Scalable ab initio approaches

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The nuclear *ab initio* endeavour

- **A systematic approach to describe nuclei**

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

Happy 100th b-day!

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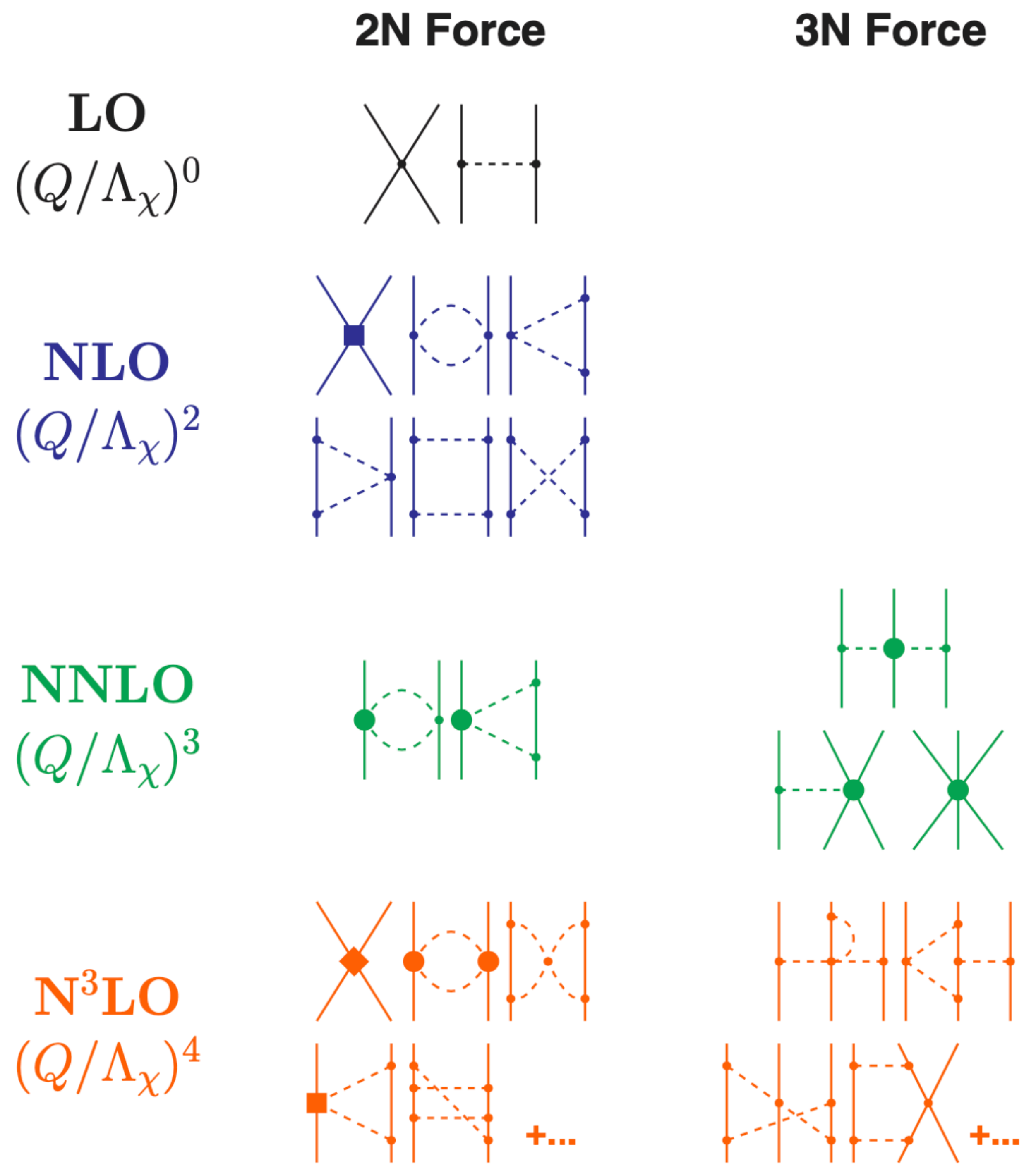
1. Model Hamiltonian

Inter-nucleon forces from chiral EFT

○ Low-energy limit of QCD

○ Nucleons and pions as d.o.f.

○ Power counting → expansion of H



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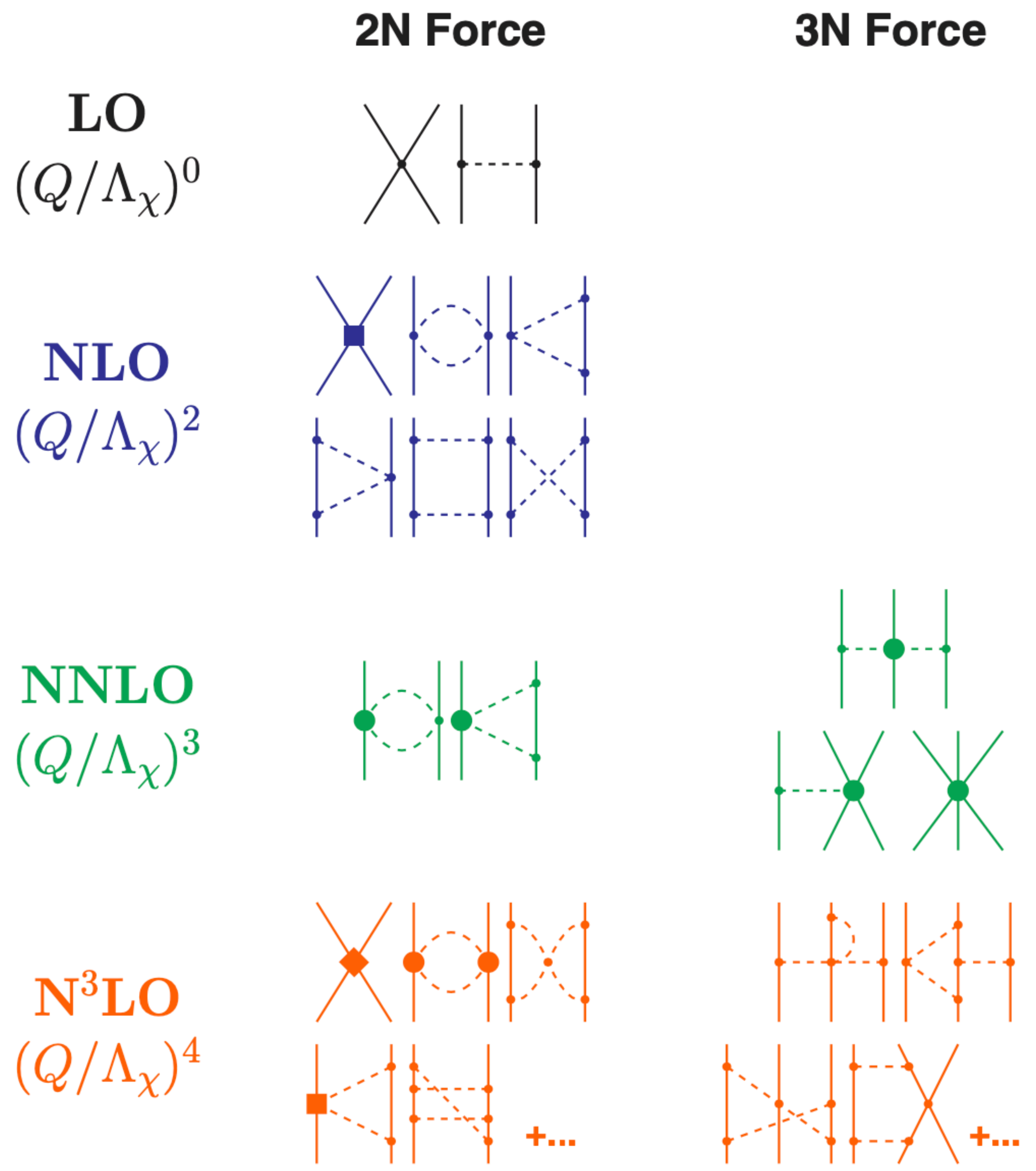

Option 1: Exact solutions have factorial or exponential scaling $\mathbf{e}^n$ → limited to light nuclei

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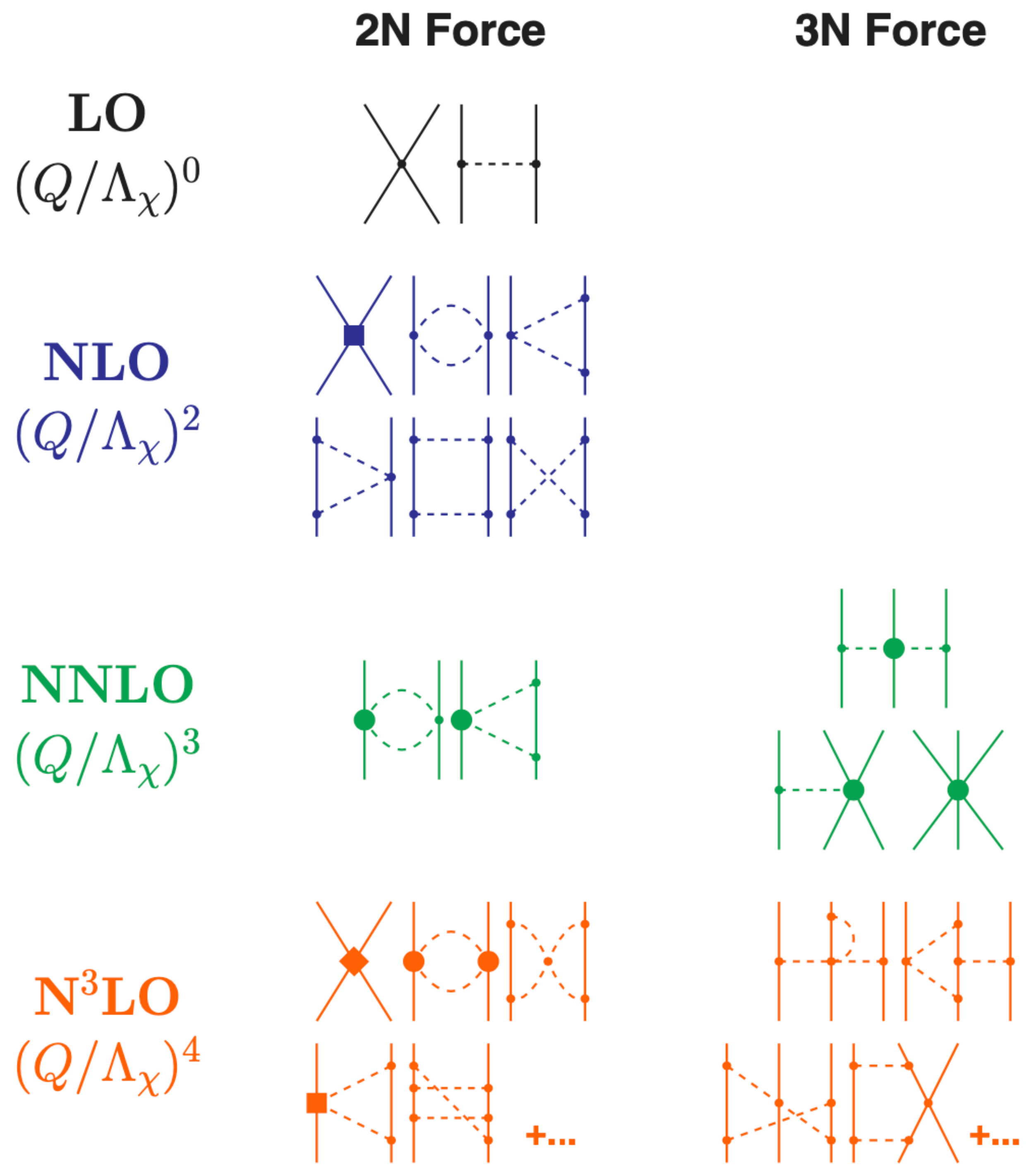

Option 1: Exact solutions have factorial or exponential scaling **e***ⁿ* → limited to light nuclei

Option 2: Correlation-expansion methods to achieve **polynomial** scaling

○ Hamiltonian partitioning $H = H_0 + H_1$

○ Reference state $H_0|\Phi_k^{(0)}\rangle = E_k^{(0)}|\Phi_k^{(0)}\rangle$

○ Wave-operator expansion $|\Psi_k^A\rangle = \Omega_k|\Phi_k^{(0)}\rangle = |\Phi_k^{(0)}\rangle + |\Phi_k^{(1)}\rangle + |\Phi_k^{(2)}\rangle + \ldots$

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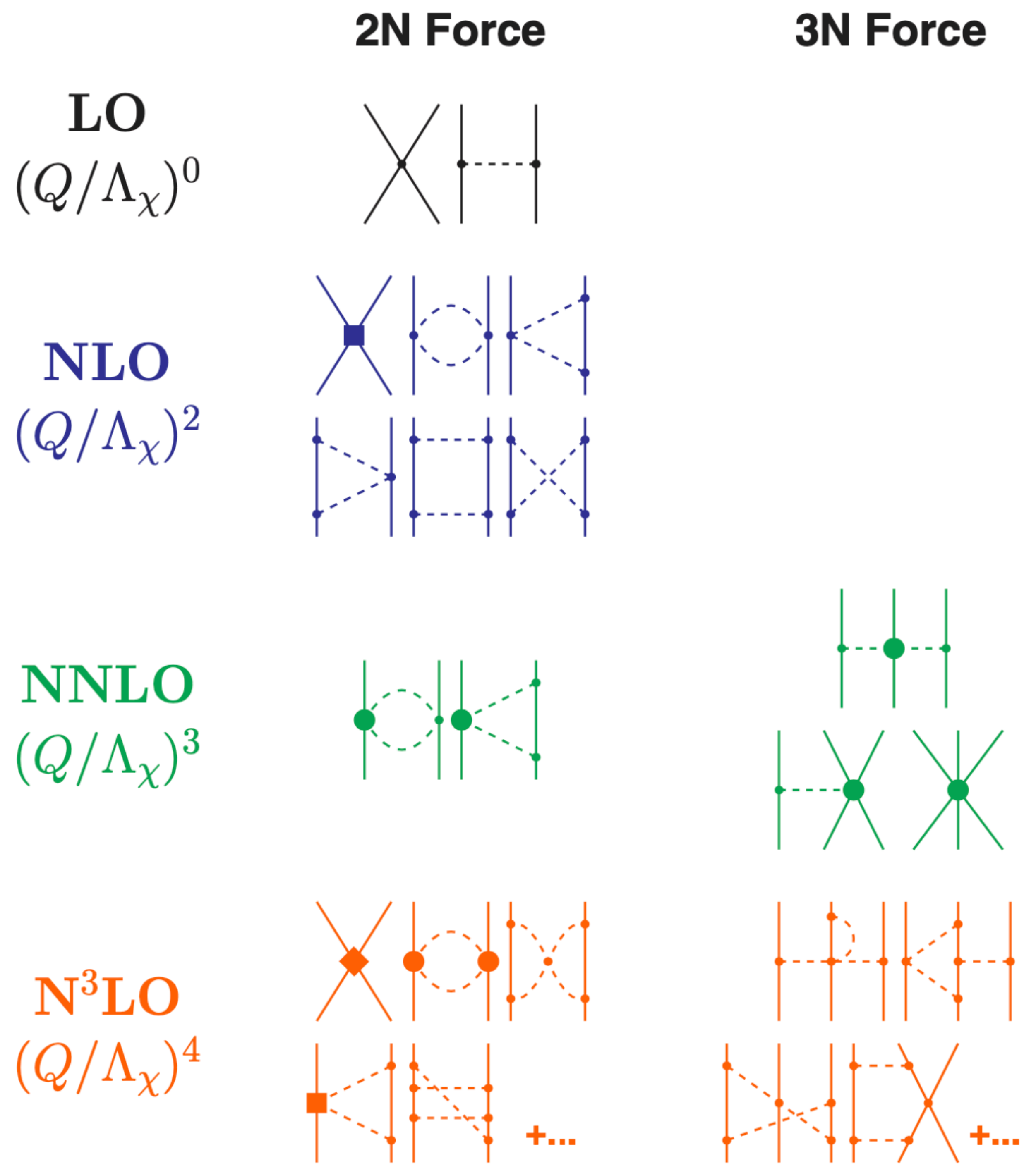

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CPU-scalable to **heavy masses**?

- Hamiltonian partitioning $H = H_0 + H_1$
- Reference state $H_0|\Phi_k^{(0)}\rangle = E_k^{(0)}|\Phi_k^{(0)}\rangle$ → scaling $\boldsymbol{n^4}$
- Wave-operator expansion $|\Psi_k^A\rangle = \Omega_k|\Phi_k^{(0)}\rangle = |\Phi_k^{(0)}\rangle + |\Phi_k^{(1)}\rangle + |\Phi_k^{(2)}\rangle + \dots$ → scaling $\boldsymbol{n^\alpha}$ with $\alpha > 4$

The Segrè chart

Nuclear structure approaches

- Energy density functionals
- Empirical shell model
- *Ab initio*
- …

[Figure: B. Bally]

Data partly taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
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[Figure: B. Bally]

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○ Correlation expansion performed in terms of **particle-hole excitations** → **Breaks down in open-shell systems**

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Solution: start from a **symmetry-breaking reference state**

→ At some point, necessary to **restore symmetries**

$U(1)_N$ x $U(1)_Z$	→	Superfluidity
$SU(2)$	→	Deformation

→ *cf. energy density functionals*

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Dynamic correlations

Static correlations

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○ Keep **polynomial cost** (with higher pre-factor)

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Dynamic correlations

Static correlations

○ Keep **polynomial cost** (with higher pre-factor)

○ **Many different strategies exist**

→ Break which symmetries?

→ Restore then expand or expand then restore?

Most efficient option will depend on

○ Nucleus

○ Observables

○ Required precision

○ …

Necessity to develop many different, complementary approaches

Theoretical methods

○ Two approaches discussed here

1 **Self-consistent Green's functions (SCGF)**

Symmetry restoration missing

$$|\Psi_k^A\rangle = \Omega_k |\Phi_k^{(0)}\rangle = |\Phi_k^{(0)}\rangle + |\Phi_k^{(1)}\rangle + |\Phi_k^{(2)}\rangle + \dots$$

Dynamical correlations on top

[Somà, Duguet, Barbieri, 2011-2014]

[Scalesi, Somà, Duguet, Frosini, 2024]

"Simple" **symmetry-breaking** (**HFB or dHF**) reference state

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"Simple" **symmetry-breaking** (**HFB or dHF**) reference state

2 **Projected Generator Coordinate Method (PGCM)**

DRF

pan@cea

DAM DES

Problème à A nucleons au CEA

$$|\Psi_k^A\rangle = \Omega_k|\Phi_k^{(0)}\rangle = |\Phi_k^{(0)}\rangle + |\Phi_k^{(1)}\rangle + |\Phi_k^{(2)}\rangle + \dots$$

Dynamical correlations (PGCM-PT) not shown here

[Frosini *et al.*, 2022]

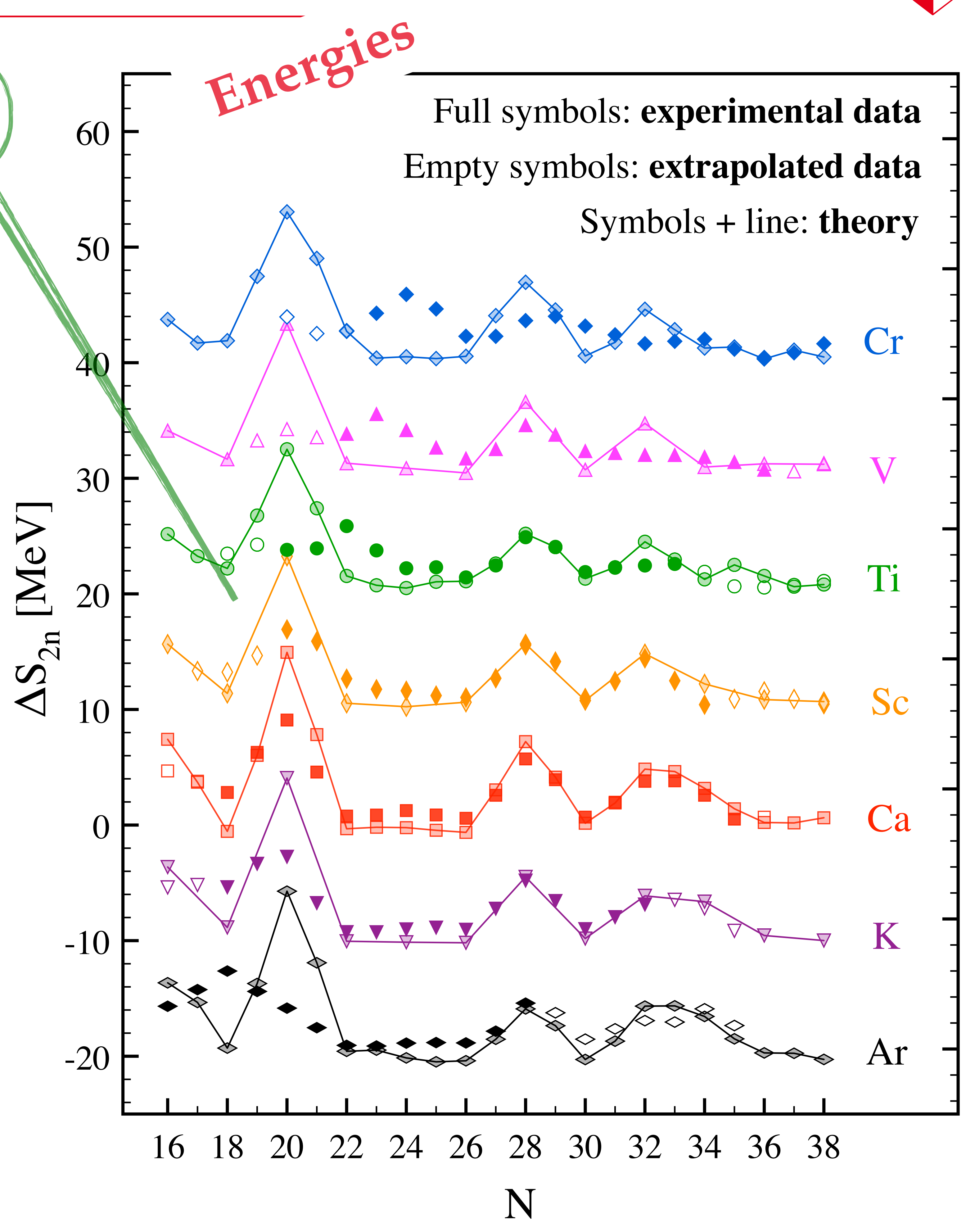
Sophisticated reference state (**linear combination of projected dHFB states**)

Superfluid self-consistent Green's functions

- ○ Symmetry breaking: particle number
- ○ Dynamical correlations at 2nd order

→ **G.s. properties of singly open-shell**

Magic numbers emerge "ab initio"



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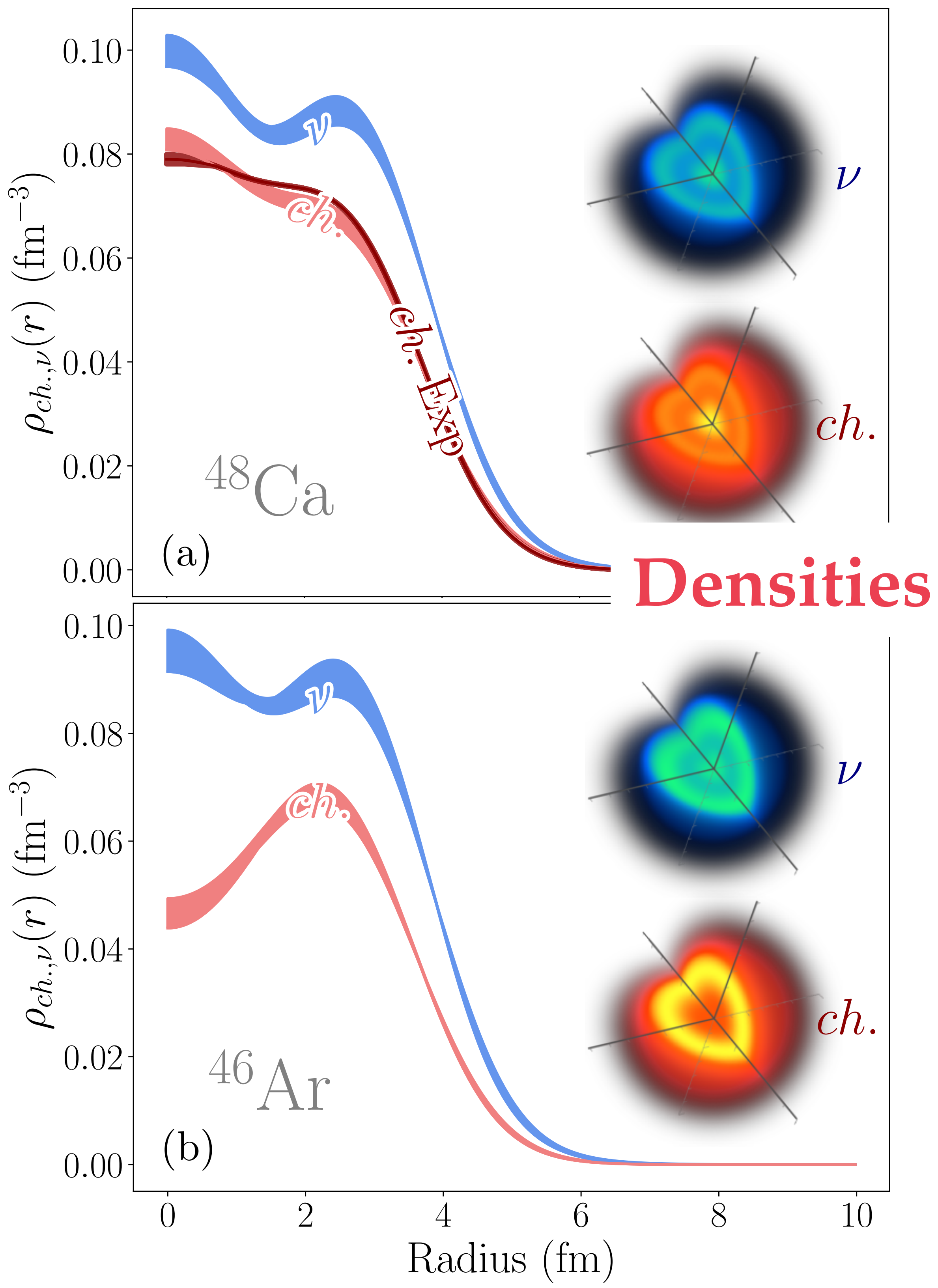
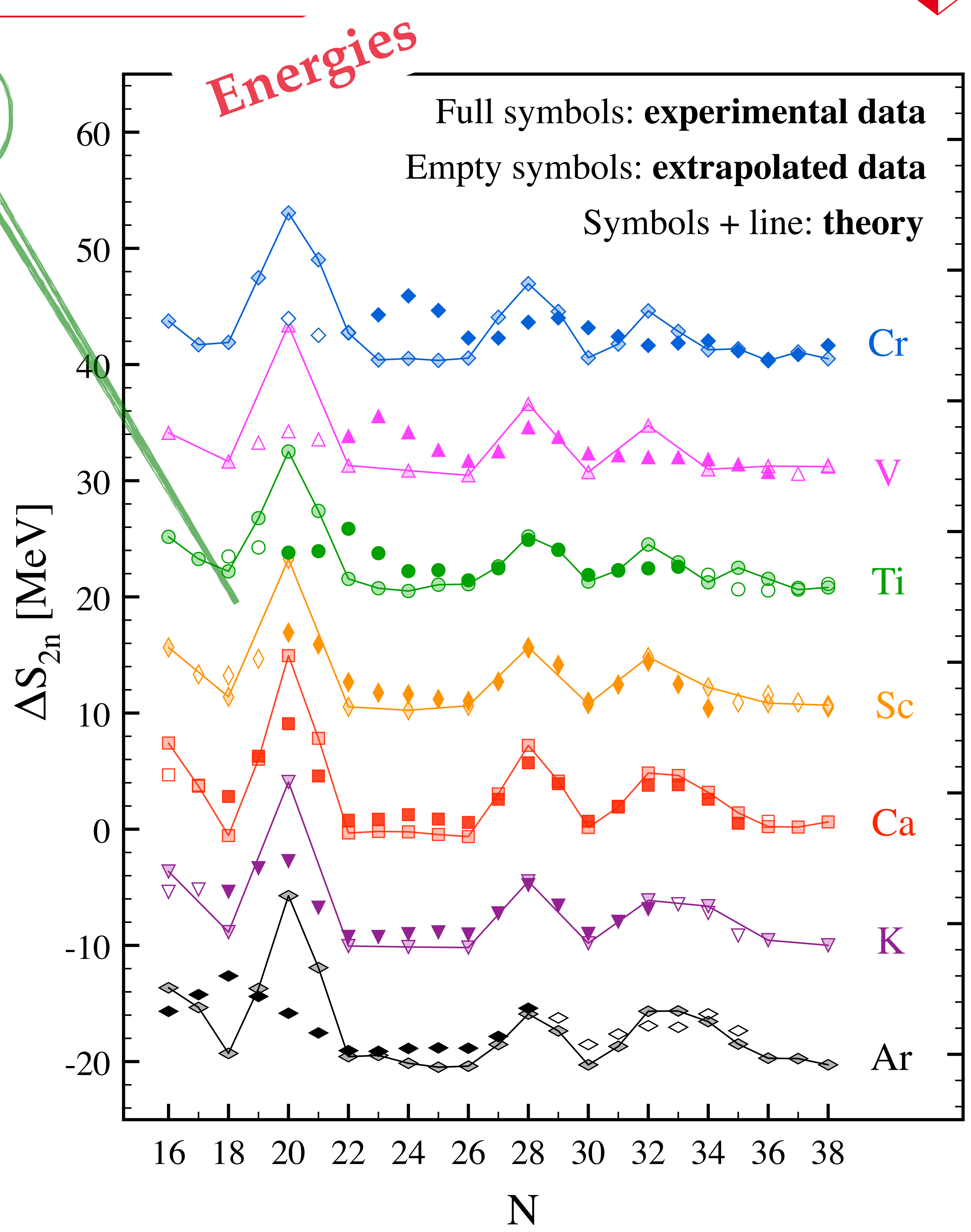
[Brugnara *et al.*, 2506.23228]





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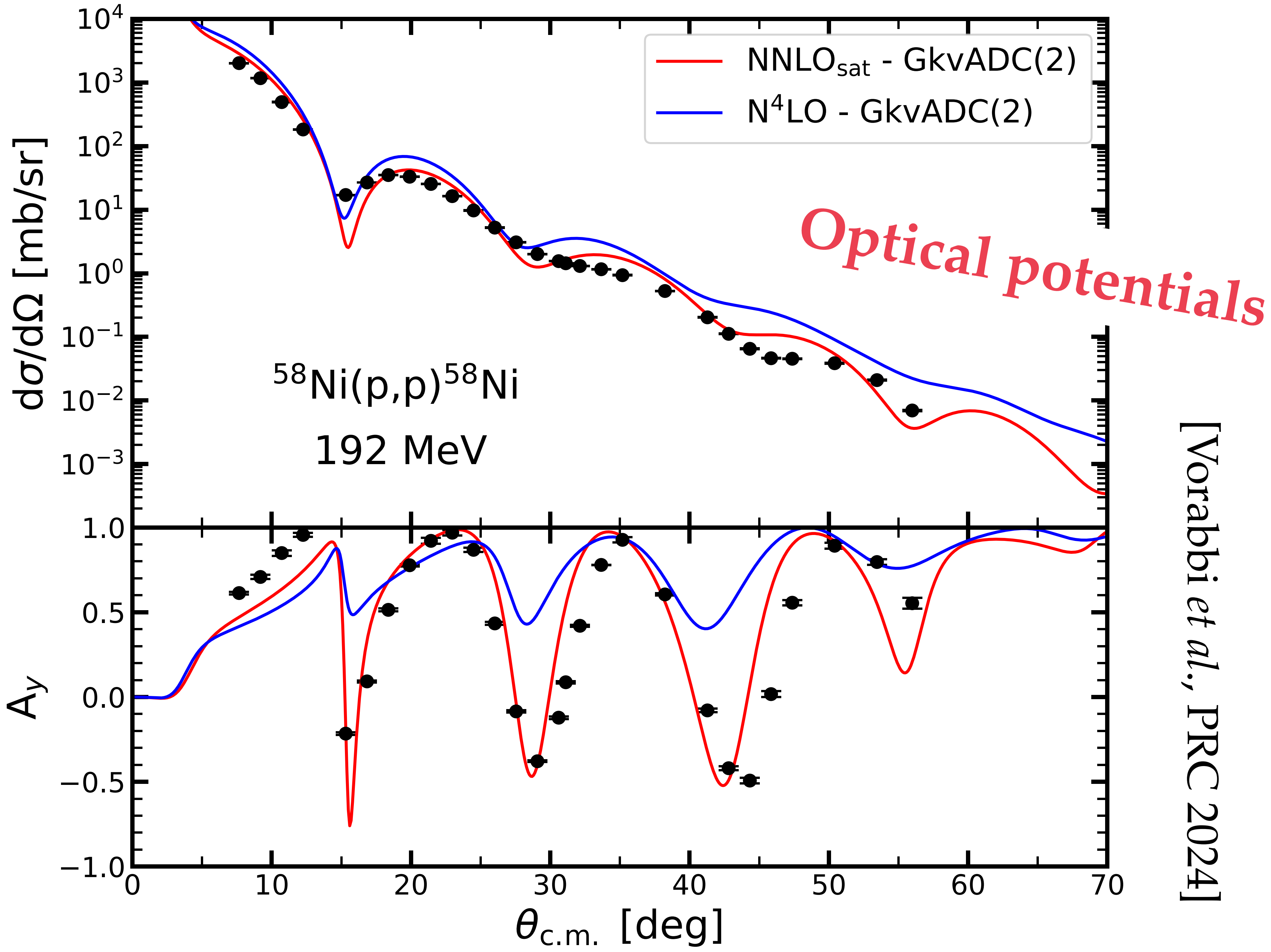

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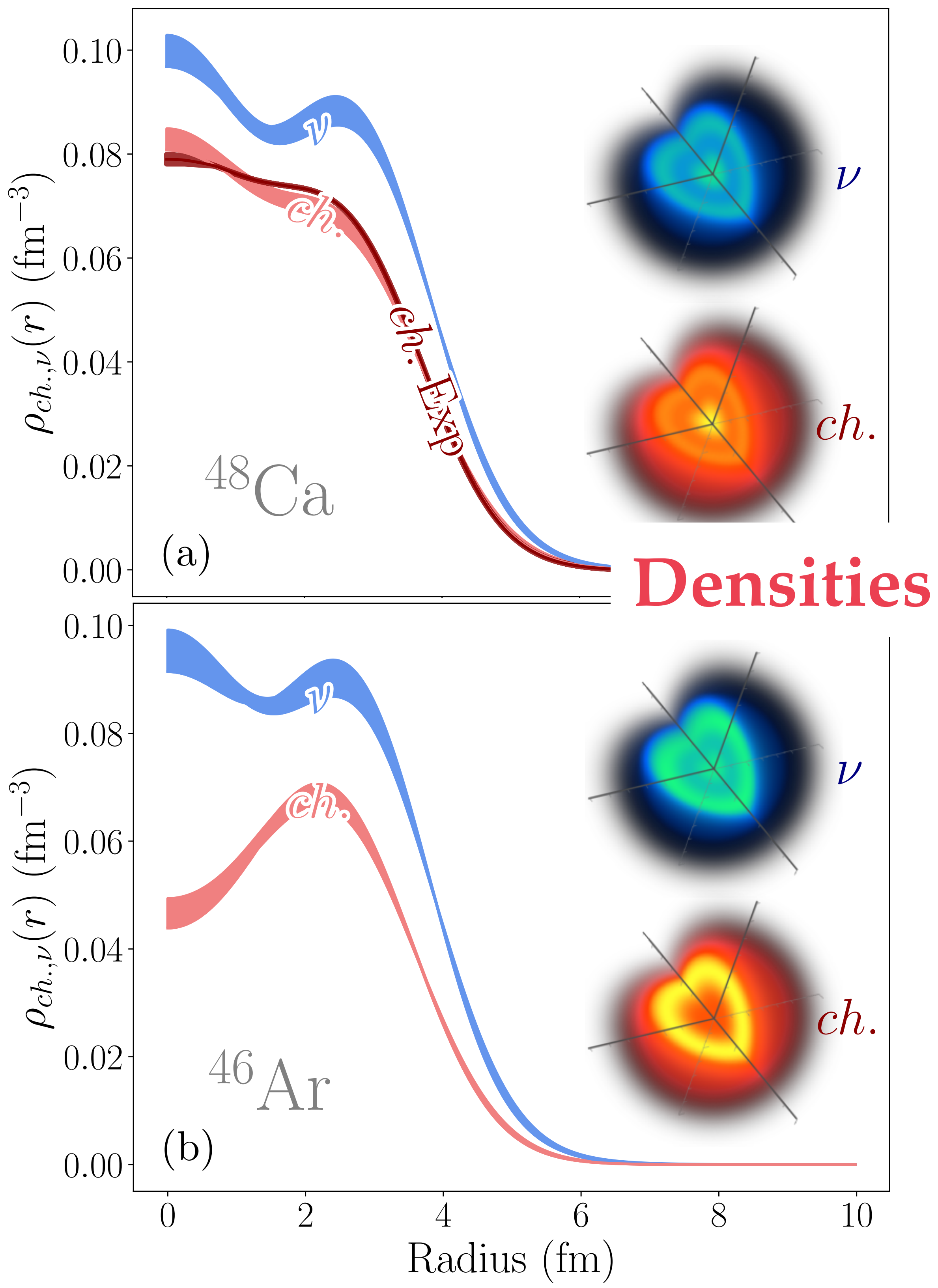

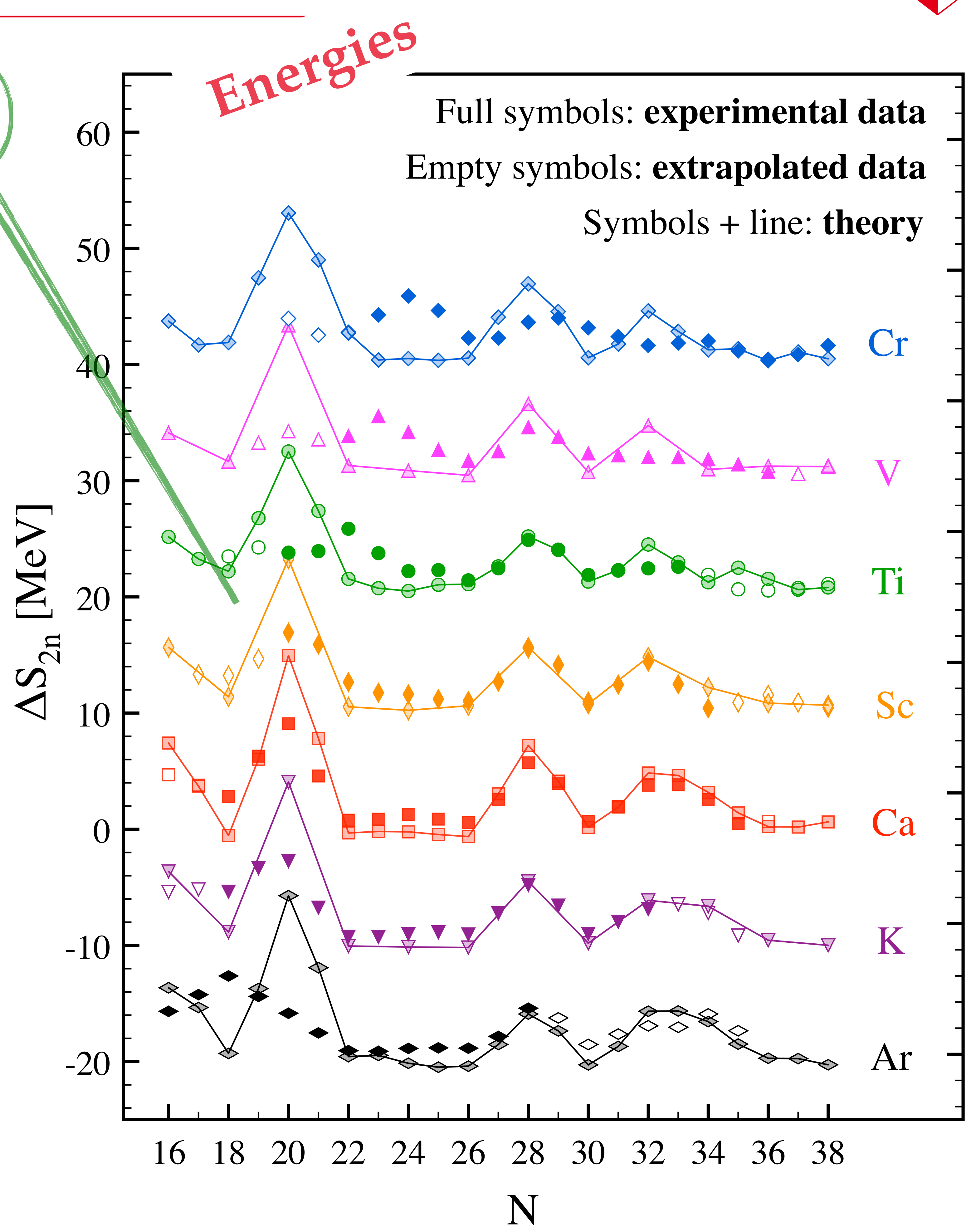

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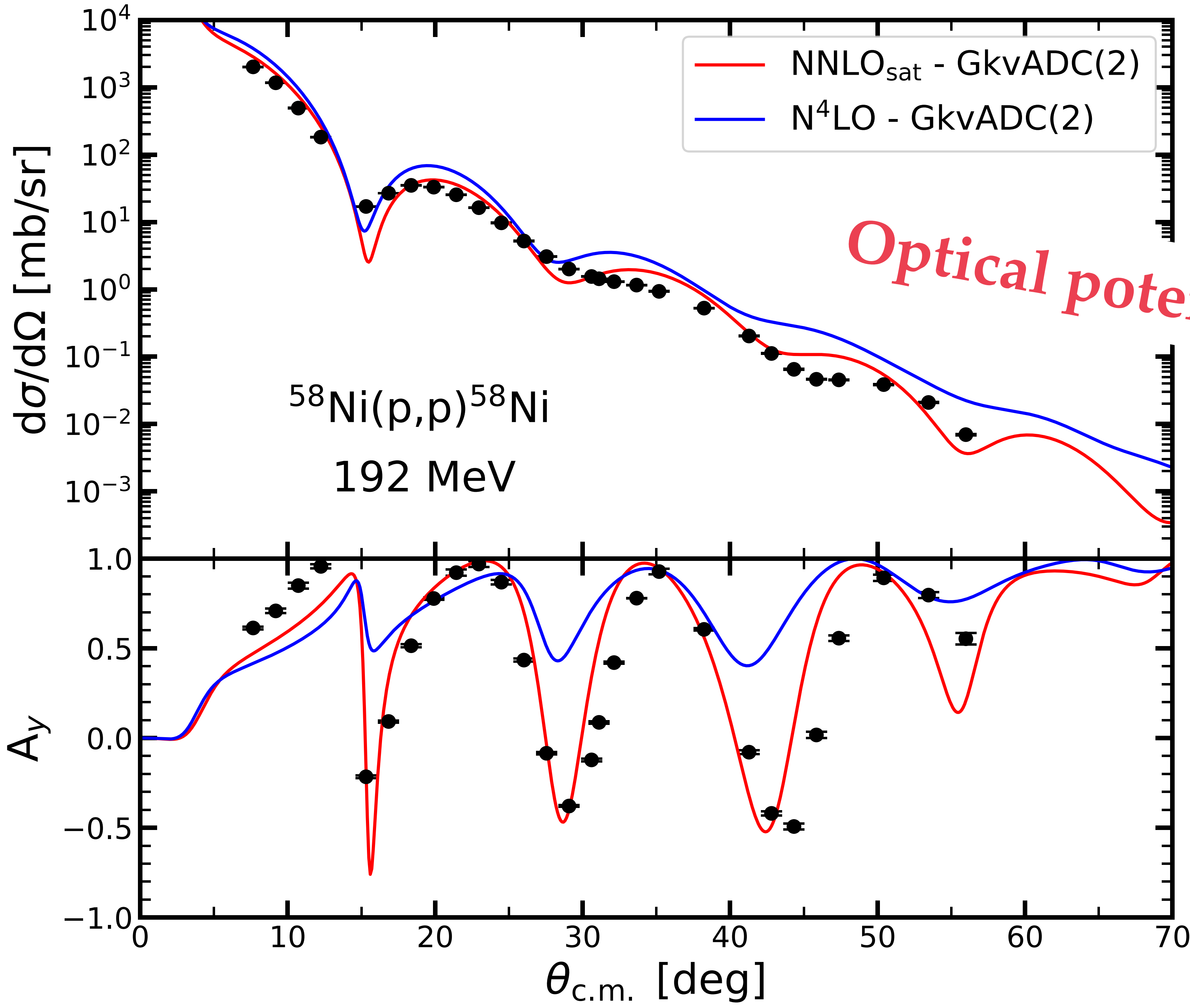
Optical potentials



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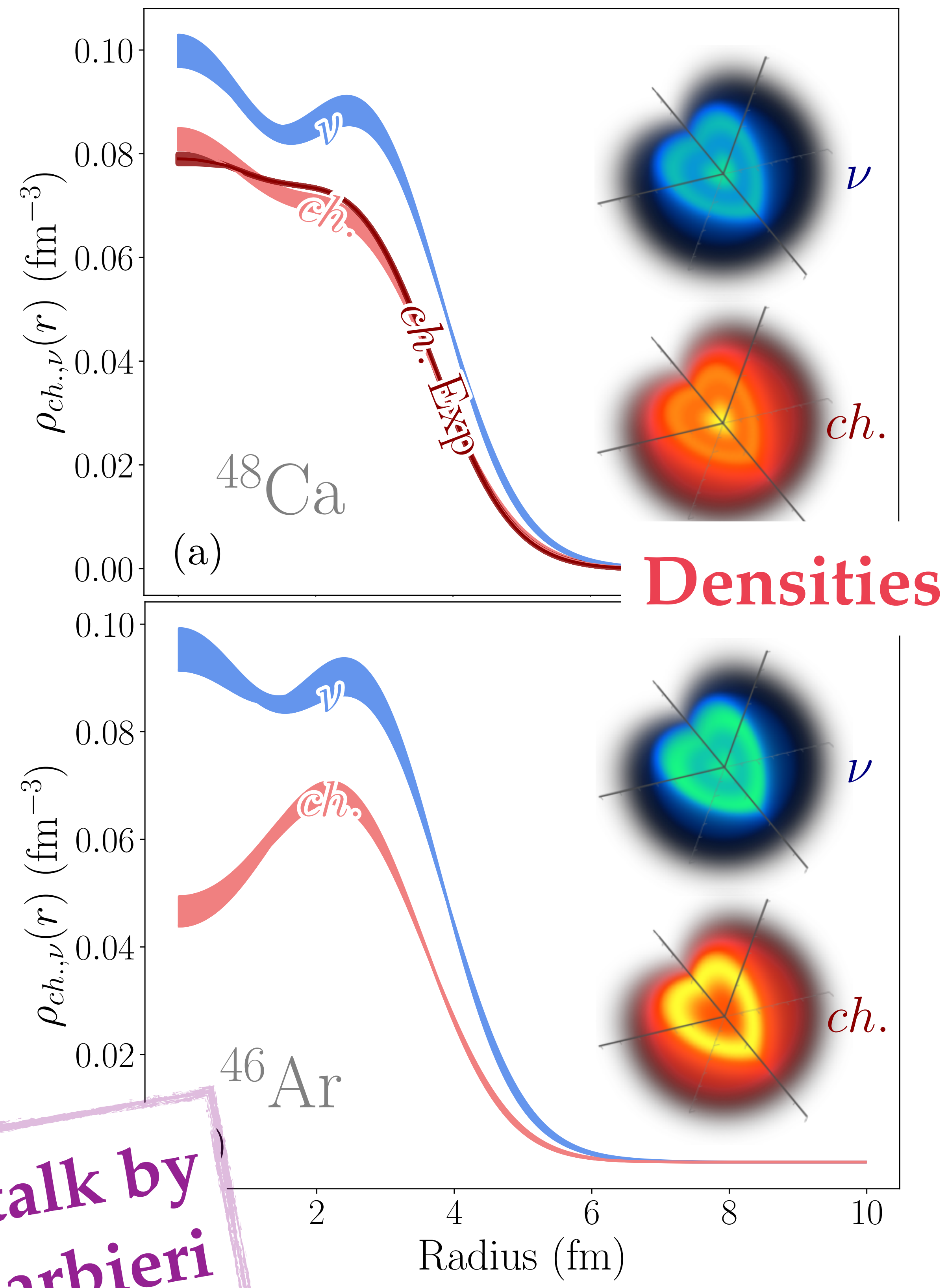
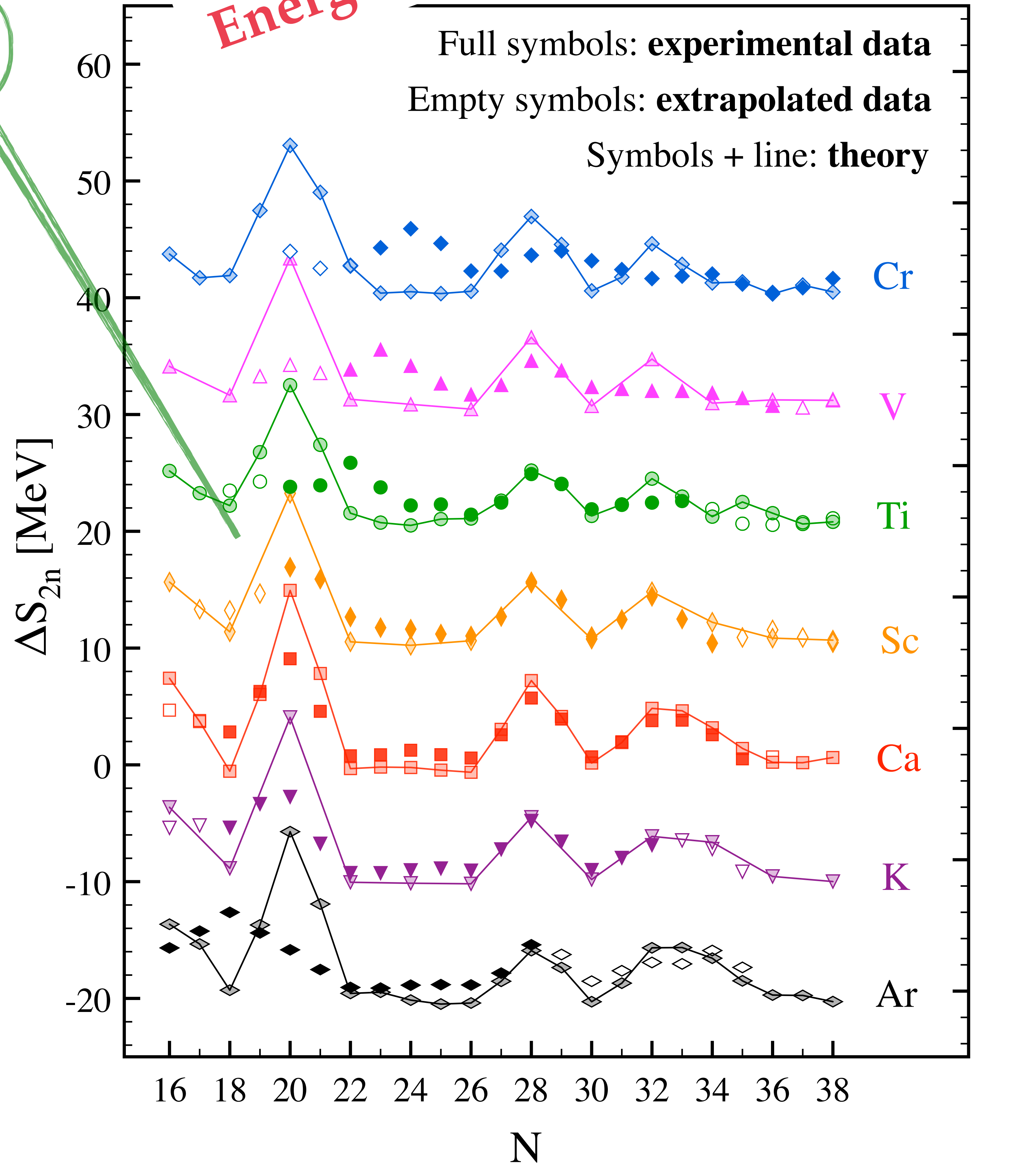


Densities

See talk by C. Barbieri

Energies



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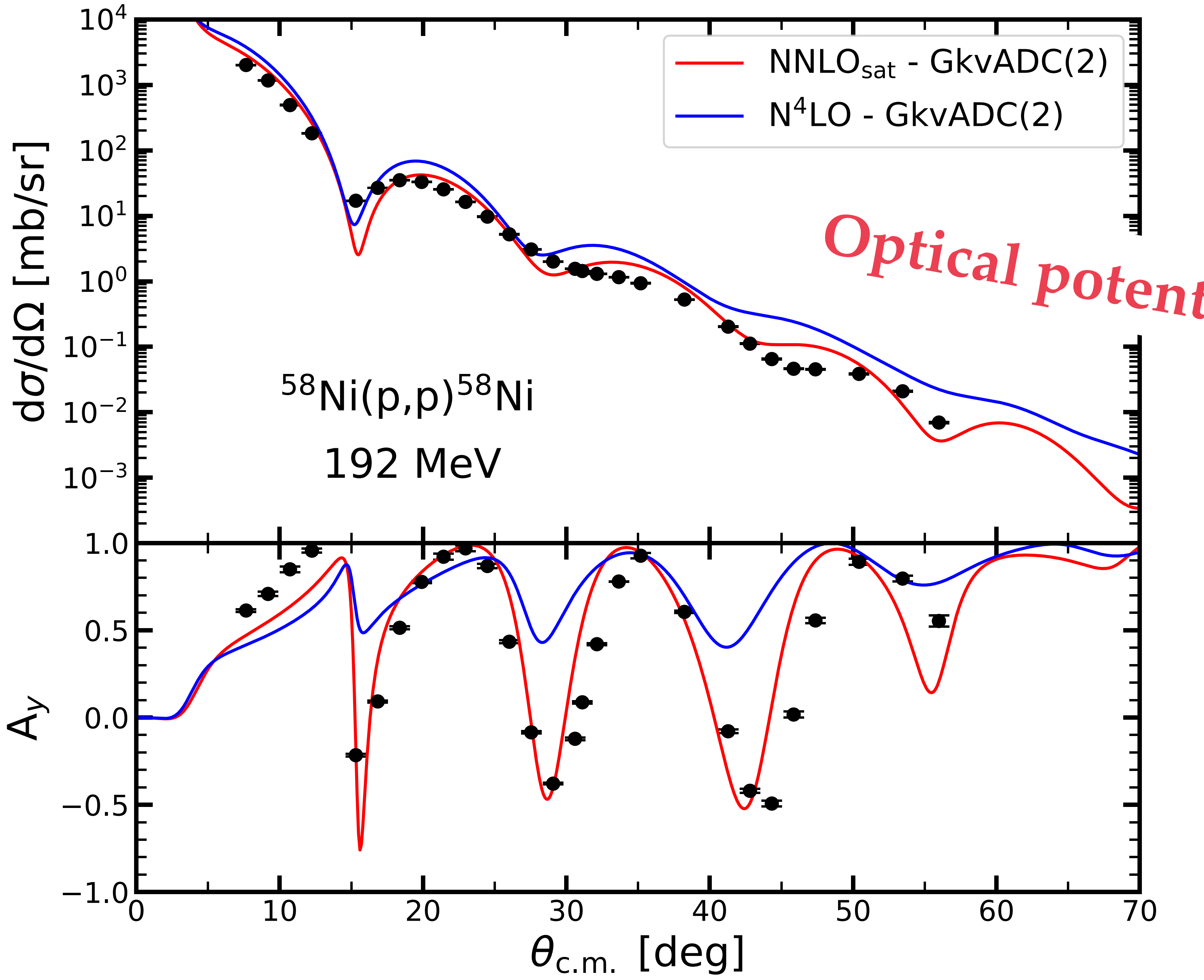

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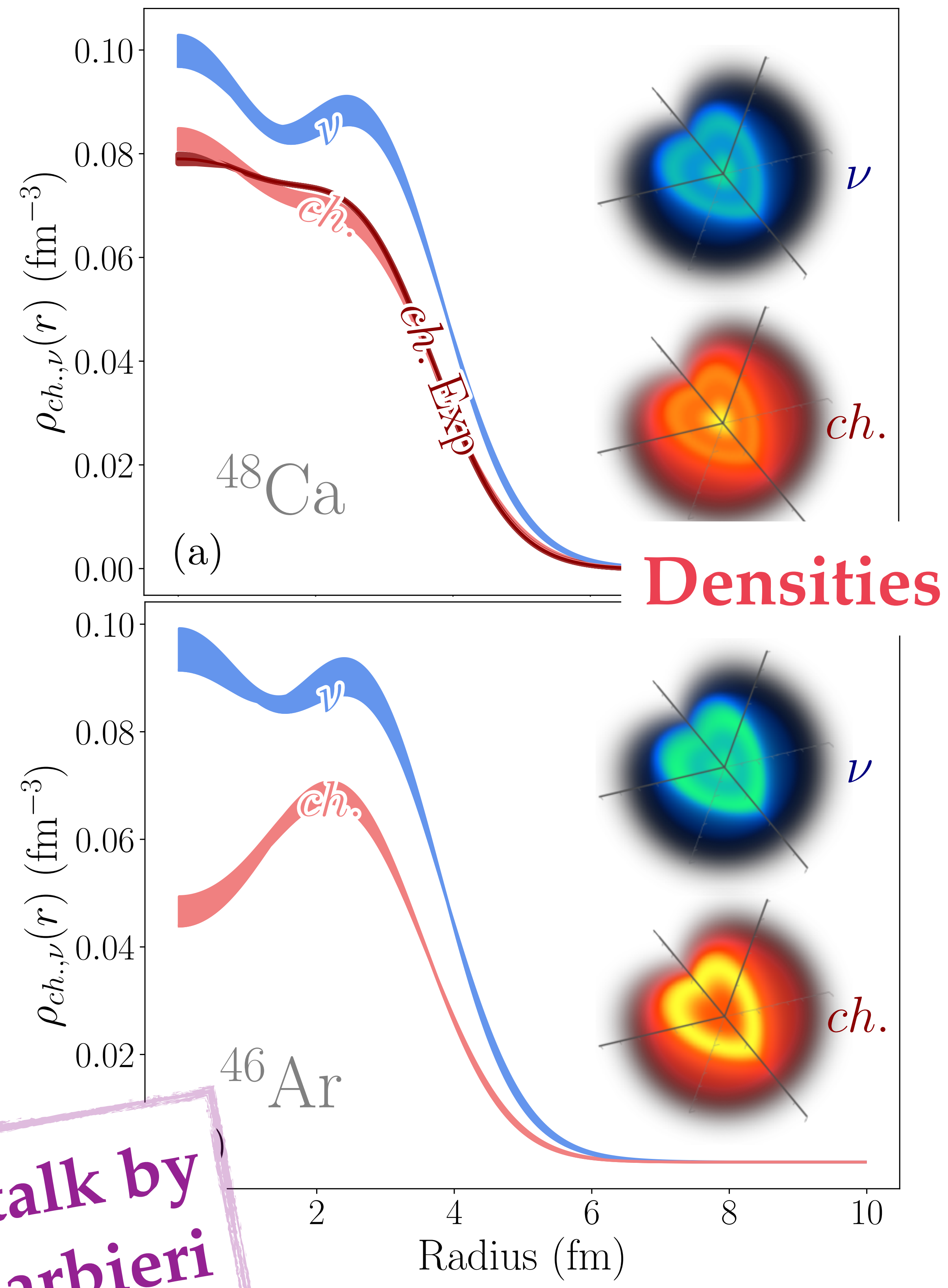

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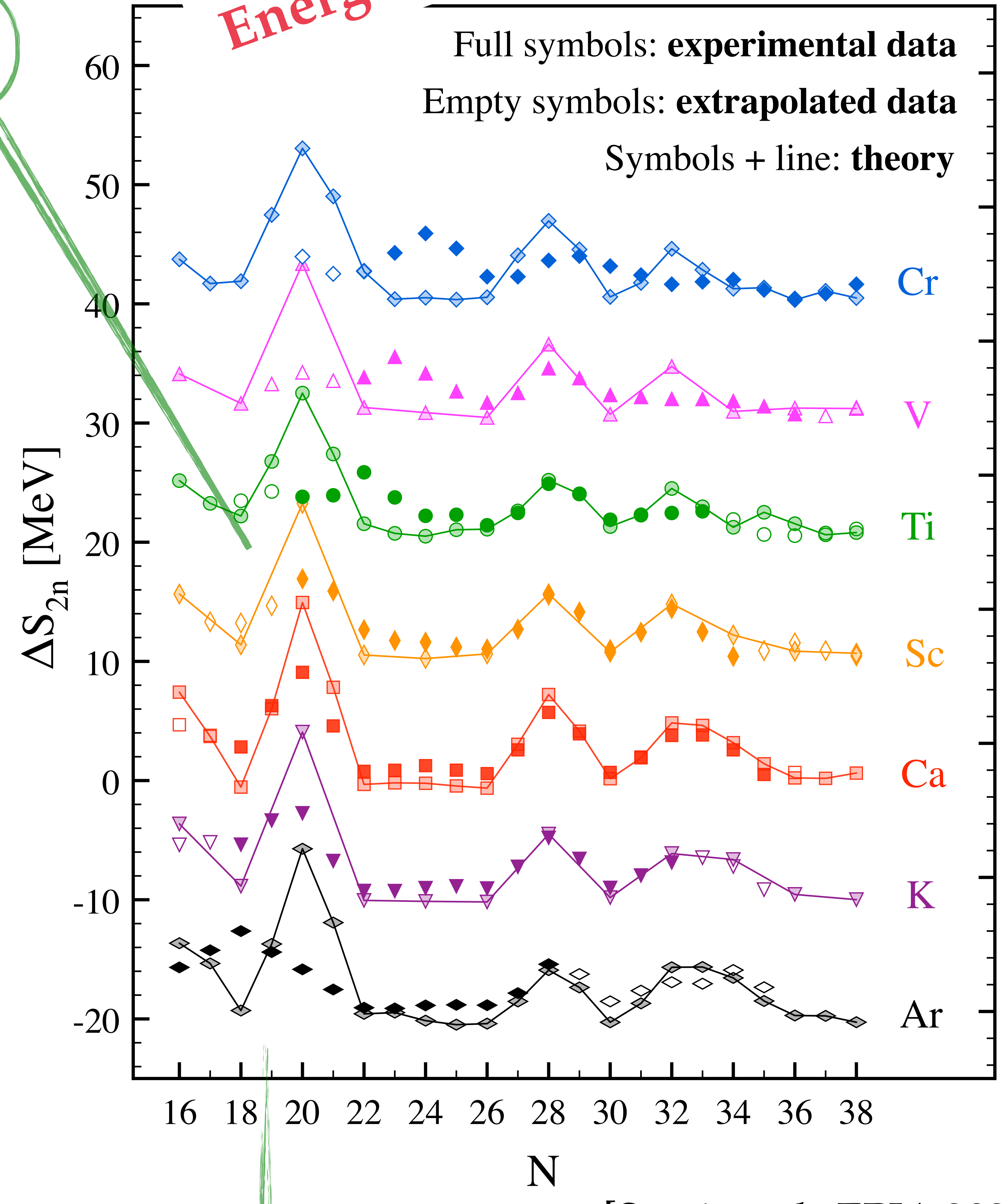

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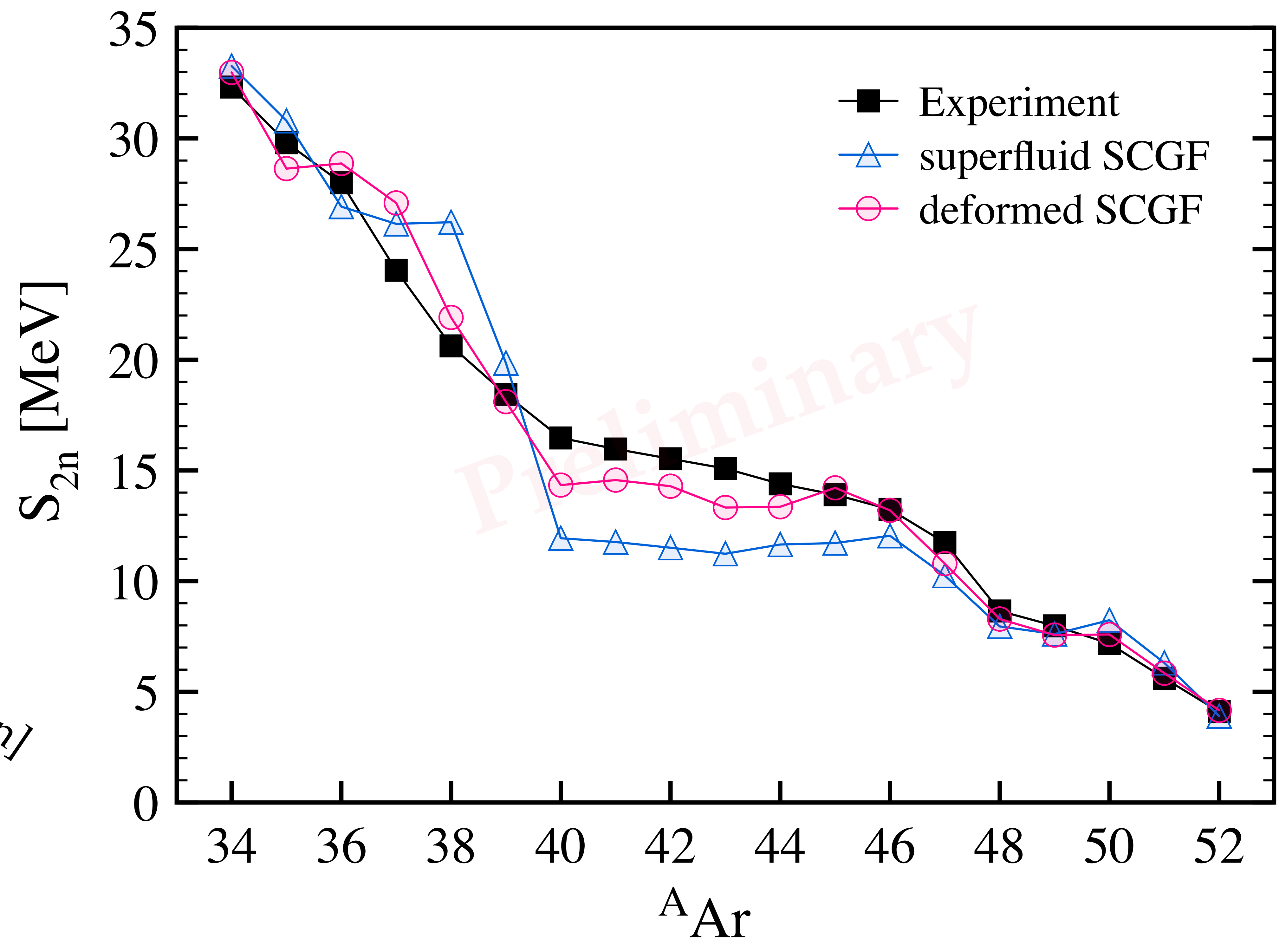
○ Accuracy degrades away from semi-magic Ca

→ Calls for **explicit inclusion of deformation**

Deformed self-consistent Green's functions

- ○ Symmetry breaking: rotational invariance
- ○ Dynamical correlations at 2nd order
- → **G.s. properties of doubly open-shell**

[Scalesi et al. in preparation]



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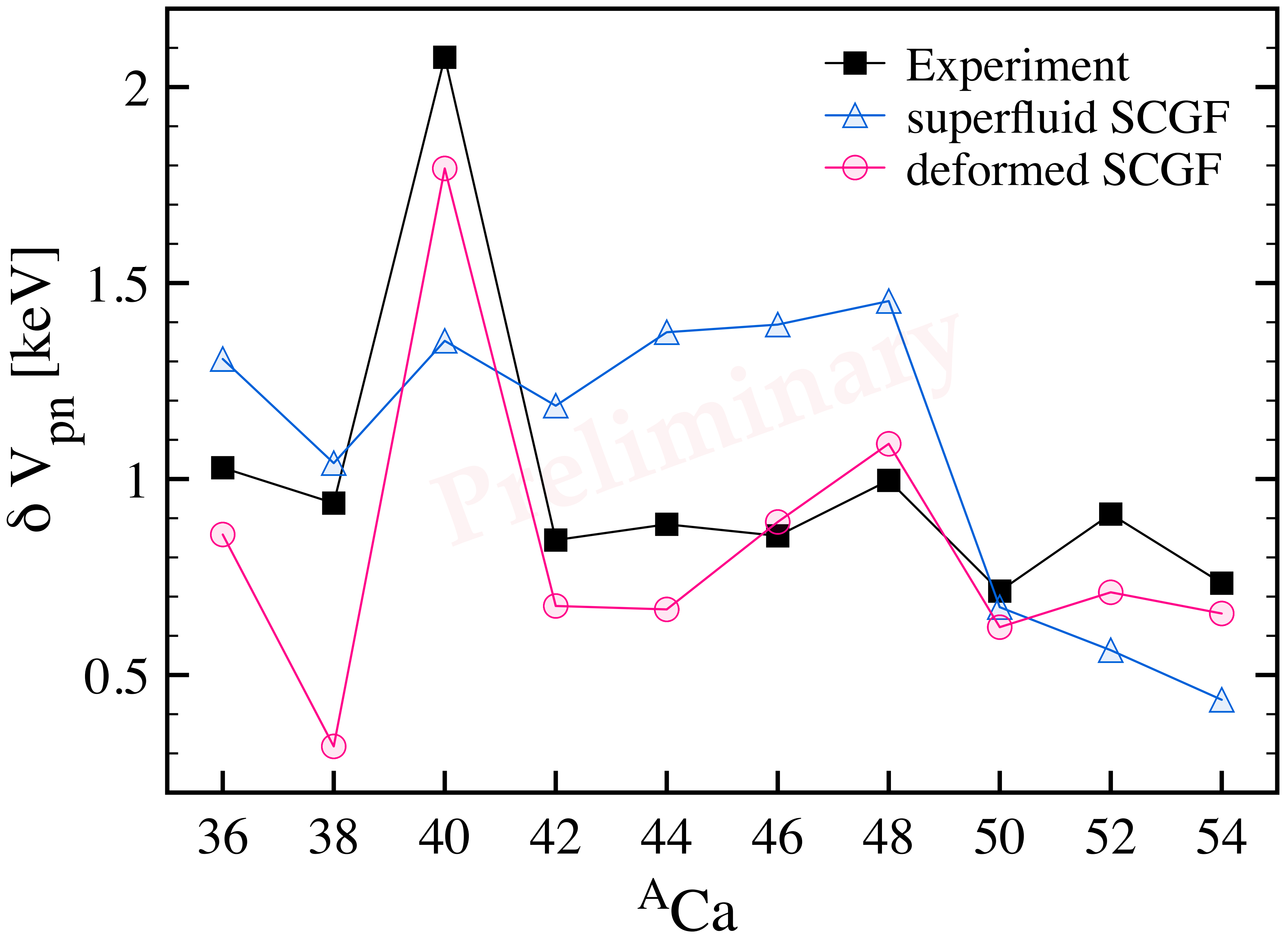

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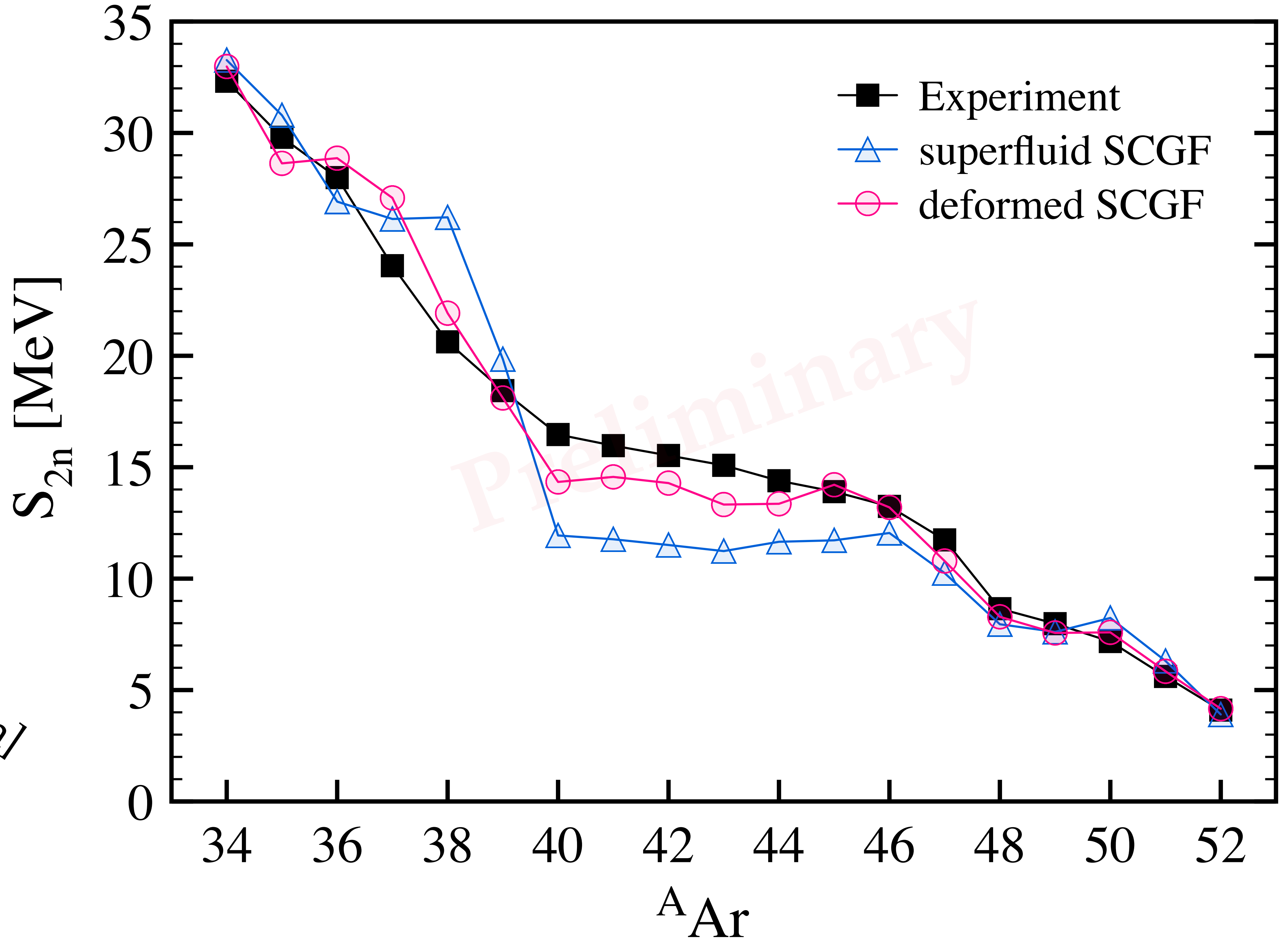

- ○ Improved description of argon chain
- ○ *np interaction* highlights **impact of deformation**

$$\delta V_{\mathrm{pn}}(N,Z) \equiv \frac{1}{4}[S_{2\mathrm{n}}(N,Z) - S_{2\mathrm{n}}(N,Z-2)]$$

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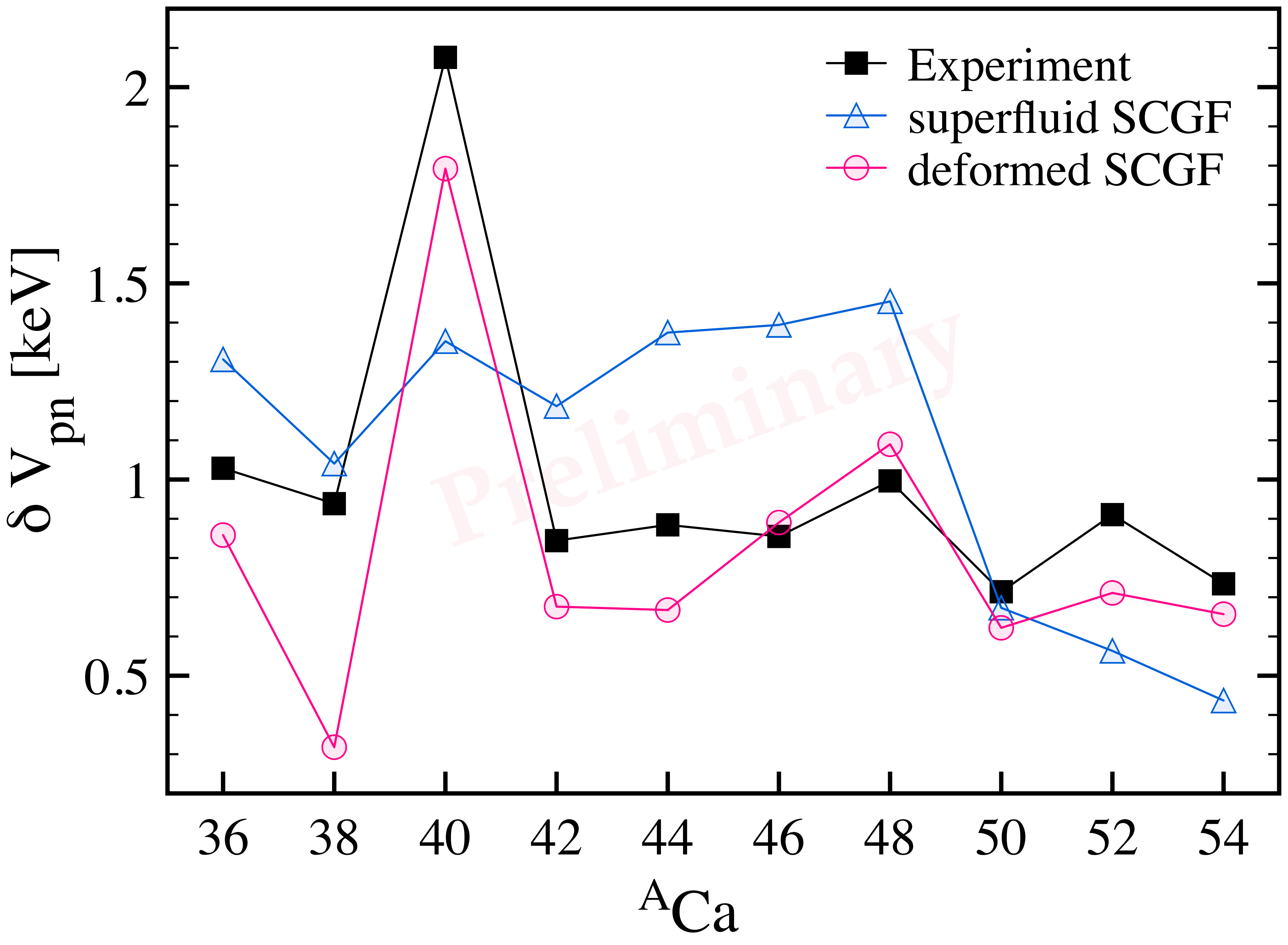

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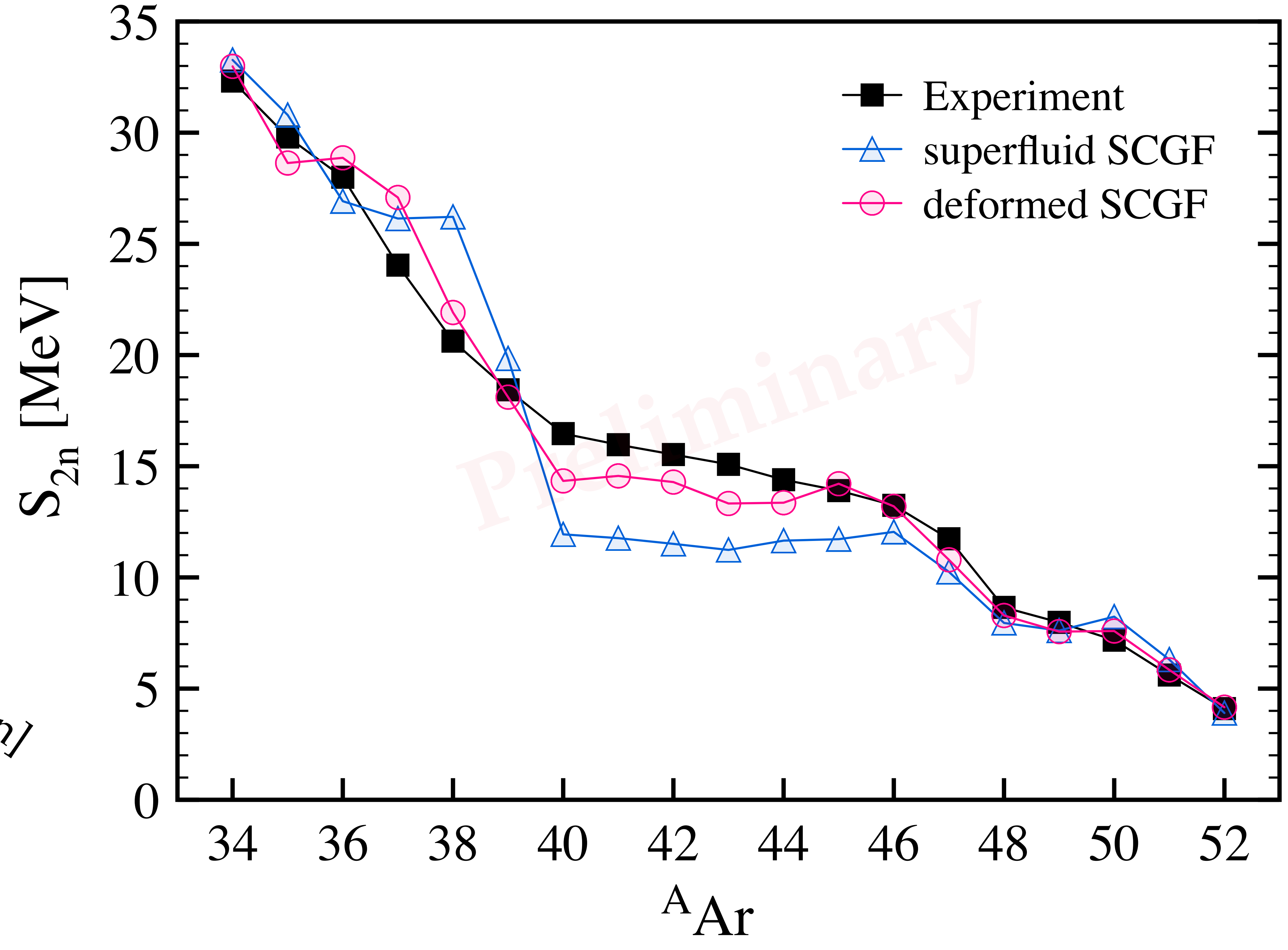

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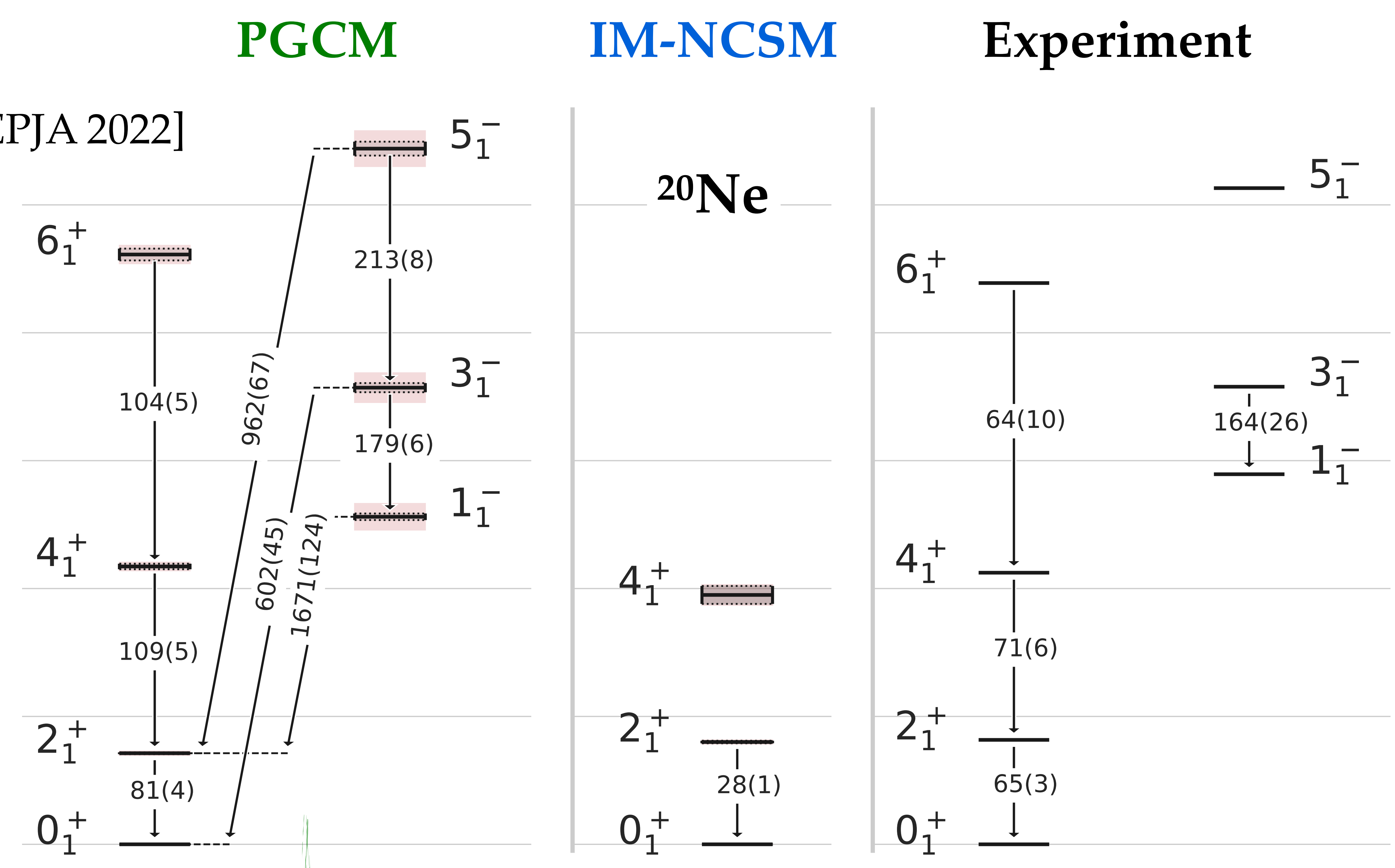
- ○ Preliminary tests in **odd-Z chains** promising

Projected generator coordinate method

- ○ Symmetry breaking & restoration
  - → particle number
  - → rotational invariance
  - → parity
- ○ No dynamical correlations
- → **Excitation spectra & collective properties**

[Frosini *et al.*, EPJA 2022]



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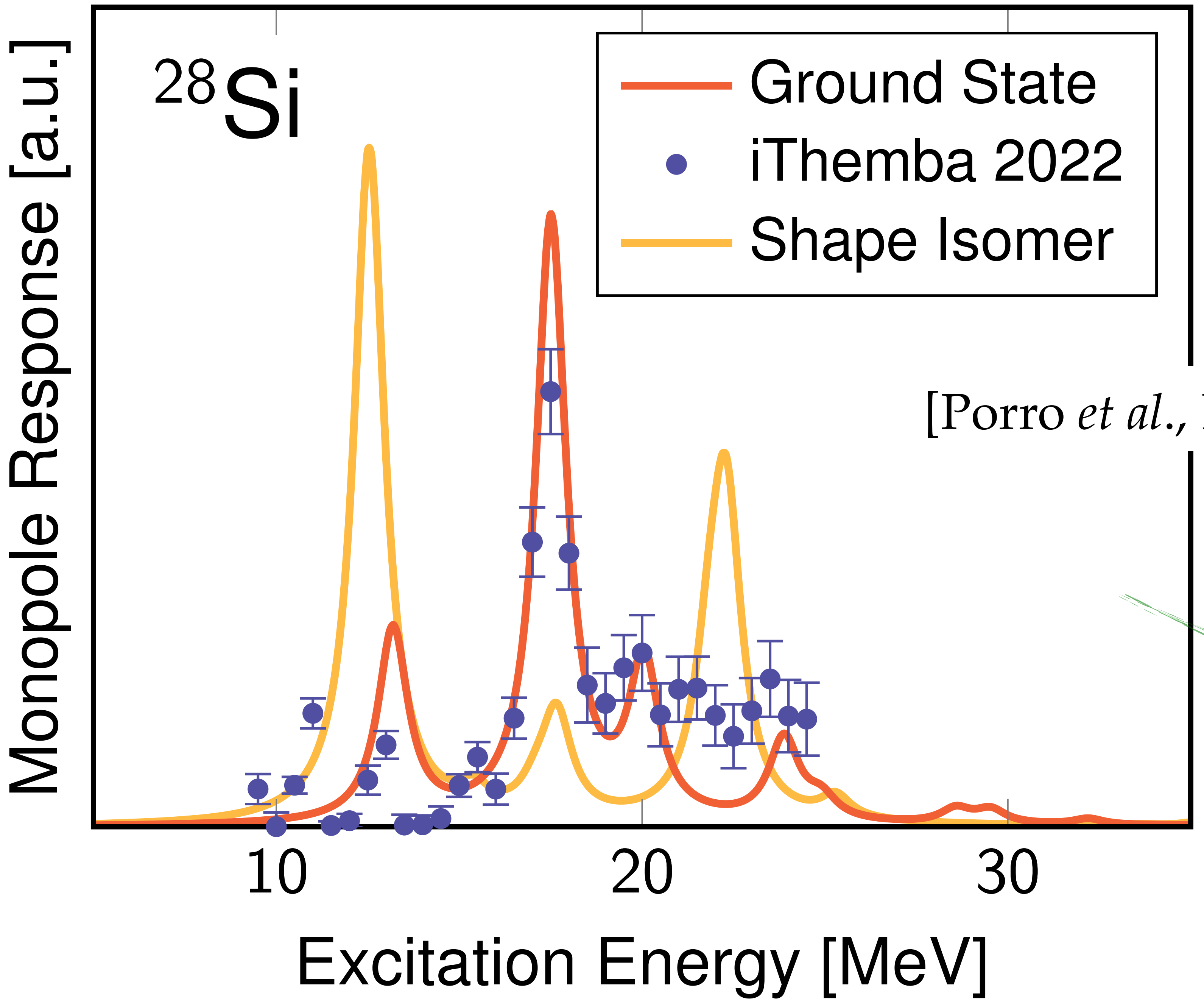

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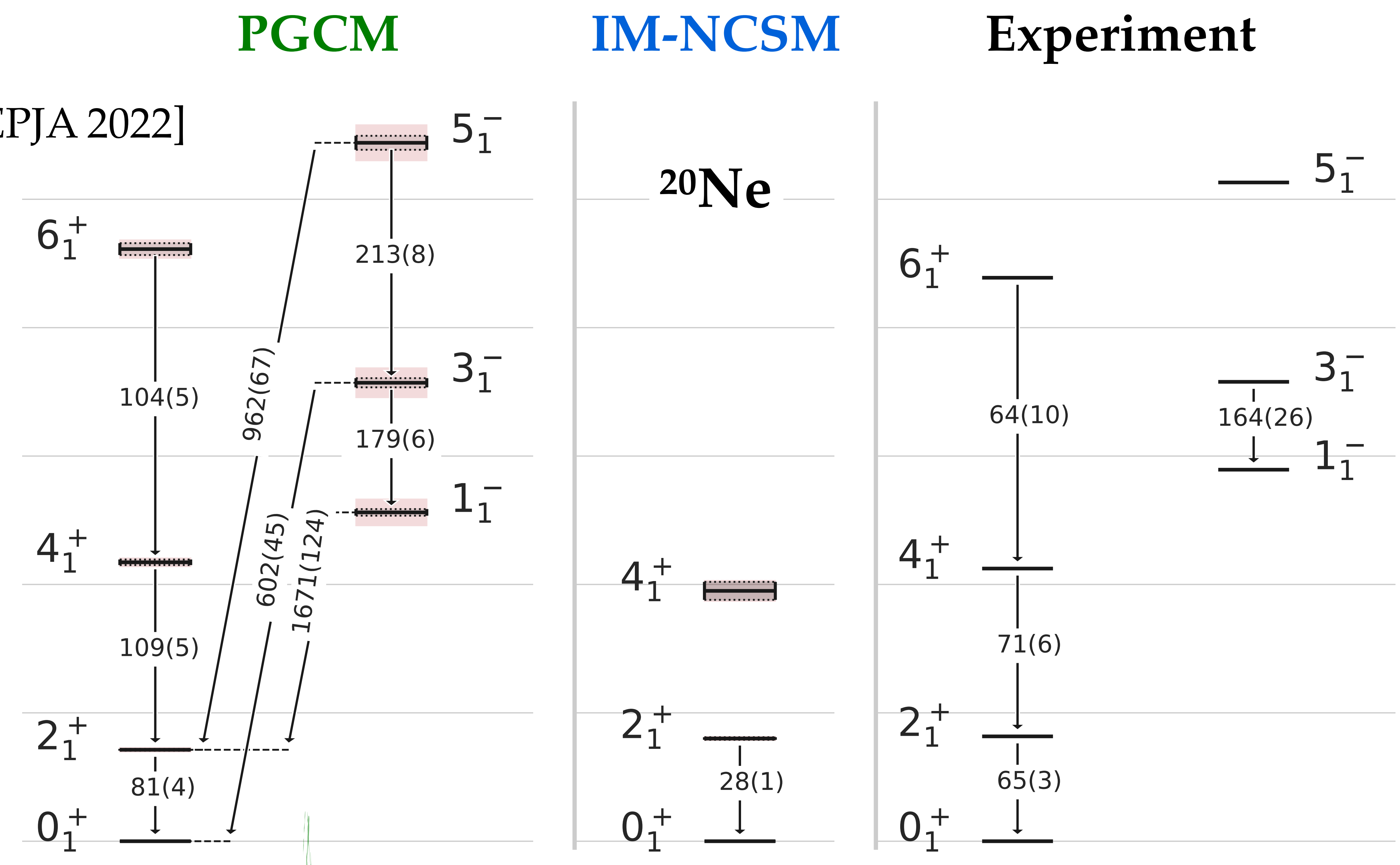

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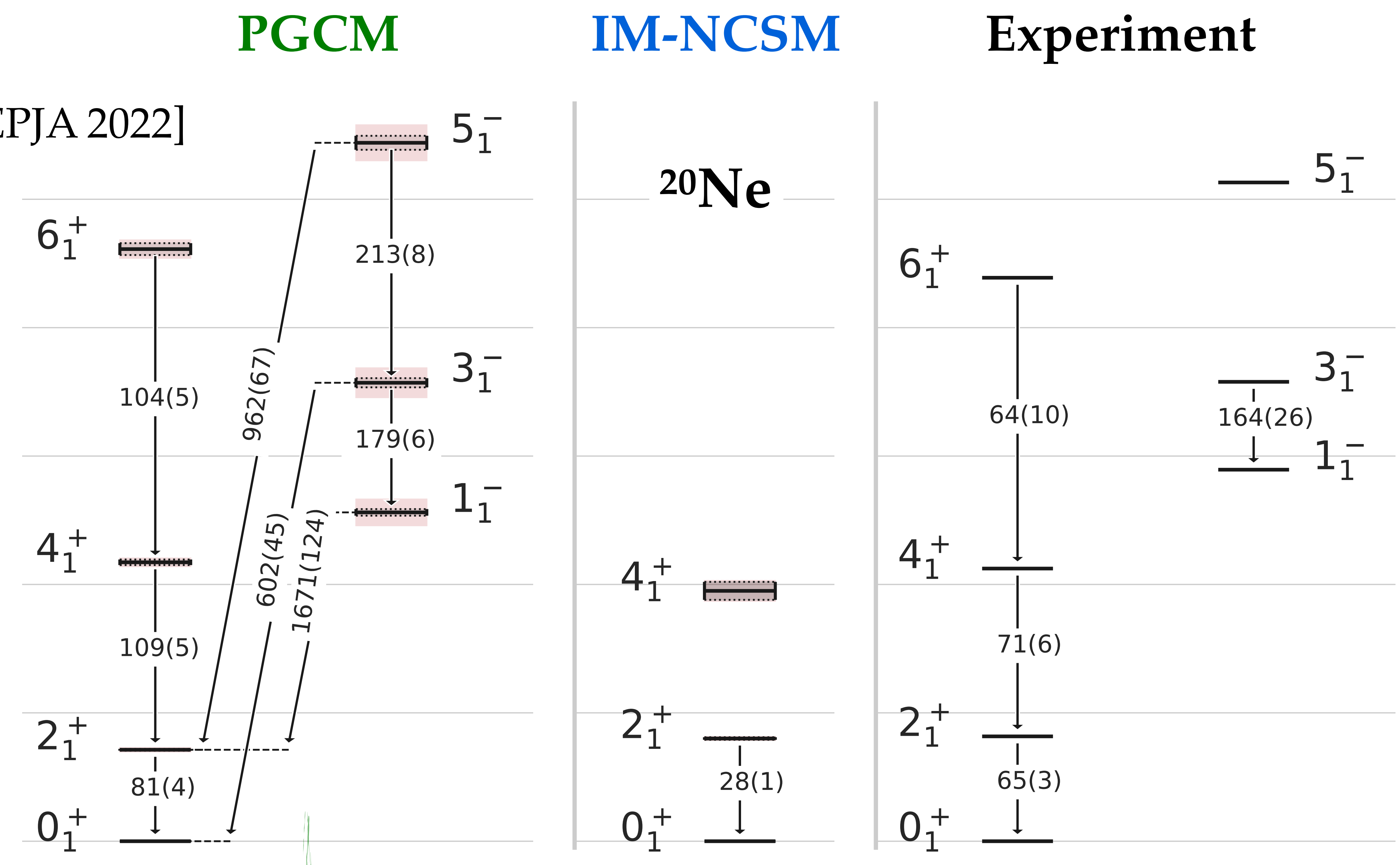

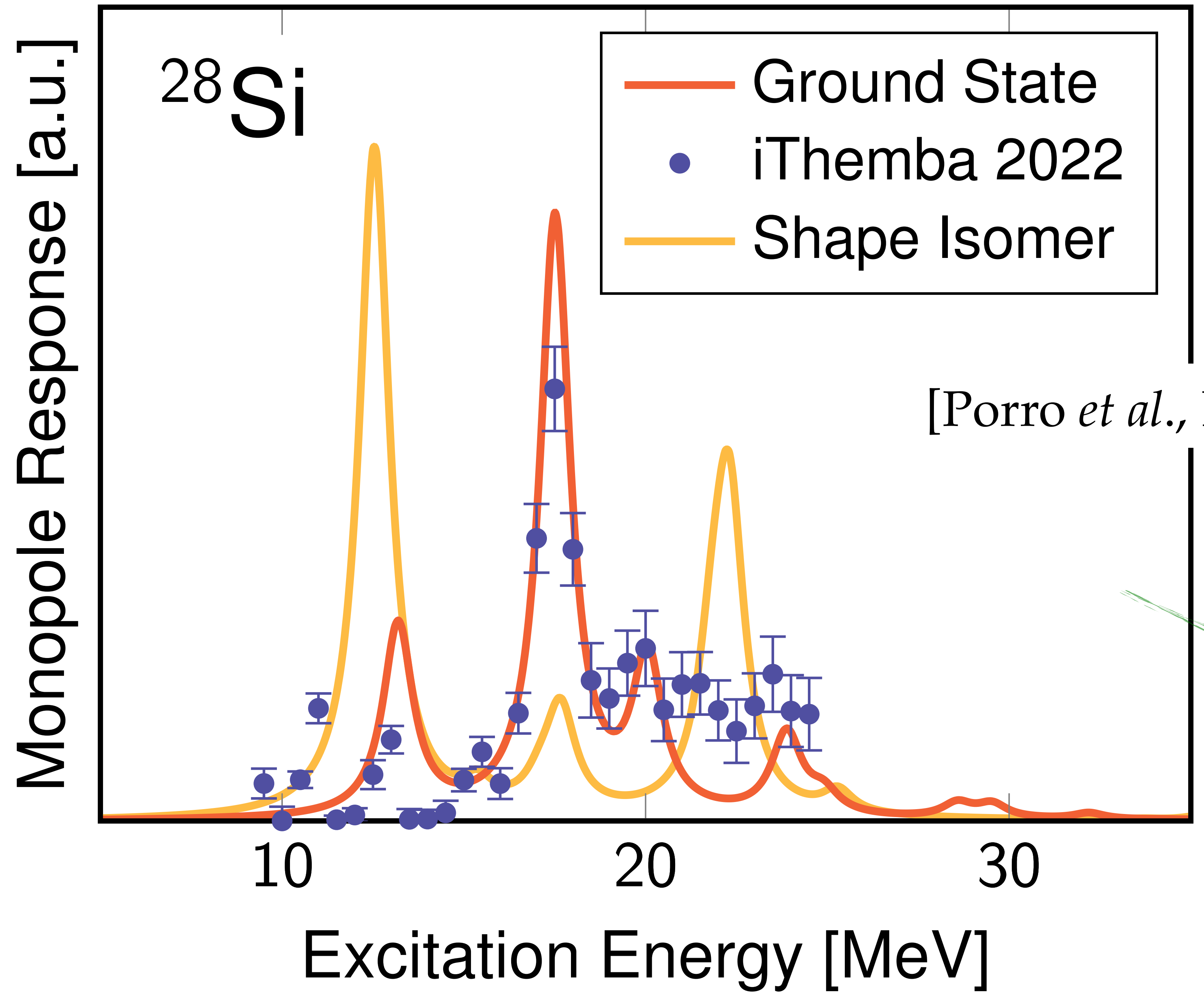

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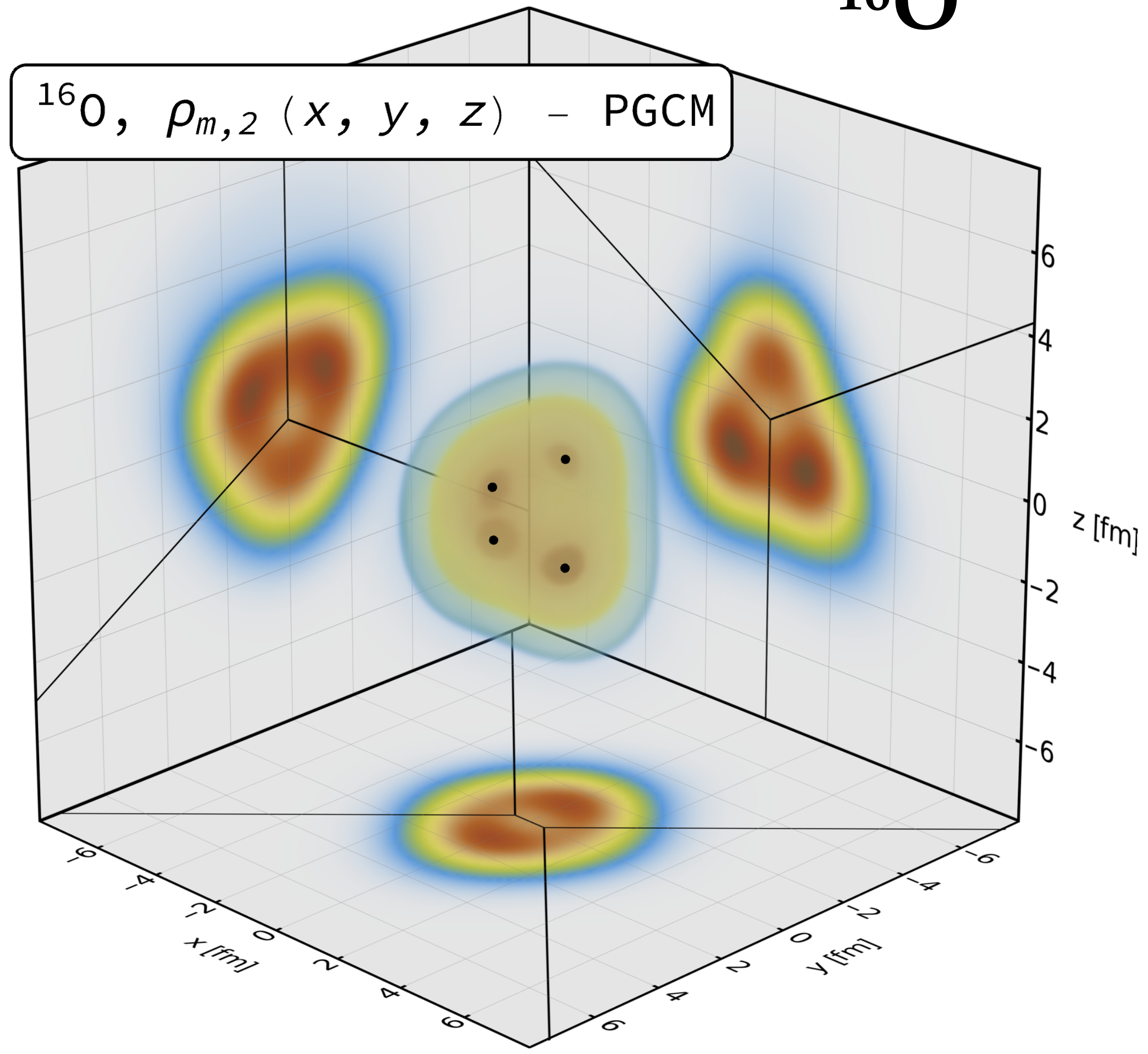
Nuclear structure & relativistic ion collisions

○ **Nuclear densities (PGCM & NLEFT) → Hydro simulation → Hadronization**

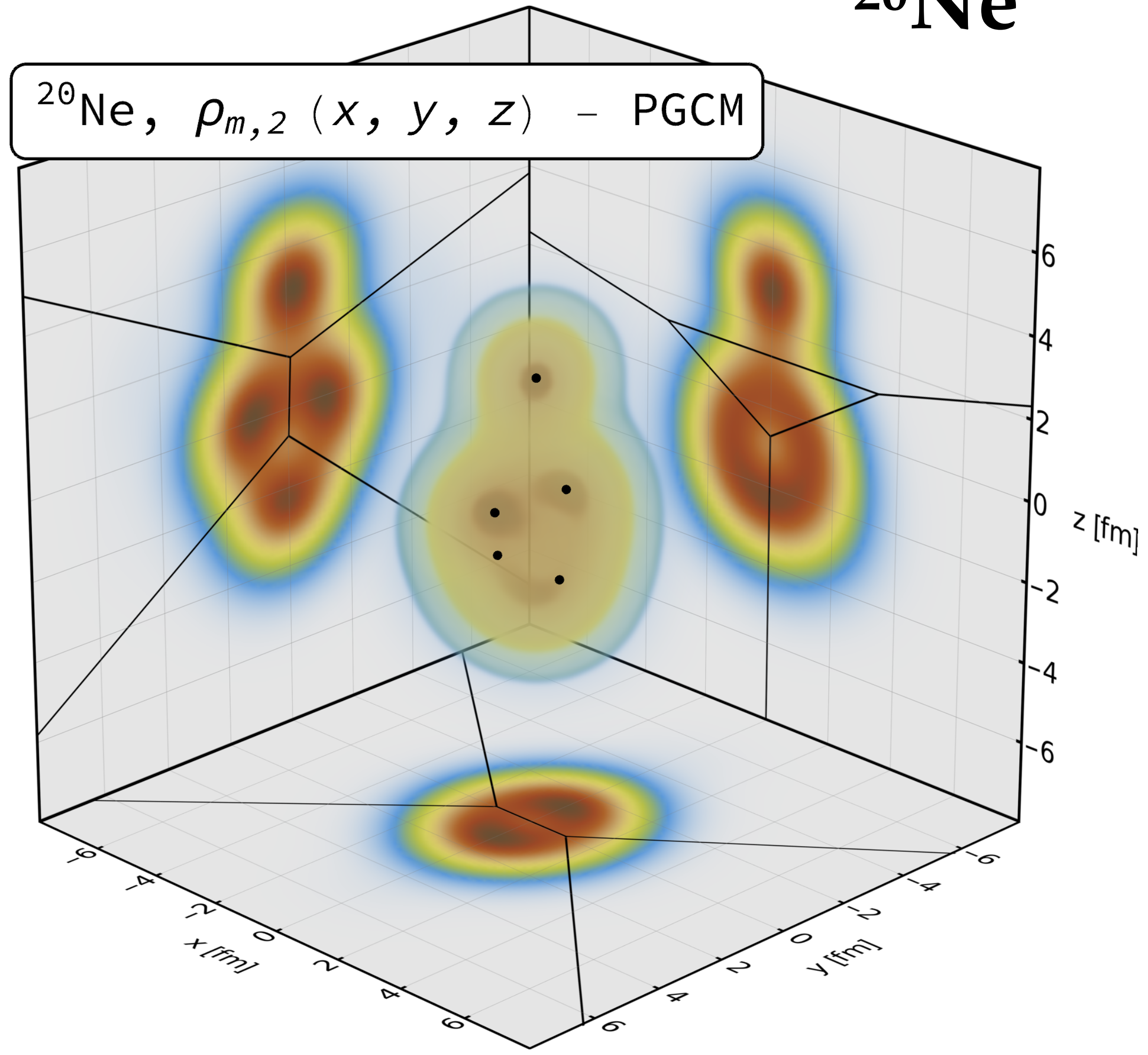
→ Test of the hydrodynamic QGP paradigm for small systems

→ New observables to test nuclear structure models

^{16}O



^{20}Ne



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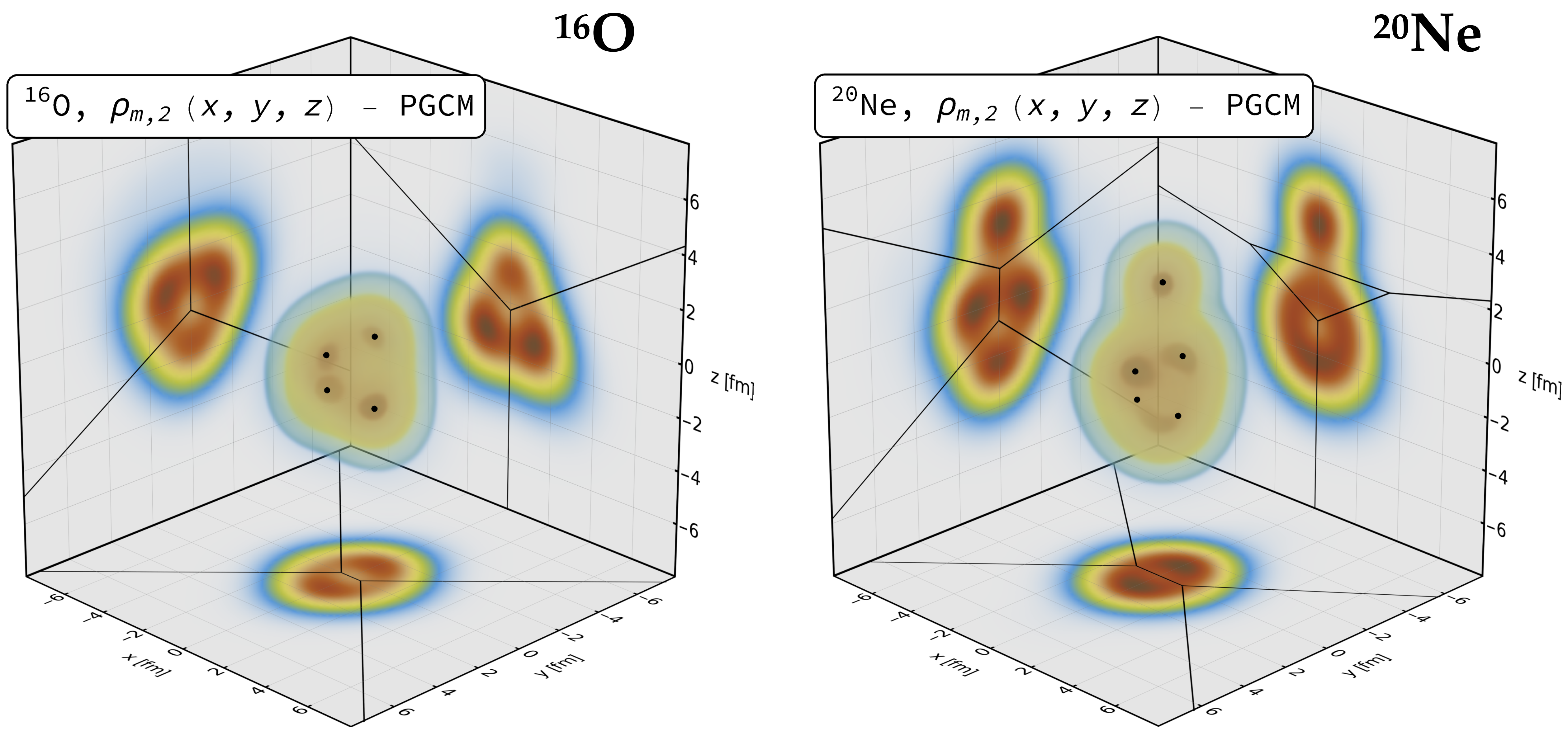

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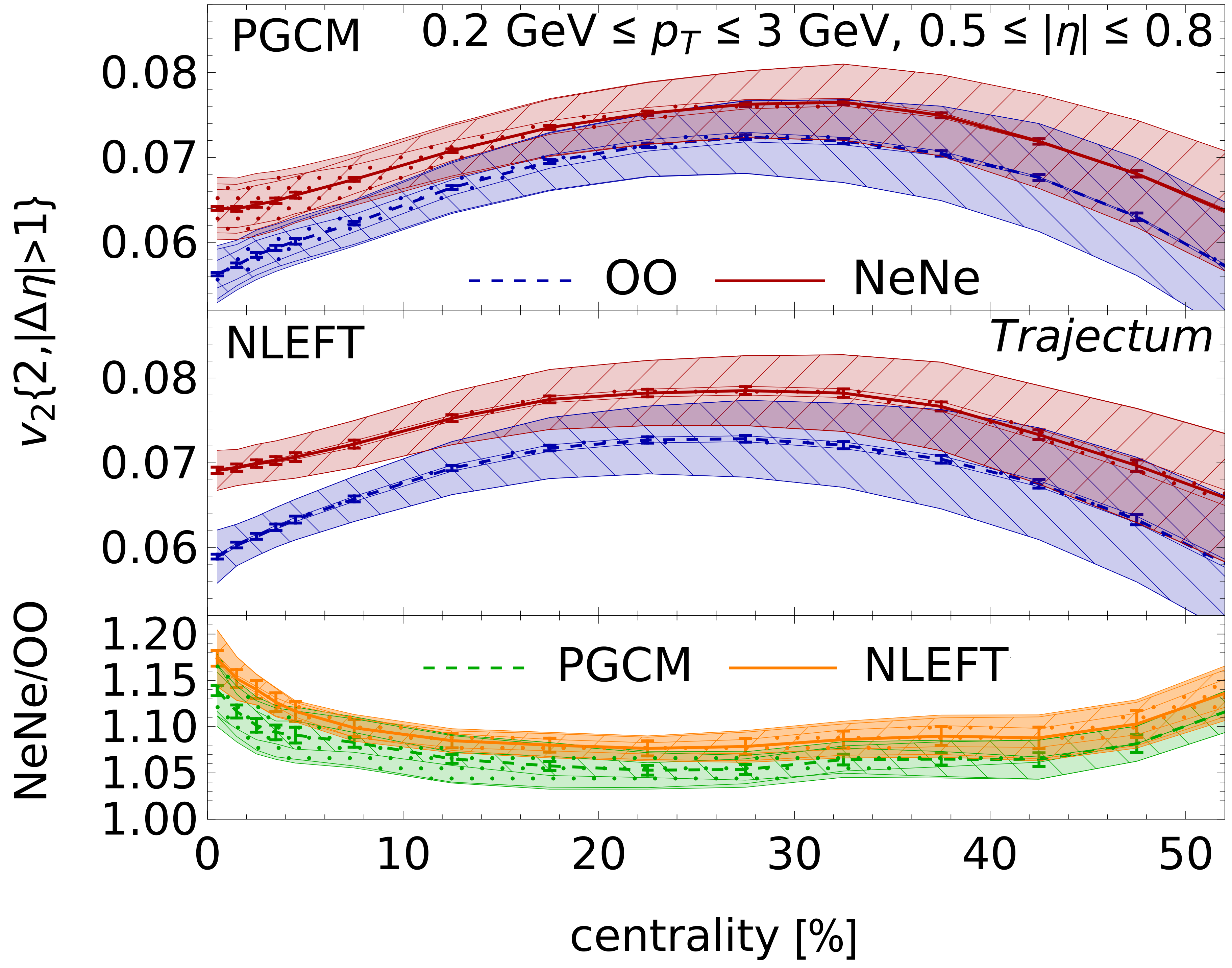
Elliptic flow



[Giacalone *et al.*, PRL 2025]

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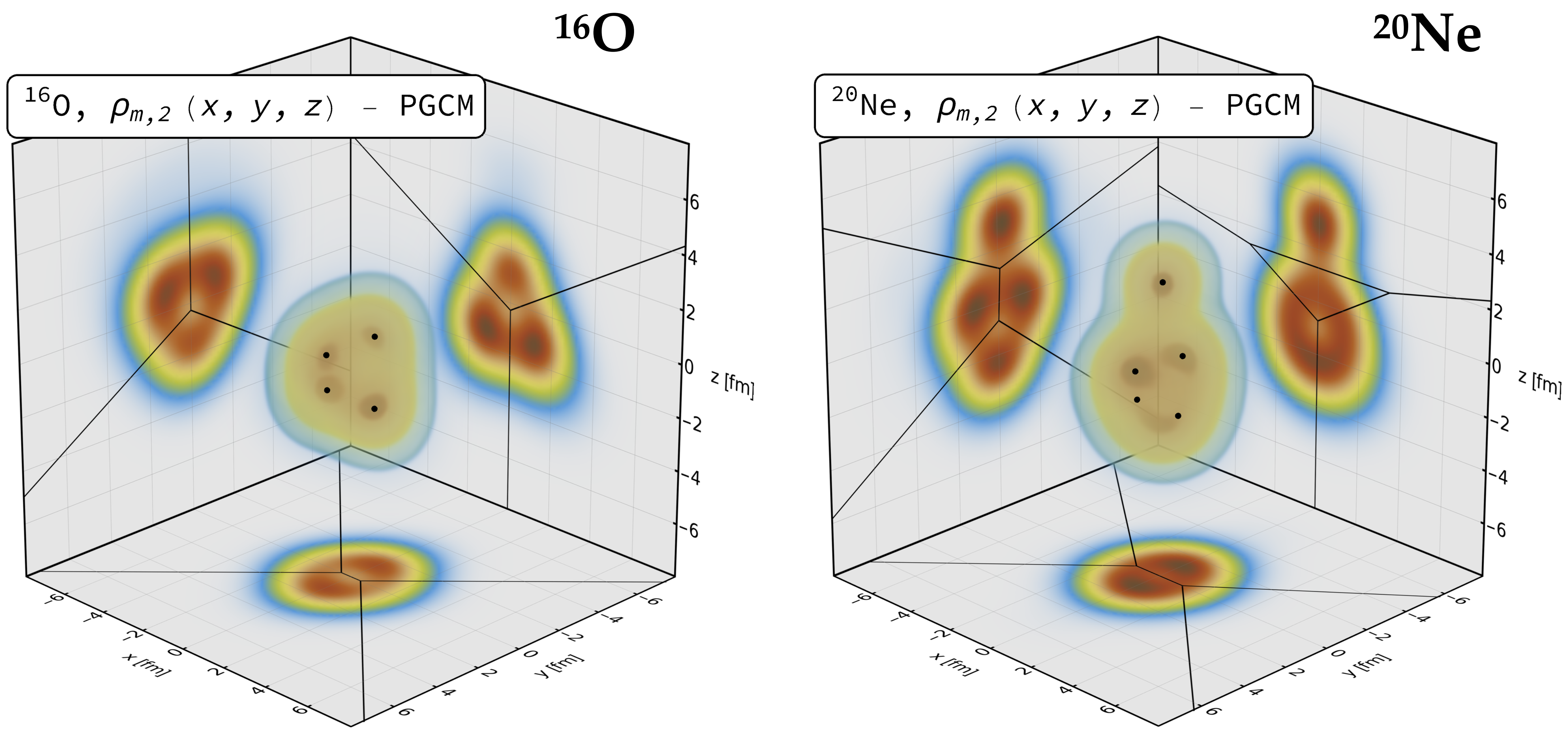

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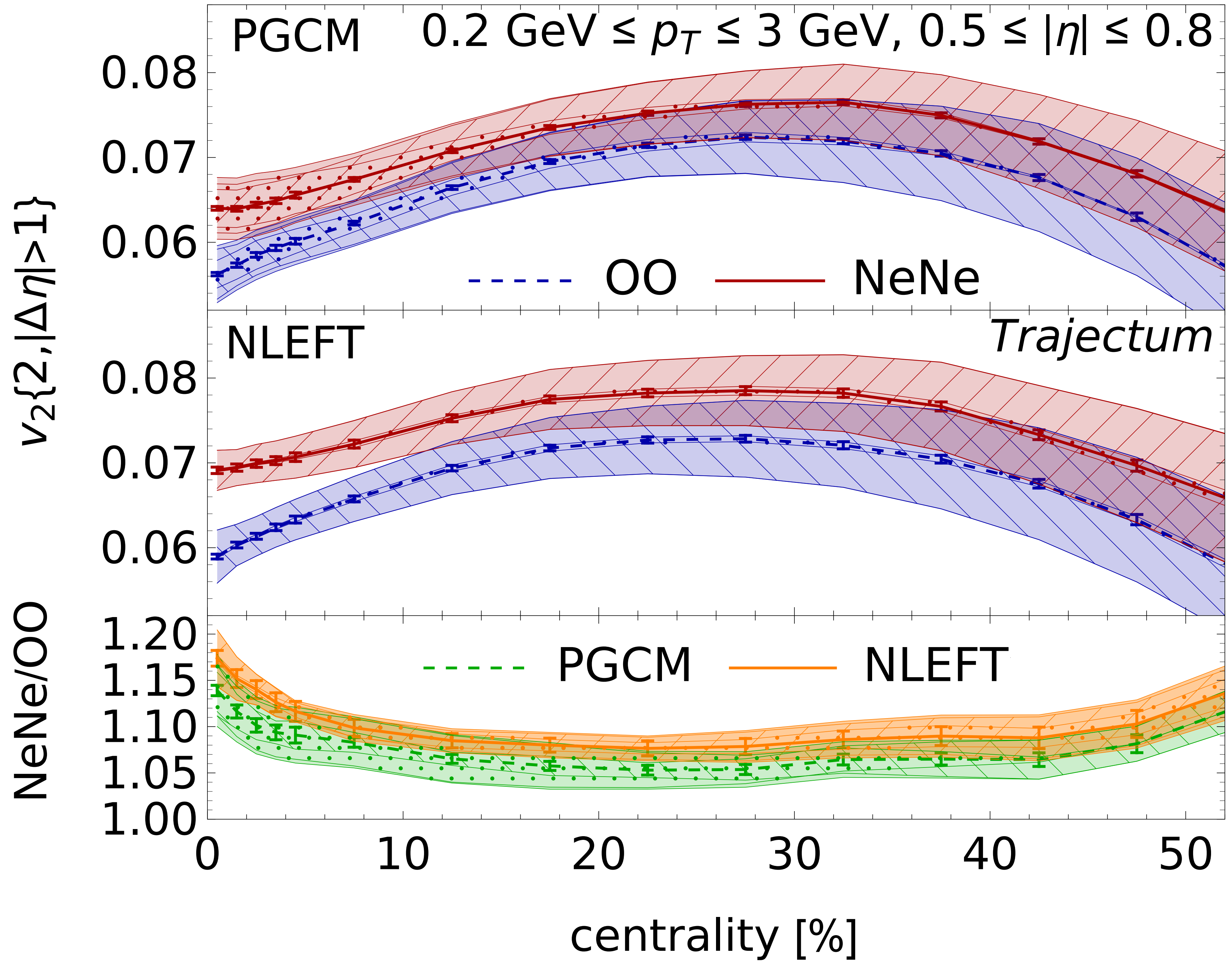

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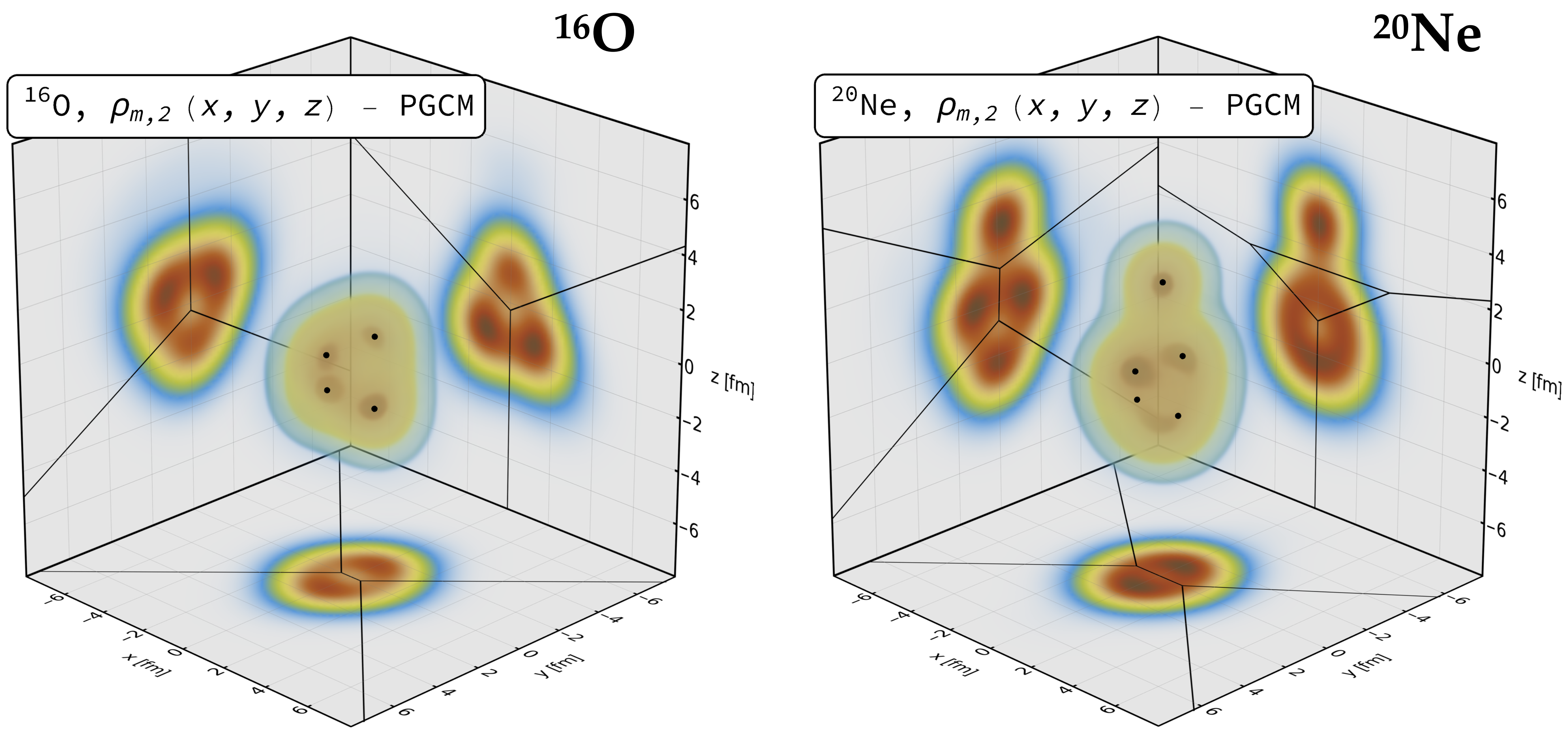

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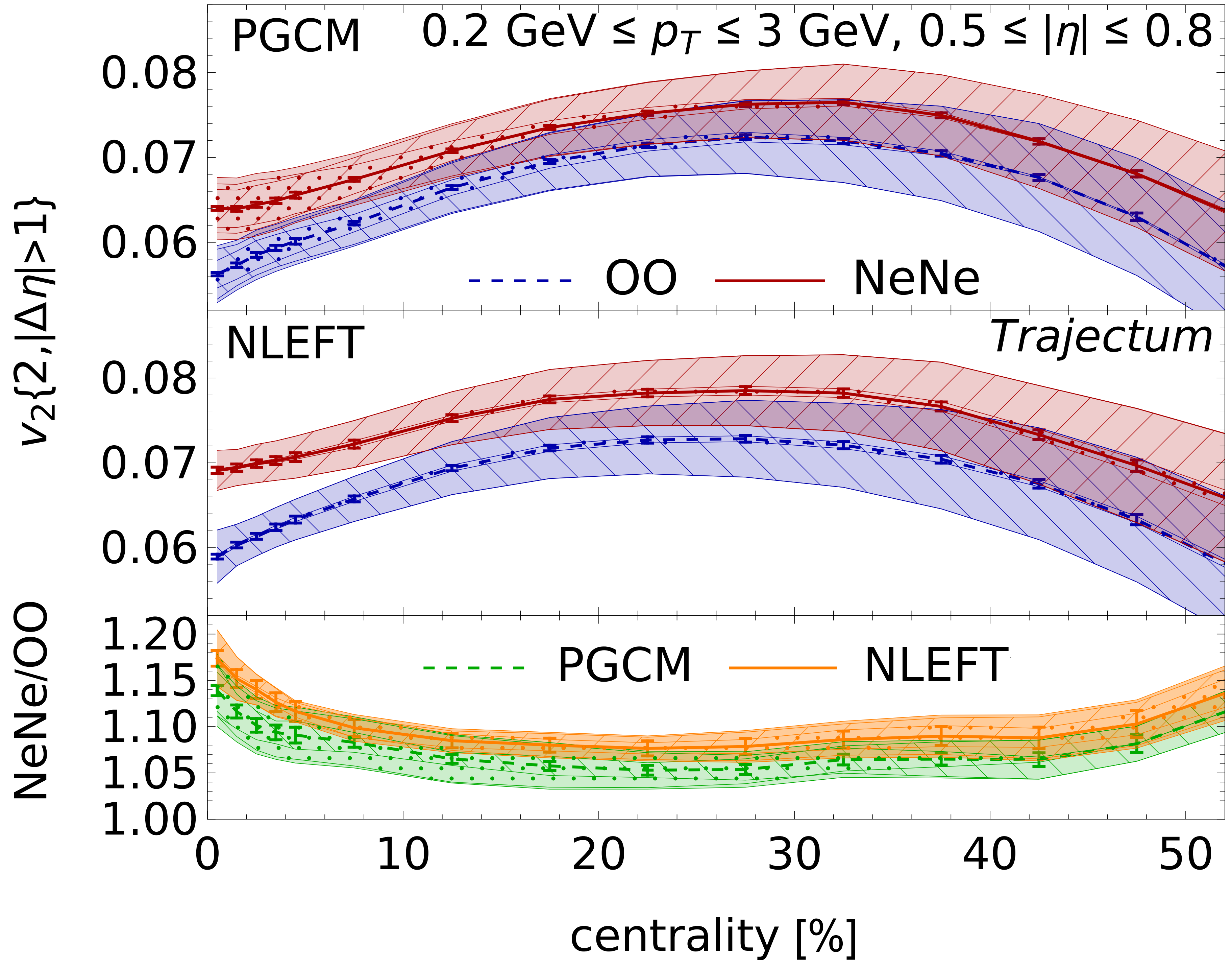

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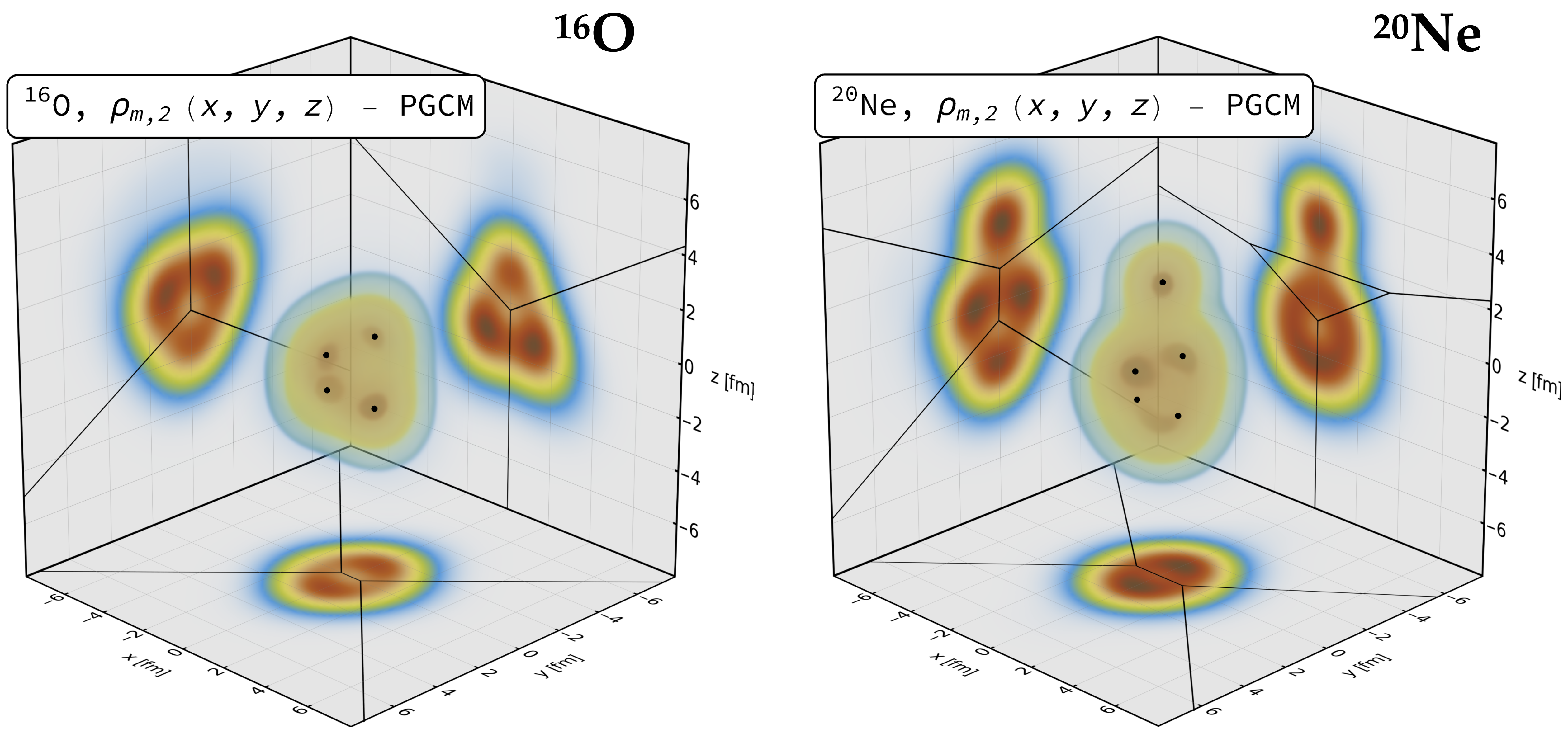

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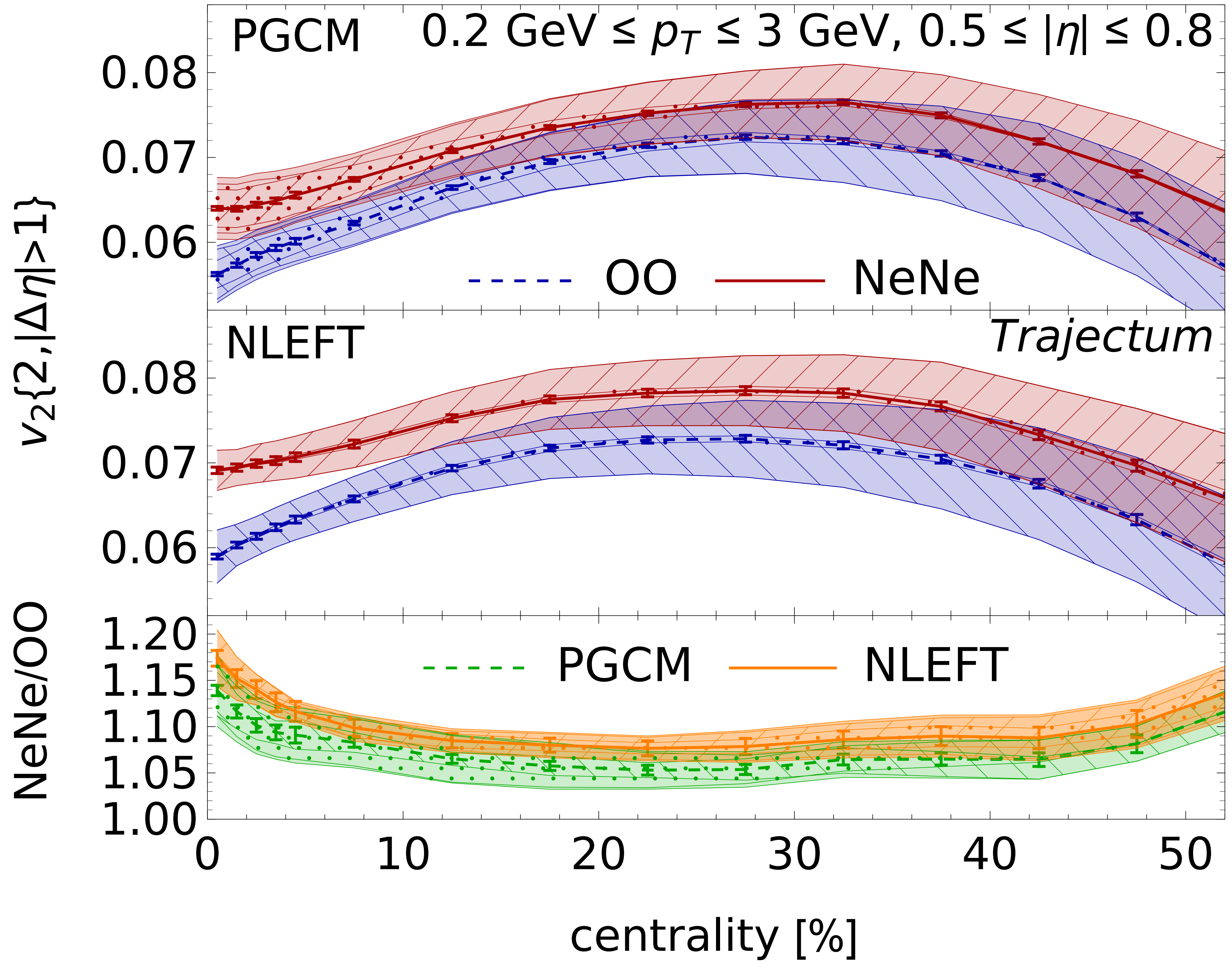

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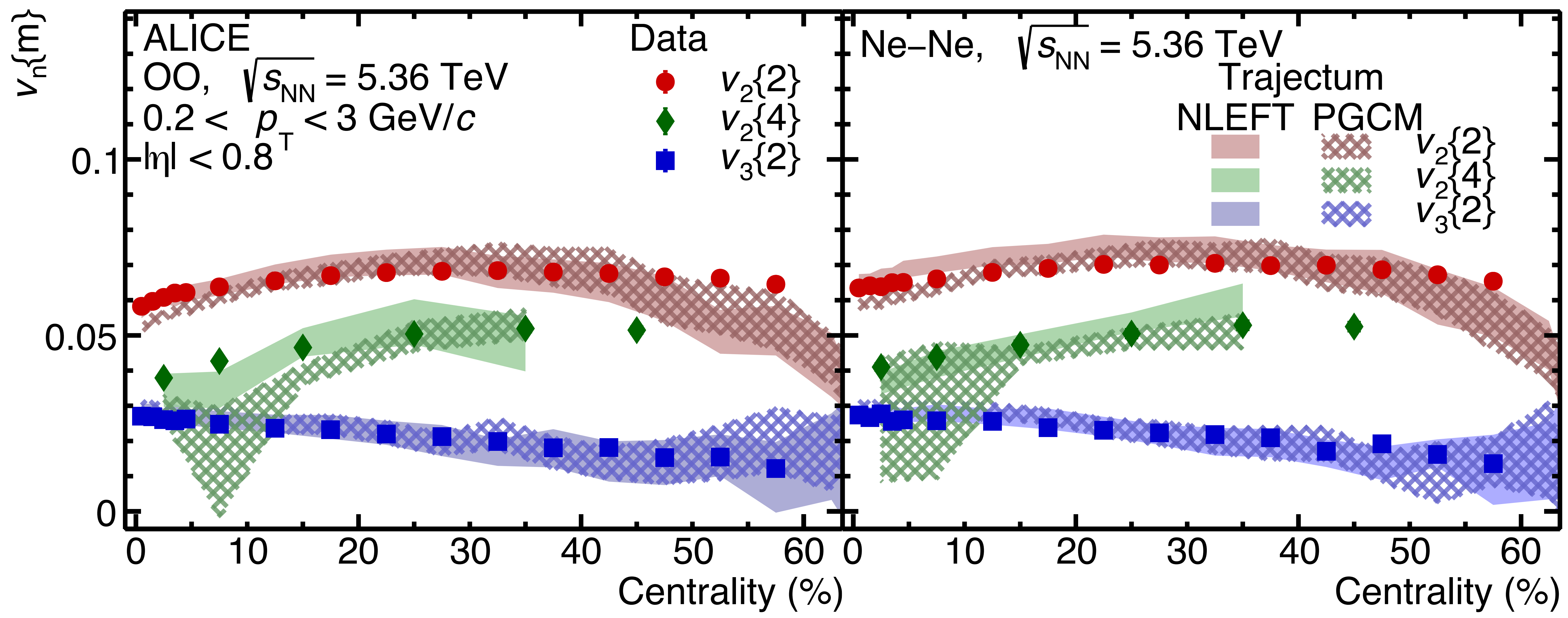
○ **Enhanced elliptic flow** in Ne collisions vs. O baseline

○ Triggered change in LHC schedule → **^{20}Ne-^{20}Ne run in July 2025!**

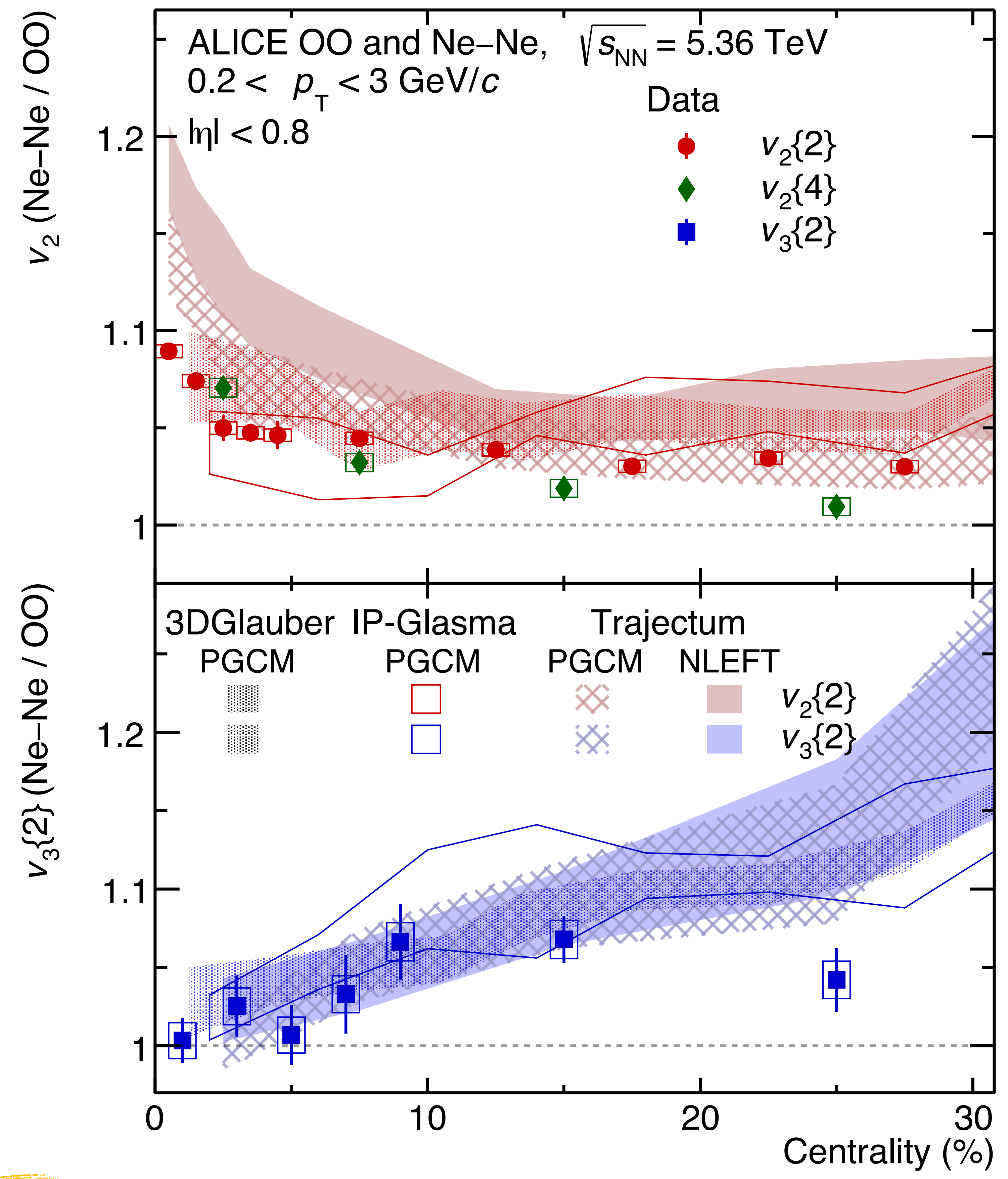
Nuclear structure & relativistic ion collisions

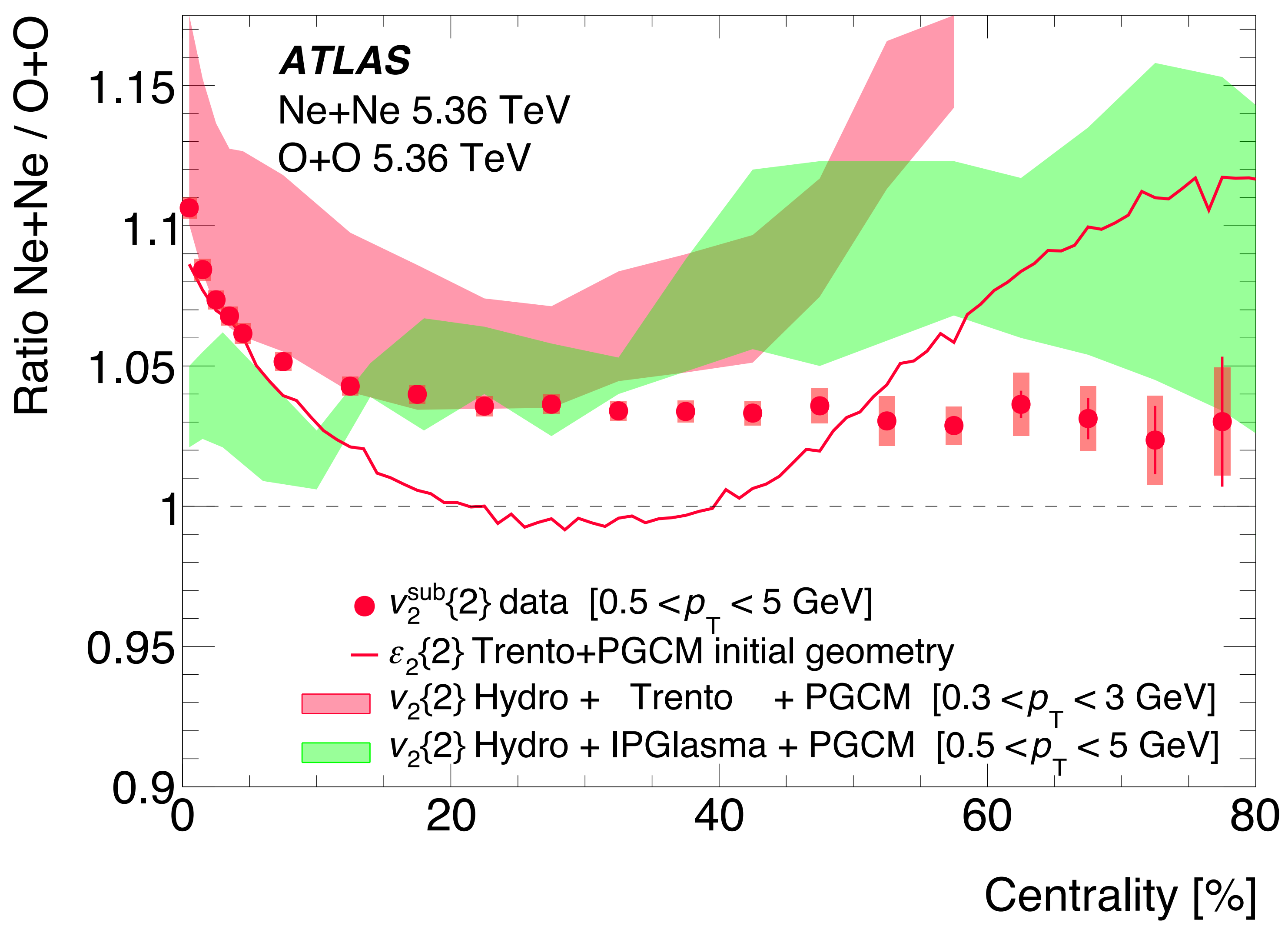
○ **First analyses of experimental measurements confirm PGCM predictions!**

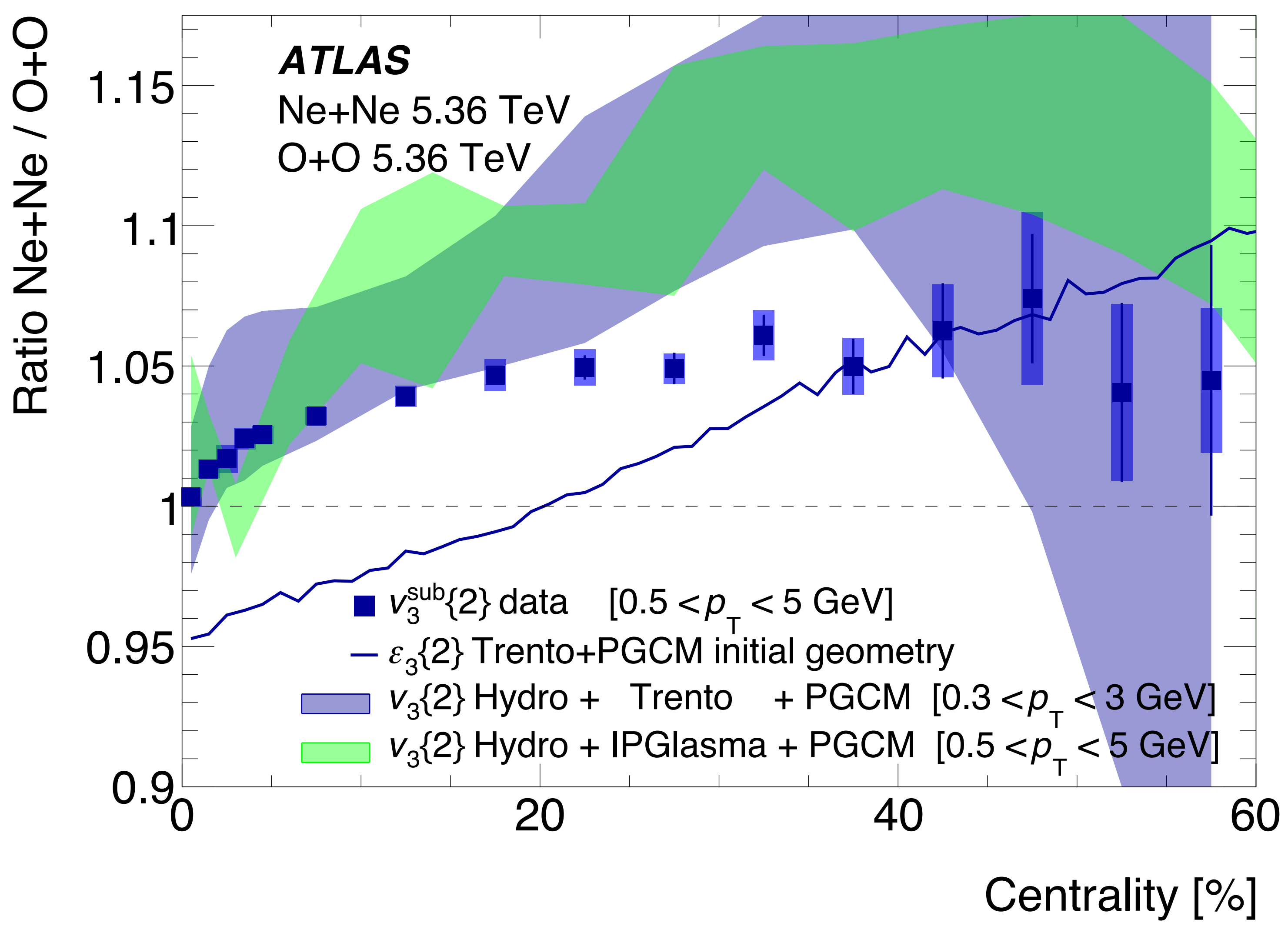
[ALICE collaboration, 2509.06428]



ALICE







ATLAS

[ATLAS collaboration, 2509.05171]

Perspectives

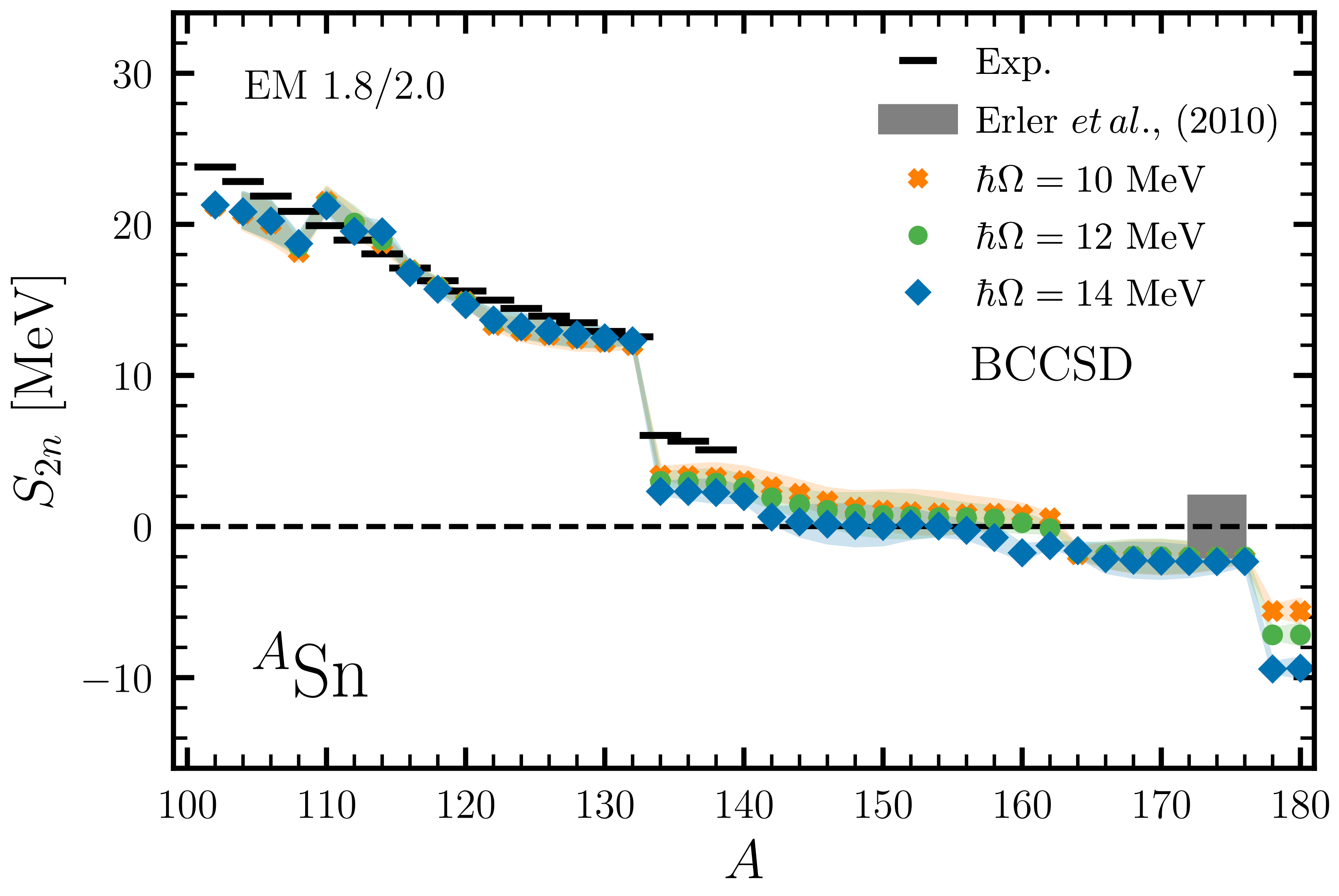
○ **How to extend such calculations to heavy systems?**

Computational obstacles

○ **Current bottleneck**: treatment of **three-nucleon forces**

→ Incorporated via rank-reduction techniques $W^{3N} \rightarrow W^{2N} = \int W^{3N} \rho$

→ Use of spherical density inadequate for large deformation



[Tichai et al., PLB 2024]

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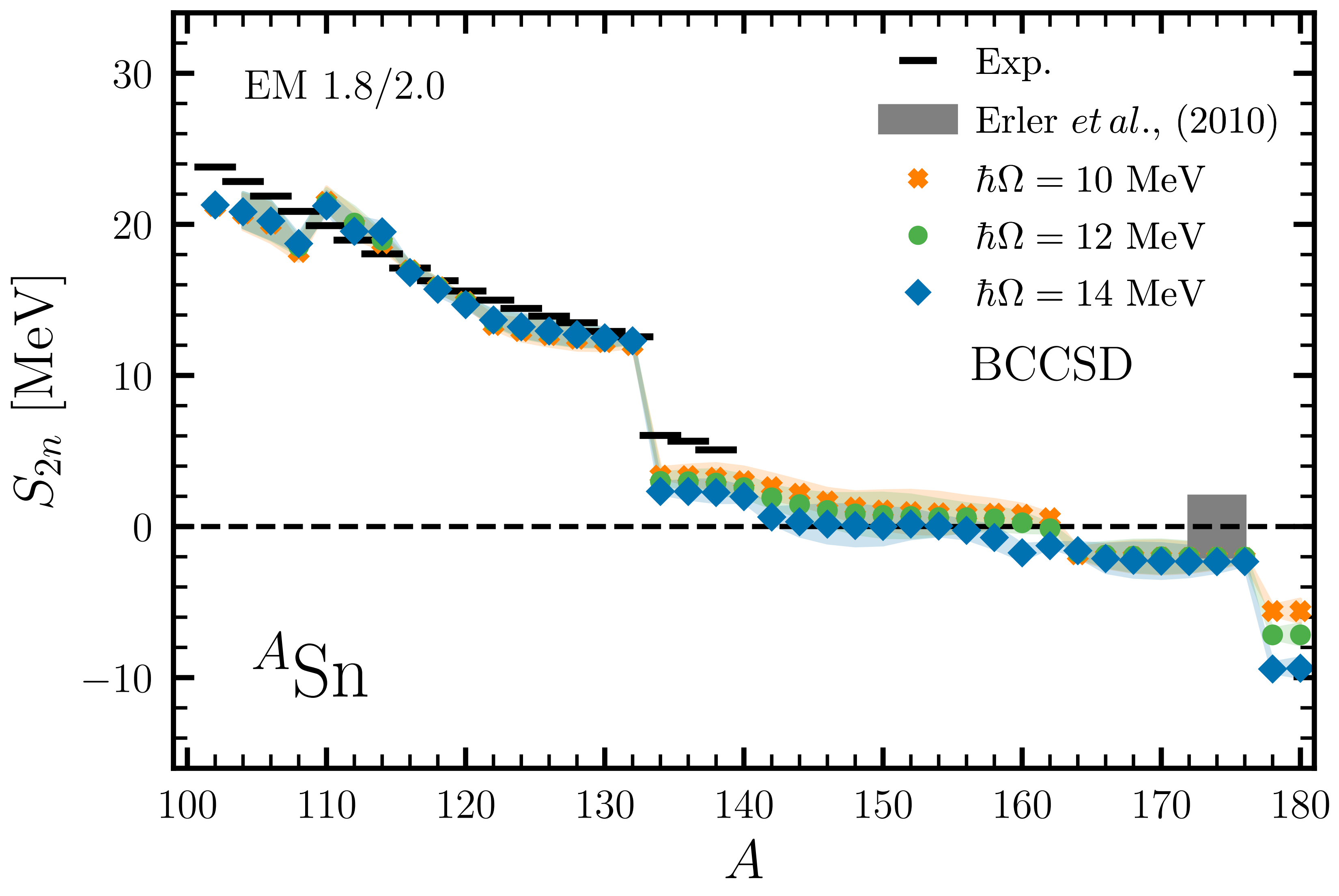
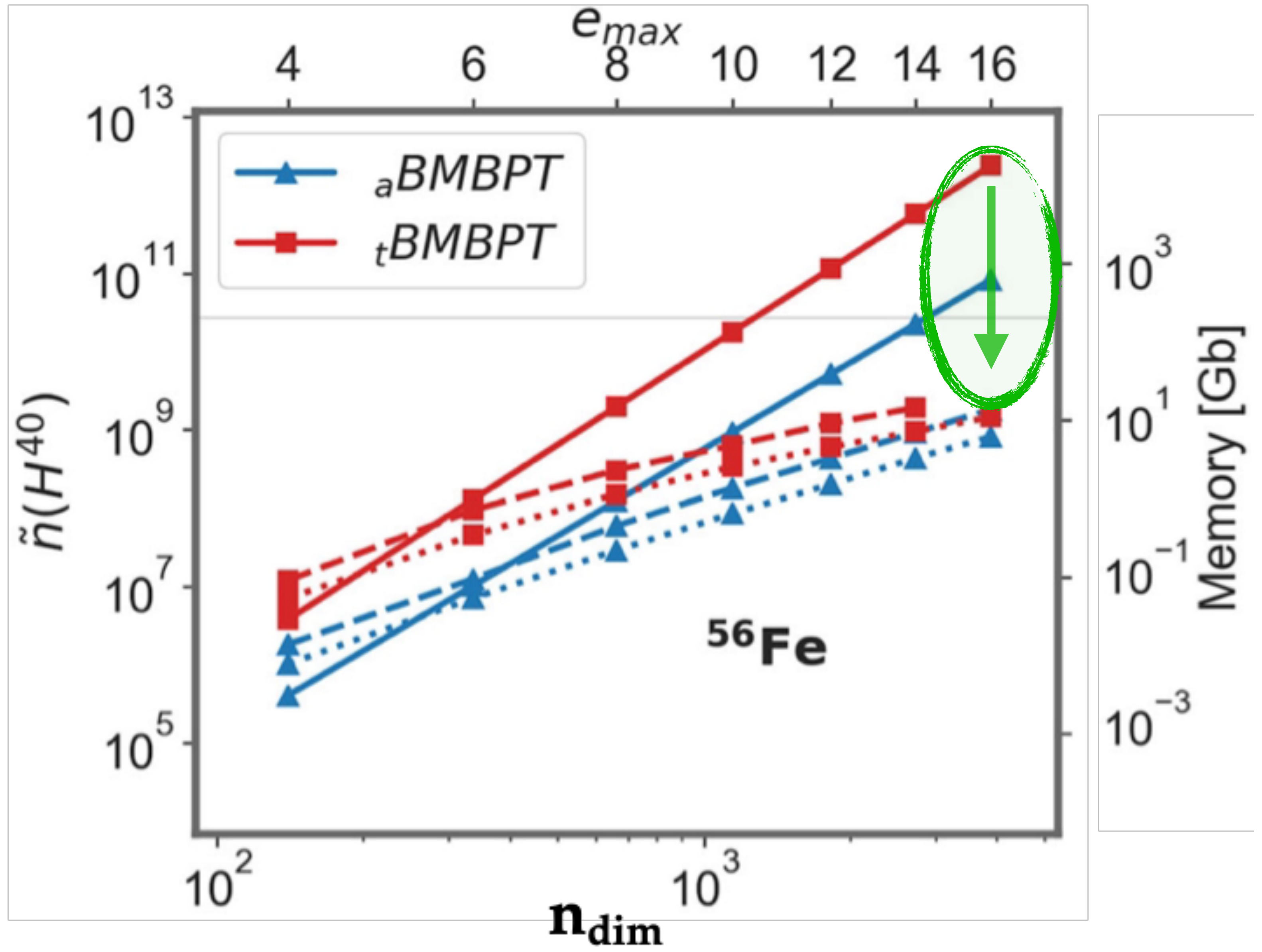
→ Development of dimensionality-reduction techniques

Importance truncation, natural orbitals, tensor factorisation

→ Use of emulators to produce statistically-relevant samples



[Tichai *et al.*, PLB 2024]



[Frosini *et al.*, EPJA 2024]

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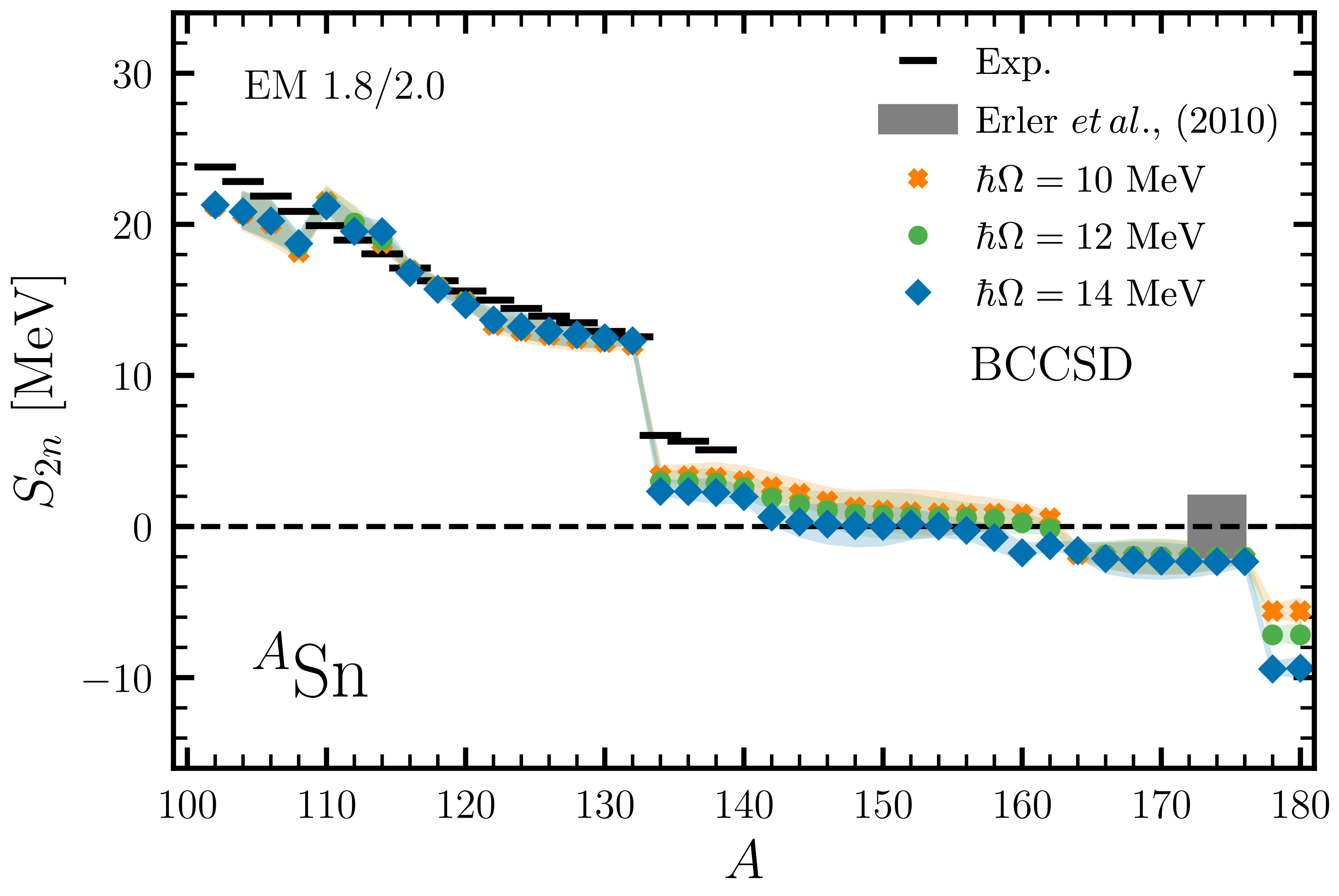
See talk by L. Zurek



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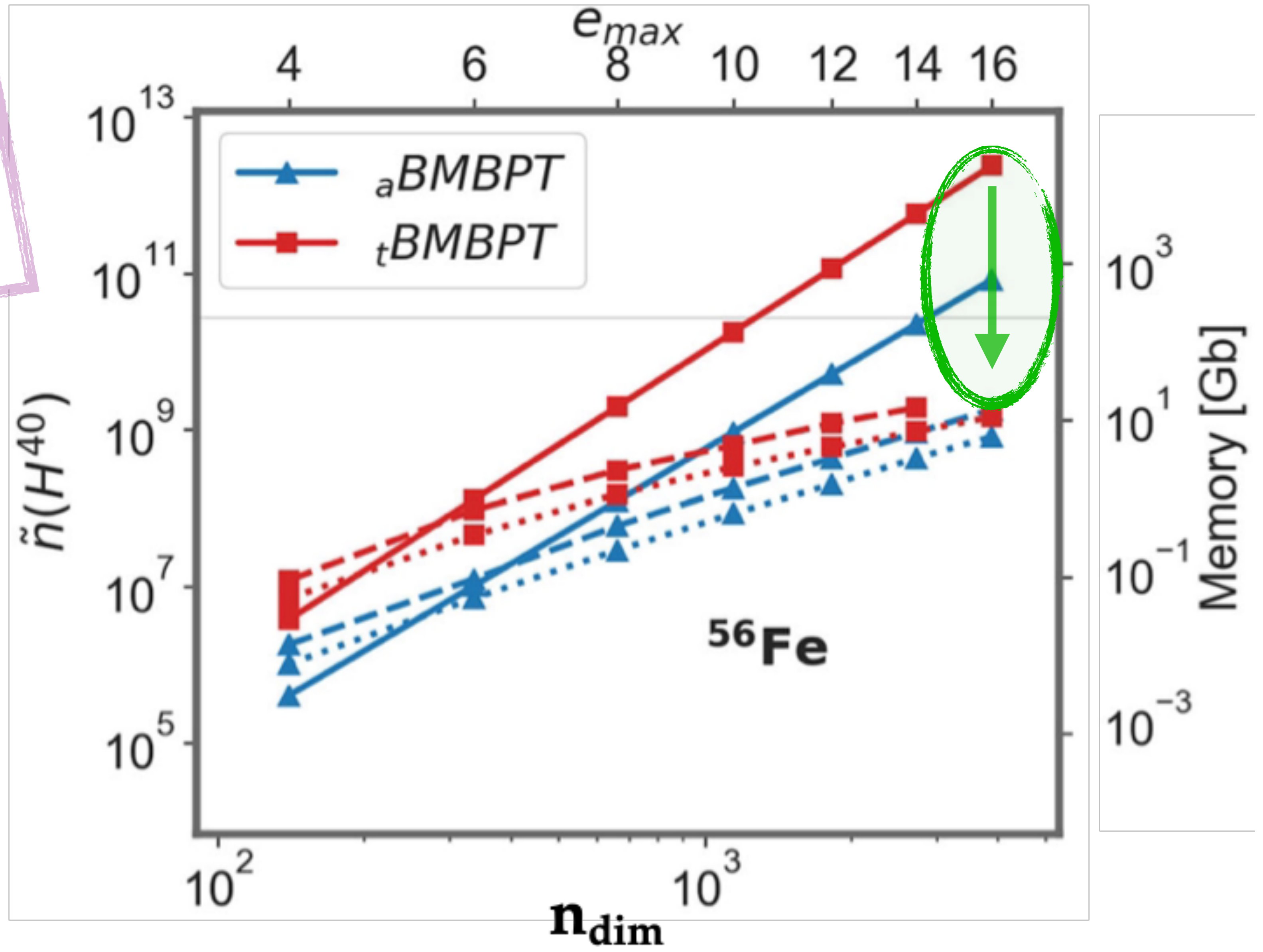

[Frosini *et al.*, EPJA 2024]