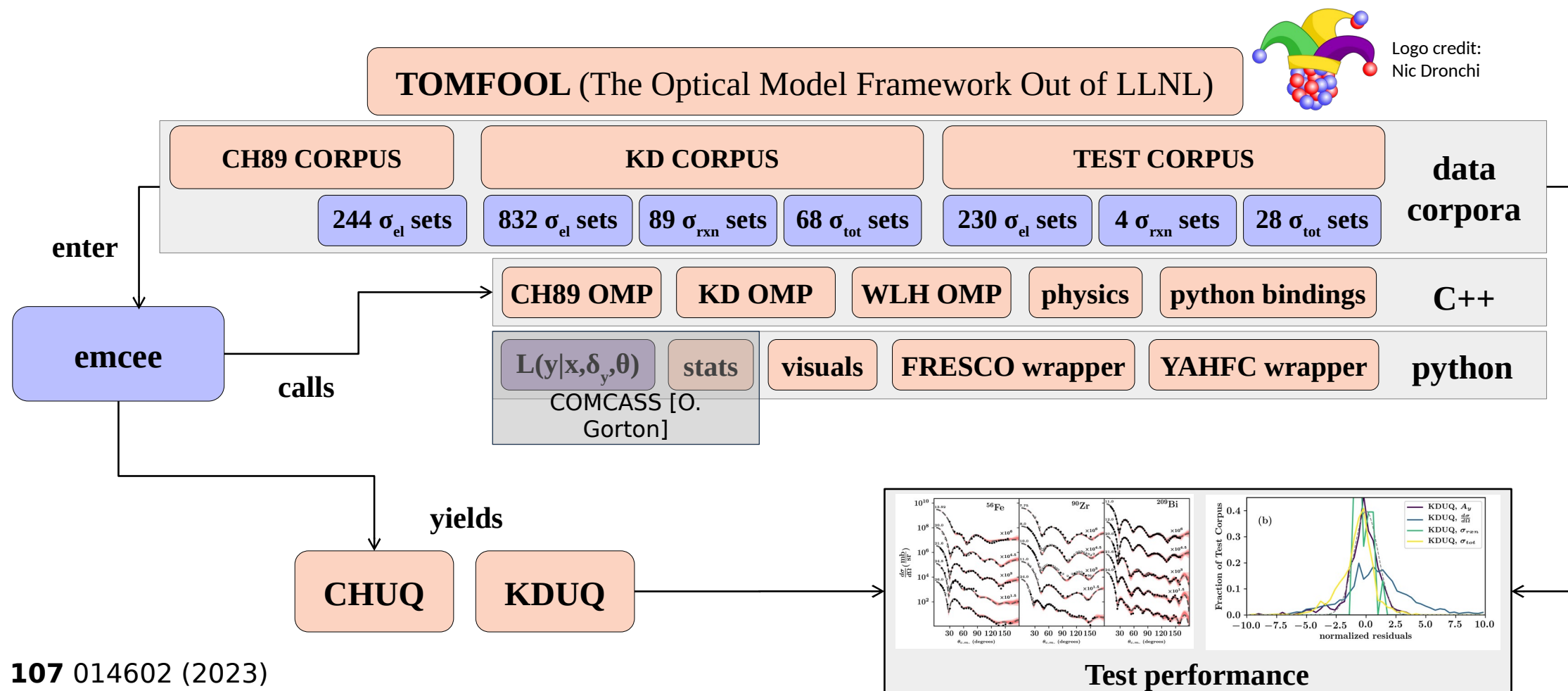
PRL **122**, 232502 (2019) G. B. King et al. PRC **110**, 064606 (2024) C. D. Pruitt et al.

ROSE: OMP emulation



PRC **109**, 044612 (2024) D. Odell et al.

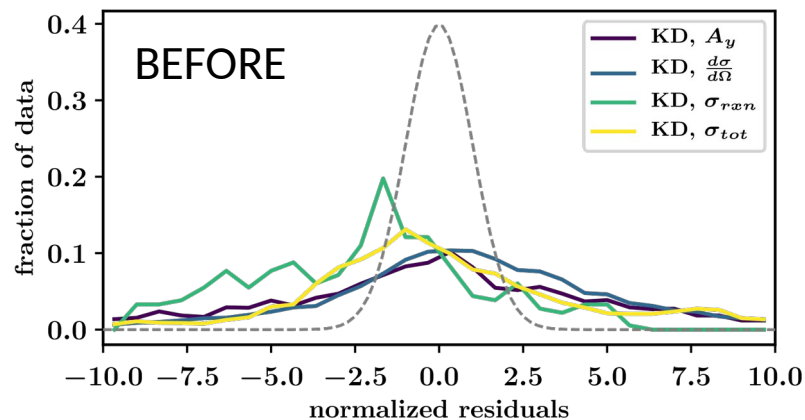
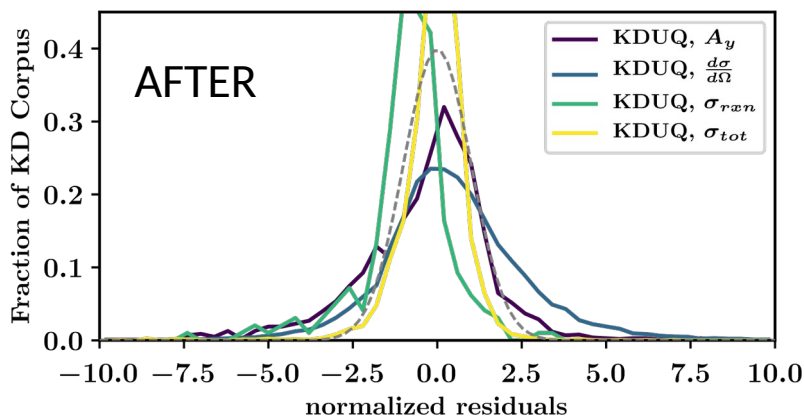
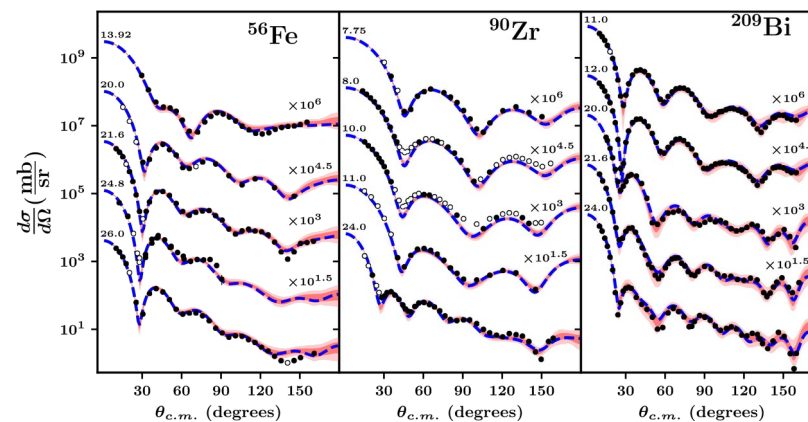
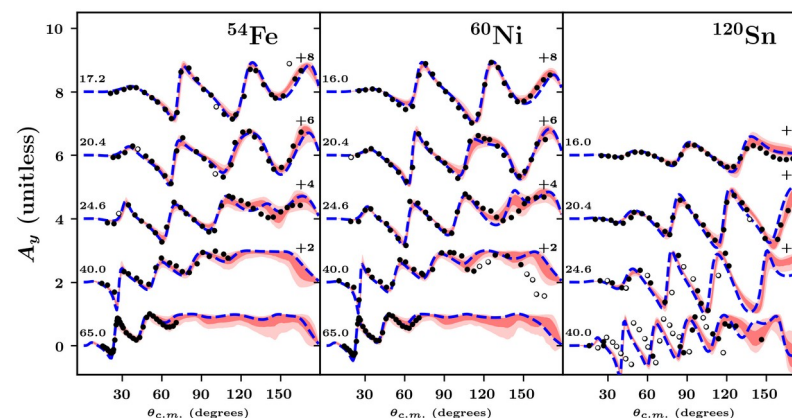
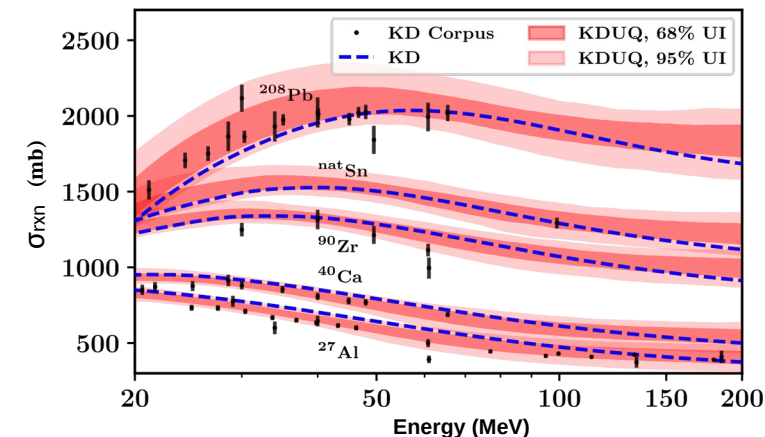
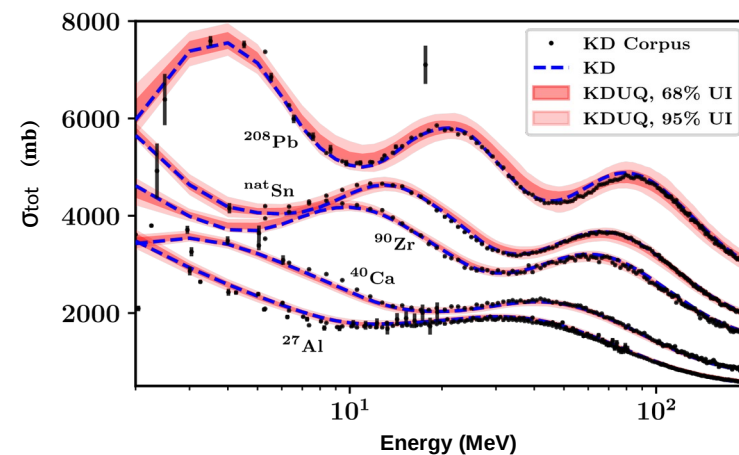
To retrain CH89 and KD with UQ, we built a pipeline using off-the-shelf MCMC and nuclear data tools



Logo credit:
Nic Dronchi

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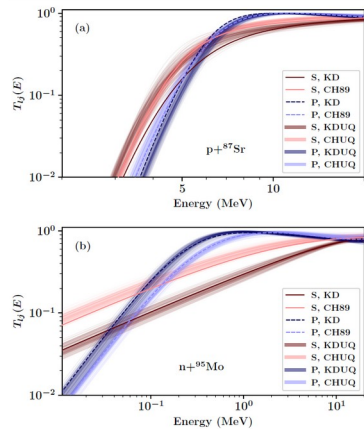
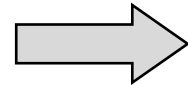
We equipped the KD OMP with uncertainties (KDUQ), enabling extrapolation consistent with known scattering data



C. D. Pruitt, J. E. Escher, R. Rahman, Phys. Rev. C **107** (2023) 014602

If you use the KD OMP, KDUQ is a drop-in extension providing model uncertainties (including correlations)

Several reaction theory studies have propagated KDUQ uncertainties into their results; TALYS integration underway



Transfer and knockout reactions

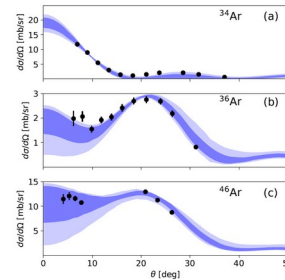


FIG. 1. Angular distributions for (a) $^{34}\text{Ar}(p,d)^{33}\text{Ar}(g.s.)$, (b) $^{36}\text{Ar}(p,d)^{35}\text{Ar}(g.s.)$ and (c) $^{46}\text{Ar}(p,d)^{45}\text{Ar}(g.s.)$ at 33.4 MeV. All theoretical distributions have been scaled to reproduce the data from Ref. [37]. The scaling factors are the extracted SFs and are listed in Table III.

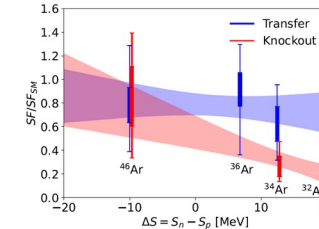
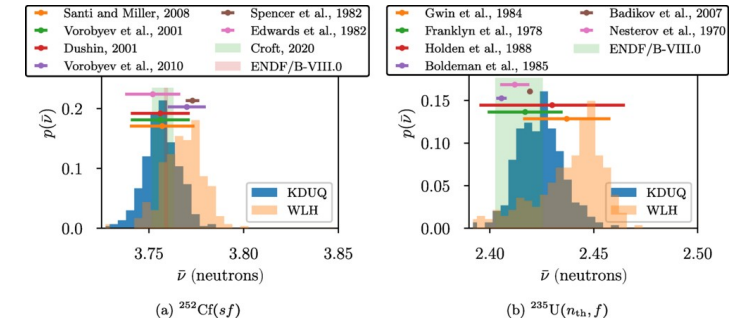


FIG. 3. Ratio of the SF extracted from data and the shell-model SF (including the center-of-mass correction) as a function of the asymmetry of the nucleus $\Delta S = S_n - S_p$. The blue error bars correspond to the SFs extracted from transfer data [37] and the red ones to the SFs extracted from knockout data [38–40]. Each error bar shows the 1 σ and 2 σ uncertainties. The shaded area correspond to the 1 σ uncertainties of a linear fit of the transfer (blue) and knockout (red) error bars.

Fission observables

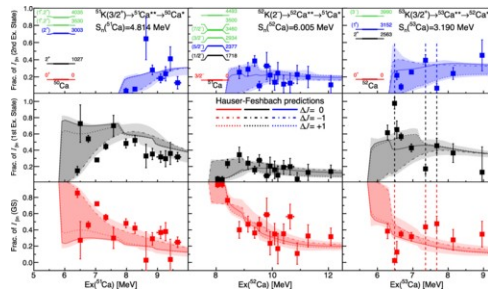


PRC **112**, 024604 (2025) K. A. Beyer et al.

KDUQ potential/transmission coeffs

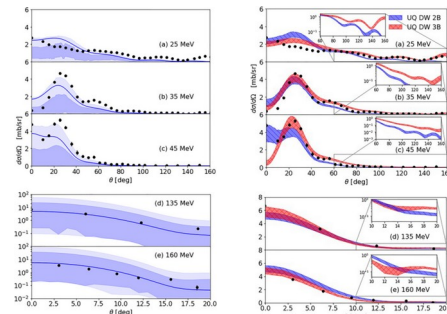
PRL **131** 212503 (2023) C. Hebborn, F. M. Nunes, A. E. Lovell

β -delayed neutron branching ratios



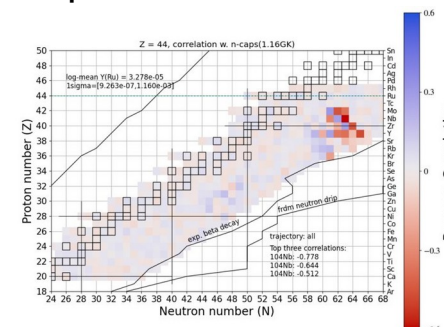
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Charge exchange reactions



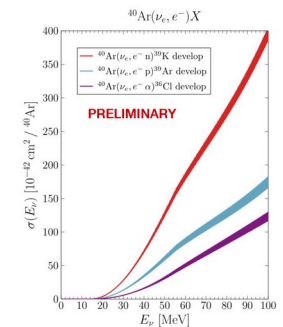
PRC **110**, 034602 (2024) A. J. Smith et al.

Weak r-process rates/abundances



Atul Kedia (NCSU)
from Nuclei in the Cosmos conference (2025)

Neutrino reactions on Ar



Steven Gardiner (Fermilab)
from NuFact conference (2024)

Model uncertainties explain where new data are (or aren't) useful

Neutron σ_{tot} , relative difference
(heavy-light)



experimental data



KD OMP (standard)



KDUQ OMP

Theory:

Nucl. Phys. A **713**, 231 (2003) Koning and Delaroche

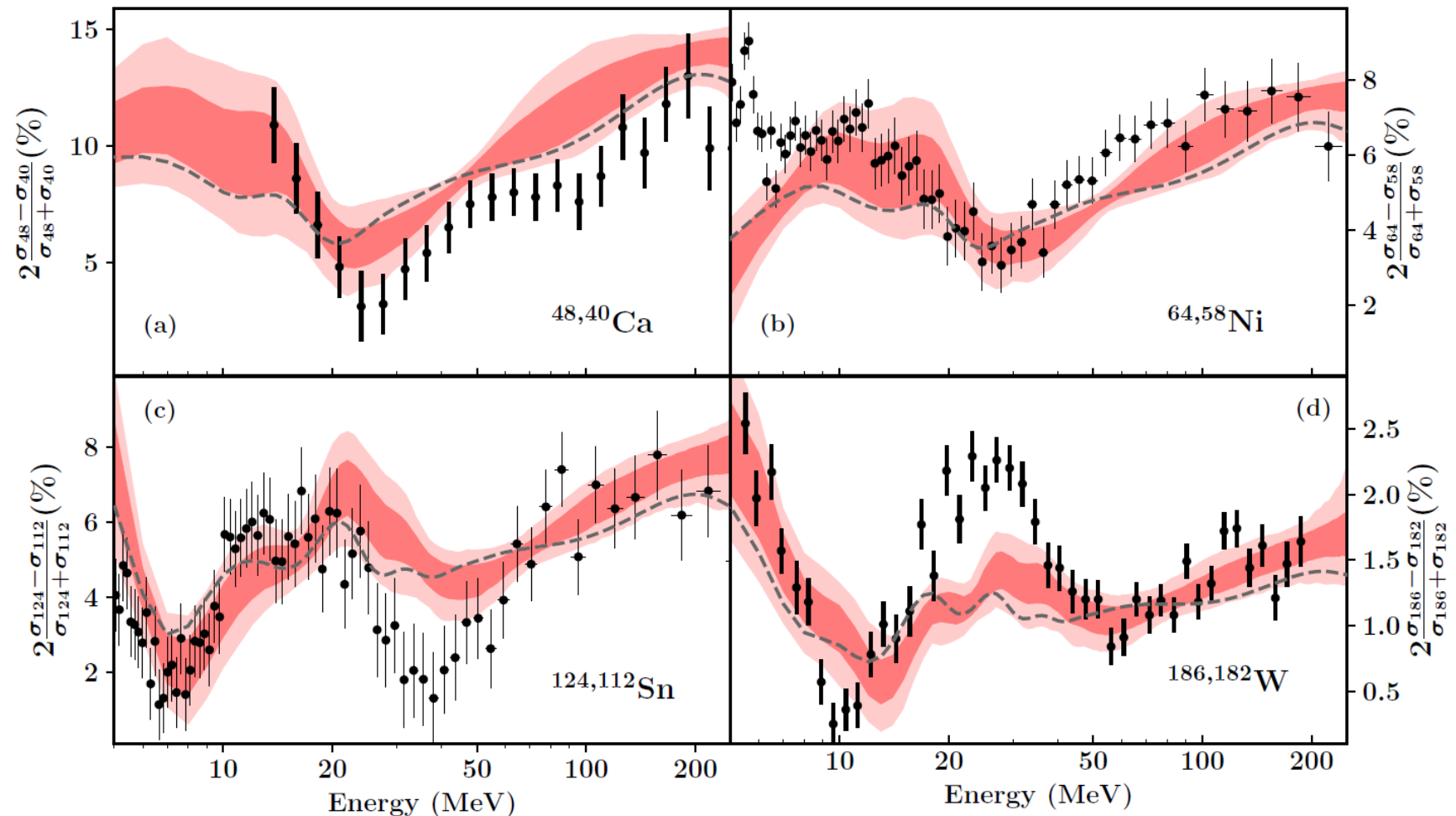
PRC **107** 014602 (2023) C. D. Pruitt, J. Escher, R. Rahman

Data:

PRC **67**, 044606 (2003) F. S. Dietrich et al.

NIM A **614**, 468 (2010) R. Shane et al.

PRC **102**, 034601 (2020) C. D. Pruitt et al.



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PRC **95**, 024611 (2017) A. E. Lovell et al.
PRC **102**, 034601 (2020) C. D. Pruitt et al.
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PRC **112**, 014302 (2025) O. C. Gorton, K. Kravvaris

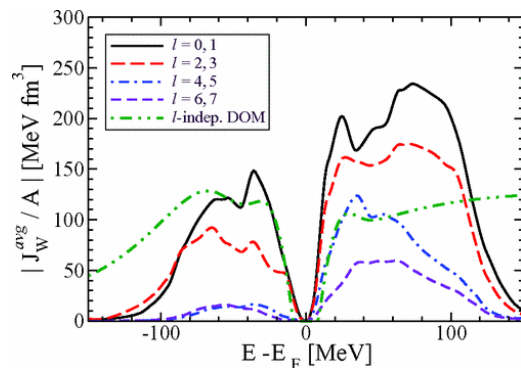
PRC **107**, 014602 (2023) C. D. Pruitt, J. Escher, R. Rahman
PRL **131**, 212503 (2023) C. Hebborn, F. M. Nunes, A. E. Lovell
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PRC **112**, 024604 (2025) K. A. Beyer et al.

PRL **119**, 222503 (2017) M. H. Mahzoon et al.
PRC **101**, 044303 (2020) M. C. Atkinson et al.
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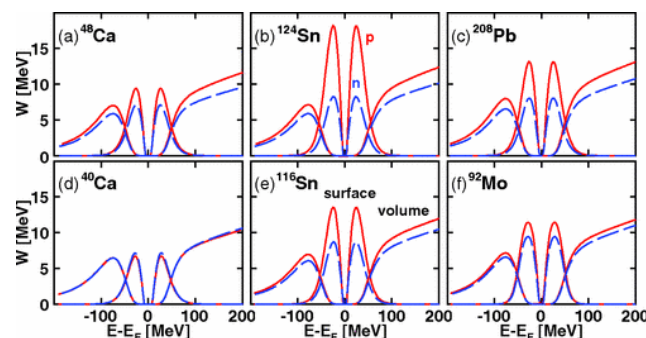
The Dispersive Optical Model (DOM) connects reactions to structure via dispersivity and non-locality physical constraints

Microscopic and DOM self-energies



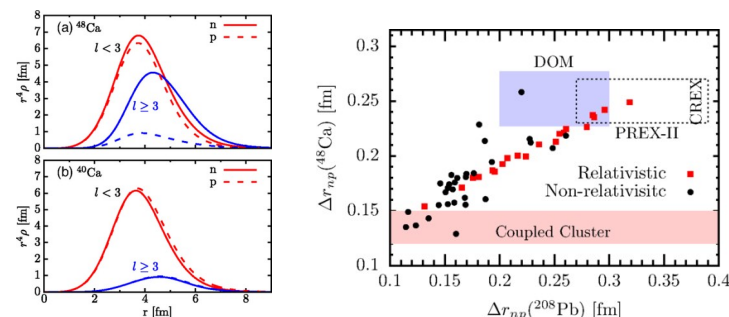
PRC **84**, 034616 (2011) S. J. Waldecker, C. Barbieri, W. H. Dickhoff

DOM asymmetry-dependence

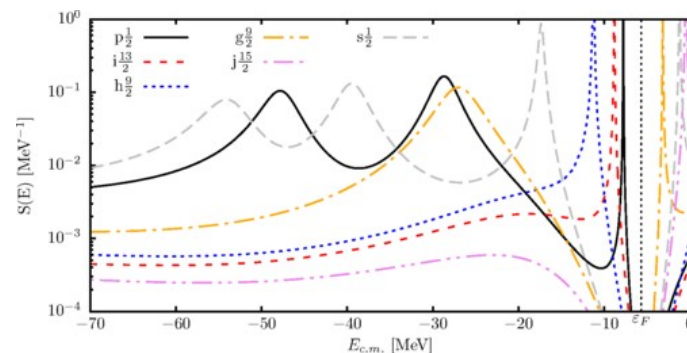


PRC **83**, 064605 (2011) J. M. Mueller et al.

Fully non-local DOM: $^{40,48}\text{Ca}$ and ^{208}Pb



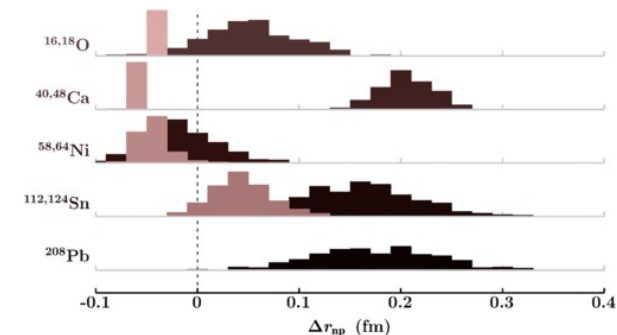
Single-particle density distributions and neutron skins



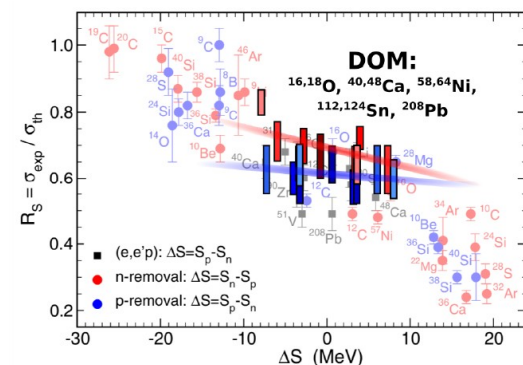
Spectral functions that agree quantitatively with (e,e'p)

PRL **119**, 222503 (2017) M. H. Mahzoon et al.
PRC **101**, 044303 (2020) M. C. Atkinson et al.

Fully non-local DOM: $^{16,18}\text{O}$, $^{40,48}\text{Ca}$, $^{58,64}\text{Ni}$, $^{112,124}\text{Sn}$, ^{208}Pb



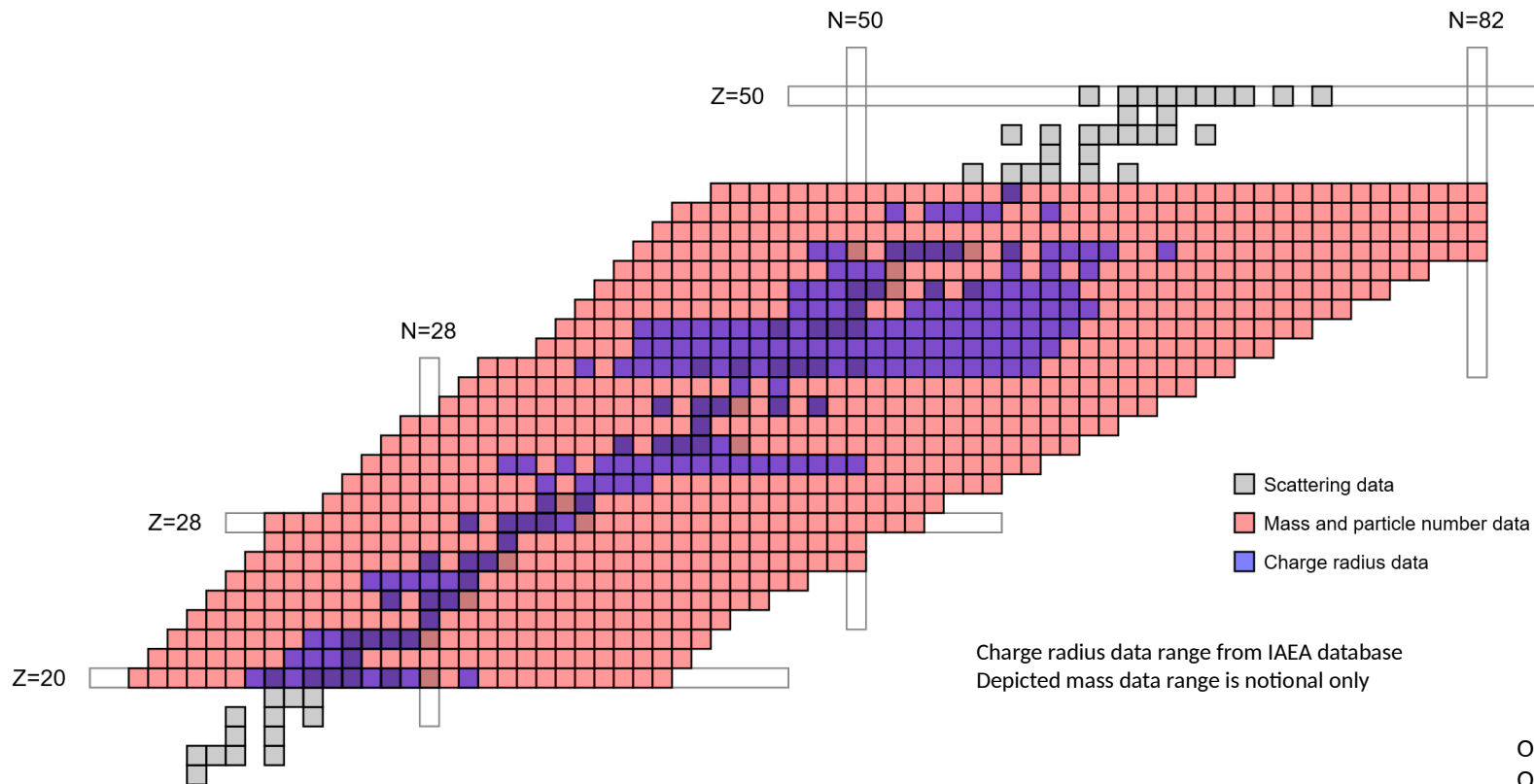
UQ neutron skins from MCMC



Spectroscopic factor trends with asymmetry

PRL **125**, 102501 (2020) C. D. Pruitt et al.
PRC **103**, 054610 (2021) J. A. Tostevin and A. Gade

Particle number, binding energy, and valence single-particle energies are powerful, universally available training data



From a non-local DOM, the hole propagator provides the **one-body density** and **structural observables**:

- Particle number (most important overall!)
- Binding energy (dictates deep-hole properties)
- Charge radius (dictates geometry)
- Single-particle energies (dictates geometry and shallow-hole properties)

The propagator also enables self-consistent treatment of **reactions combining structure and scattering**:

- (e,e'p) cross sections
- (p,2p) cross sections
- (p,n) and (n,p) cross sections
- parity-violating electron scattering (neutron skins)

On (e,e'p) and the DOM: Atkinson et al., Phys. Rev. C **98** (2018) 044627

On (p,2p) and the DOM: Yoshida et al., Phys. Rev. C **105** (2022) 014622

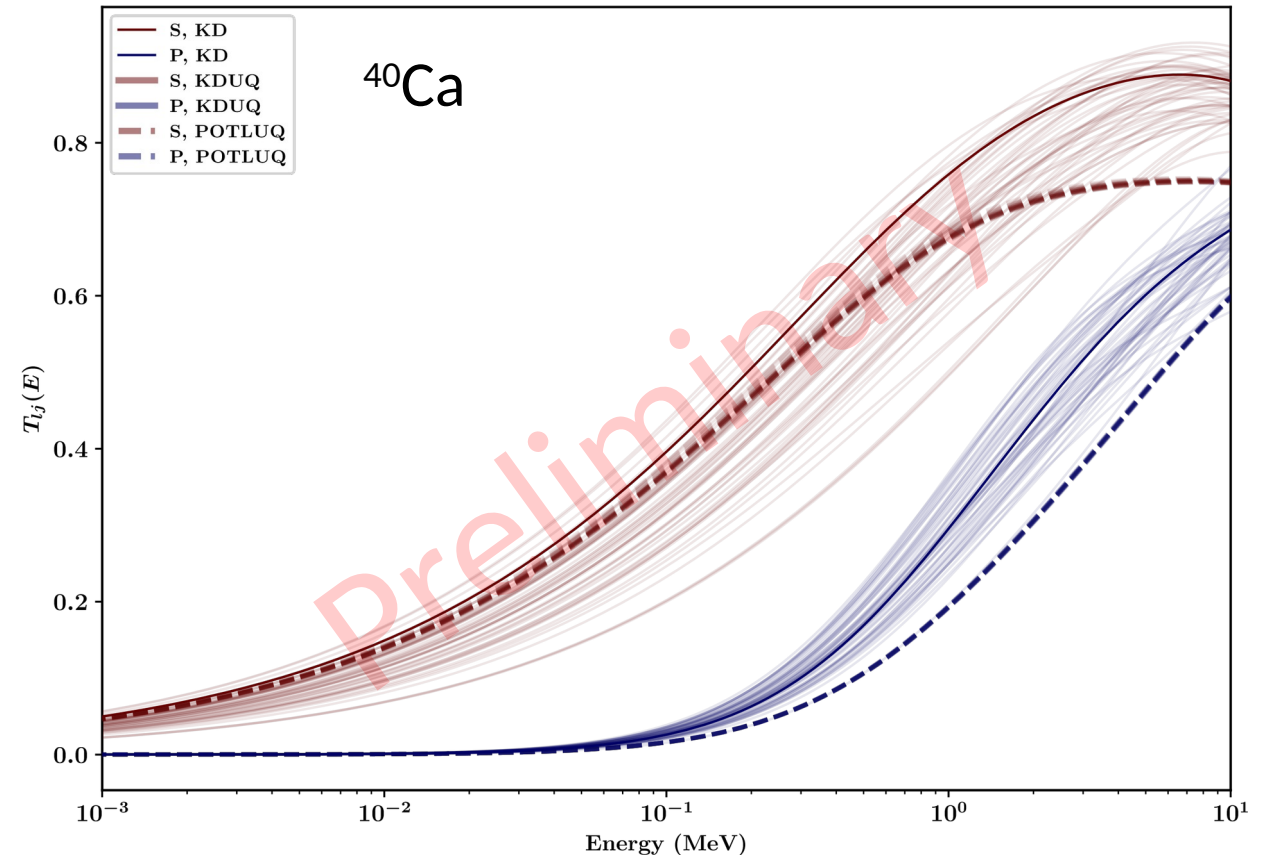
On neutron skins and the DOM: Mahzoon et al., Phys. Rev. Lett. **119** (2017) 222503

Structure data can provide meaningful constraints on scattering, even in the absence of experimental data

POTLUQ (LLNL global UQ DOM) preliminary results: $^{40,48,54,58}\text{Ca}$

Very preliminary:

- At low asymmetries ($^{40,48}\text{Ca}$), DOM neutron transmission coefficients are largely consistent with KD/KDUQ at astrophysical energies
- At high asymmetries ($^{54,58}\text{Ca}$), transmission coefficients drop dramatically, driven by shallow Fermi energy and particle-number constraint (DOM fit recovers $N=40$ for ^{60}Ca)
- Dripline imaginary surface strength likely weaker than shell model predictions of spectroscopic-factor asymmetry dependence
- Spectral functions indicate considerable broadening of deep holes, consistent with understanding from $(e,e'p)$

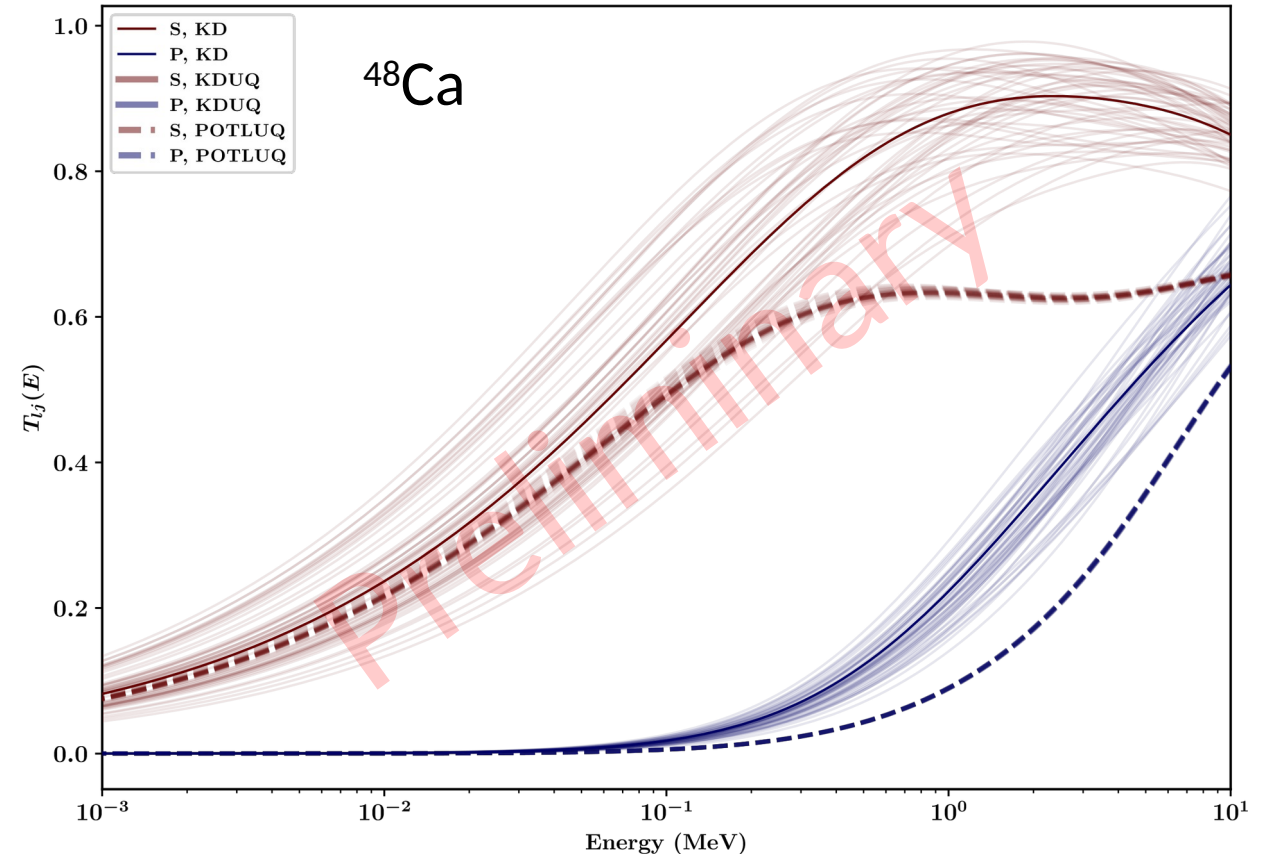


Preliminary results show a larger isovector surface asymmetry dependence compared to non-dispersive models, which would tend to reduce near-dripline (n,γ) cross section predictions

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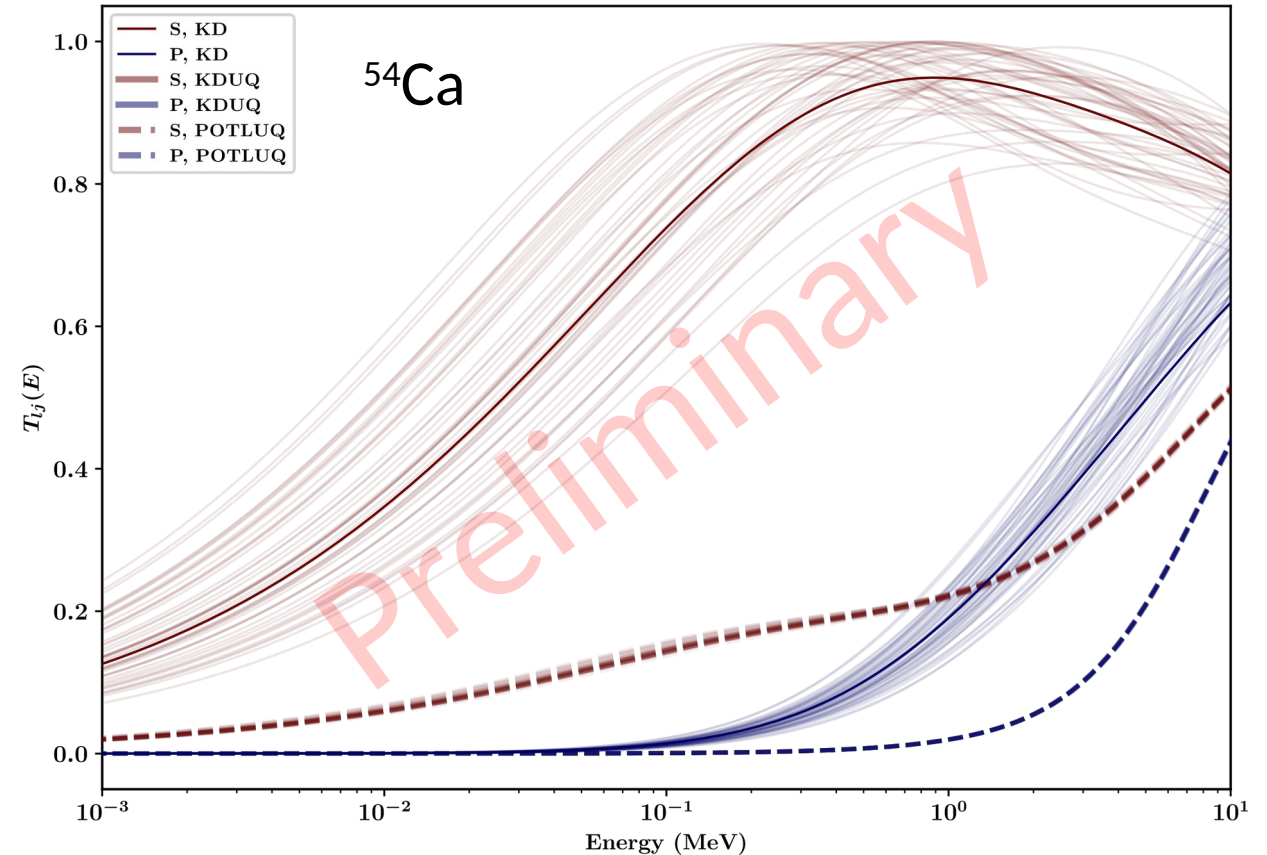


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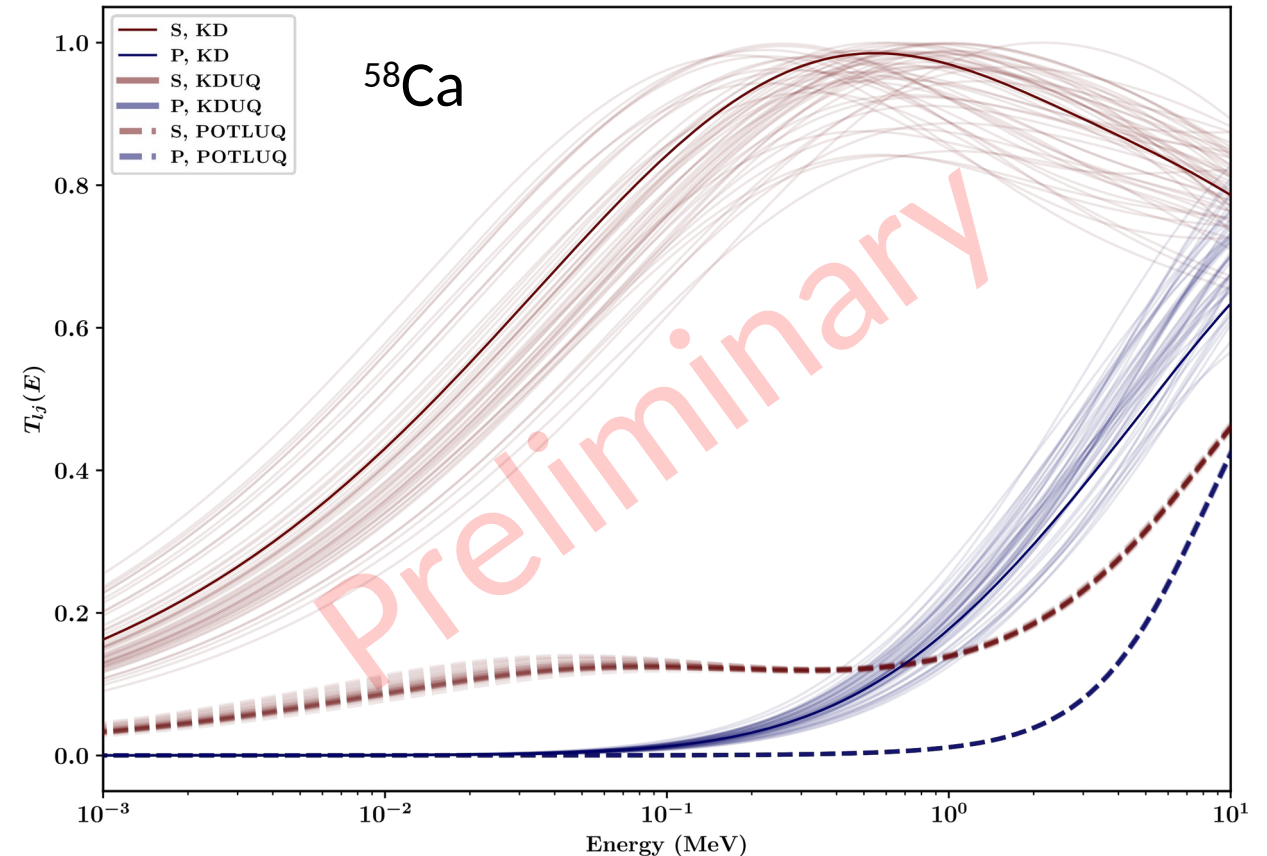


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Acknowledgments



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Bob Charity



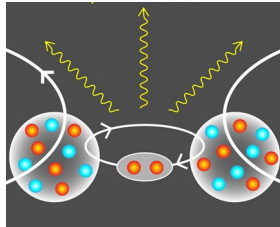
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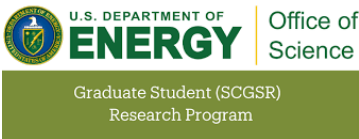
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