Scalable approaches to the ab initio description of nuclei

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The nuclear *ab initio* endeavour

- **A systematic approach to describe nuclei**

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

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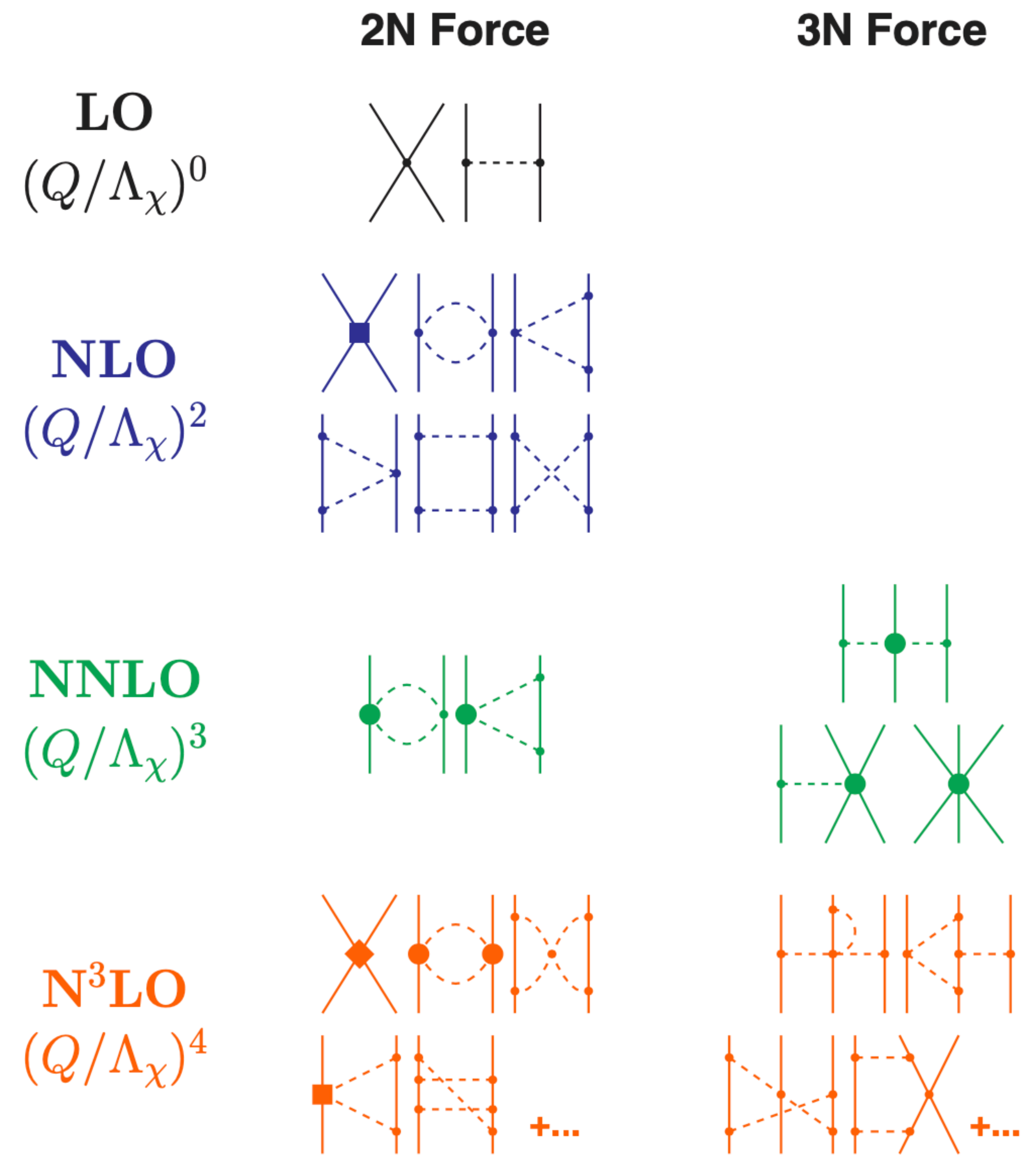
1. Model Hamiltonian

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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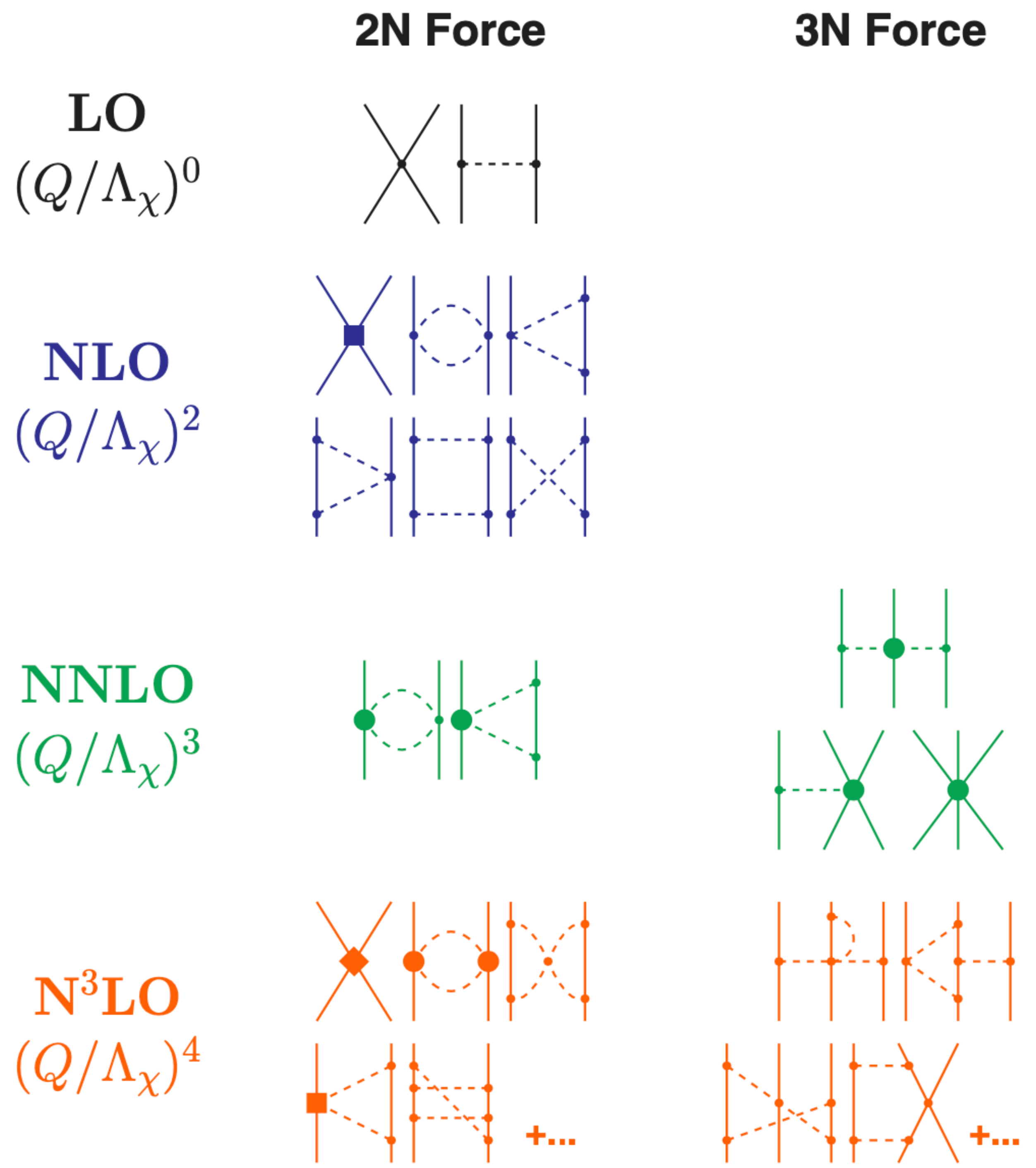

Option 1: Exact solutions have factorial or exponential scaling $\mathbf{e}^n$ → limited to light nuclei

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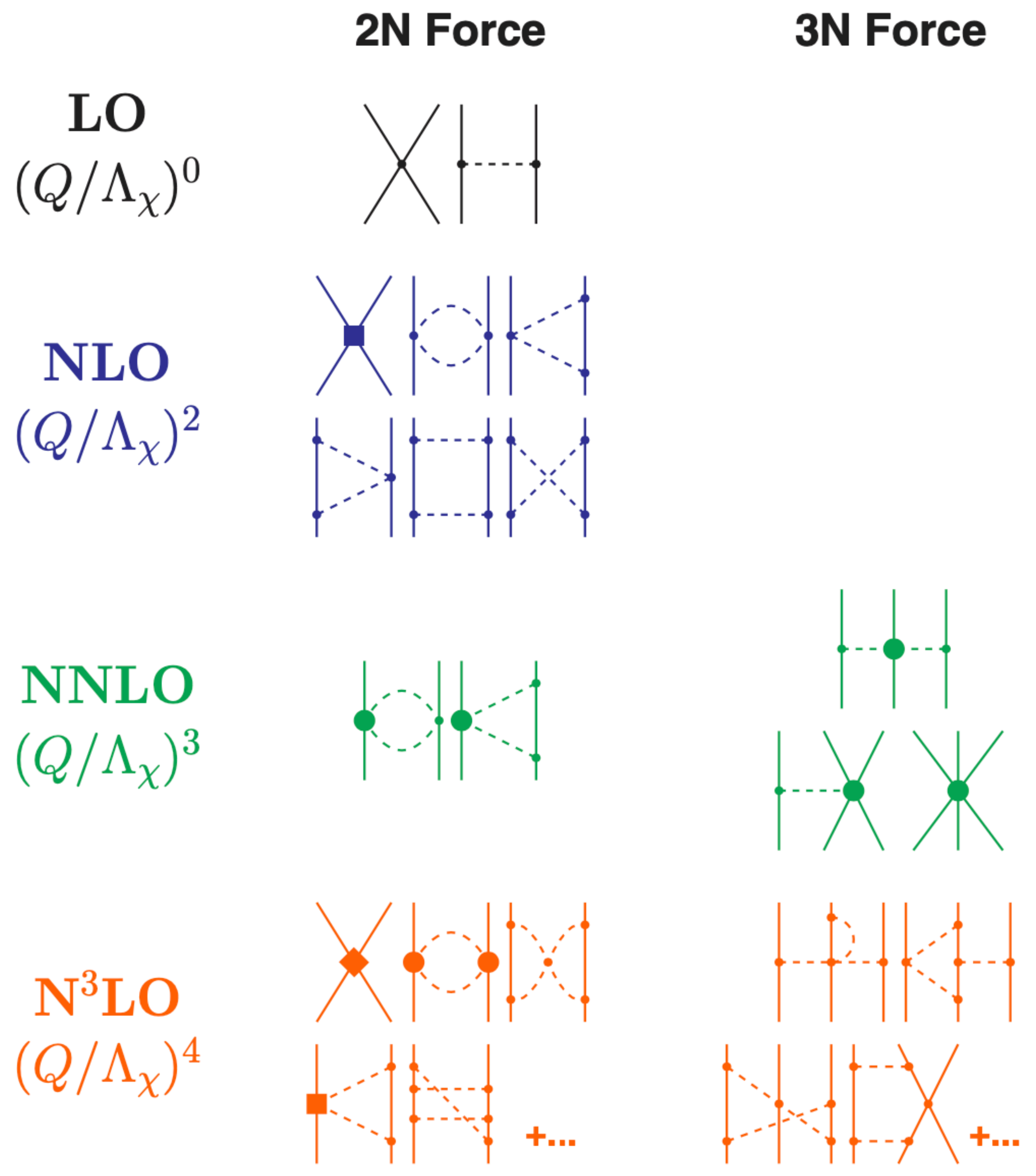

Option 1: Exact solutions have factorial or exponential scaling $\mathbf{e}^n$ → limited to light nuclei

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

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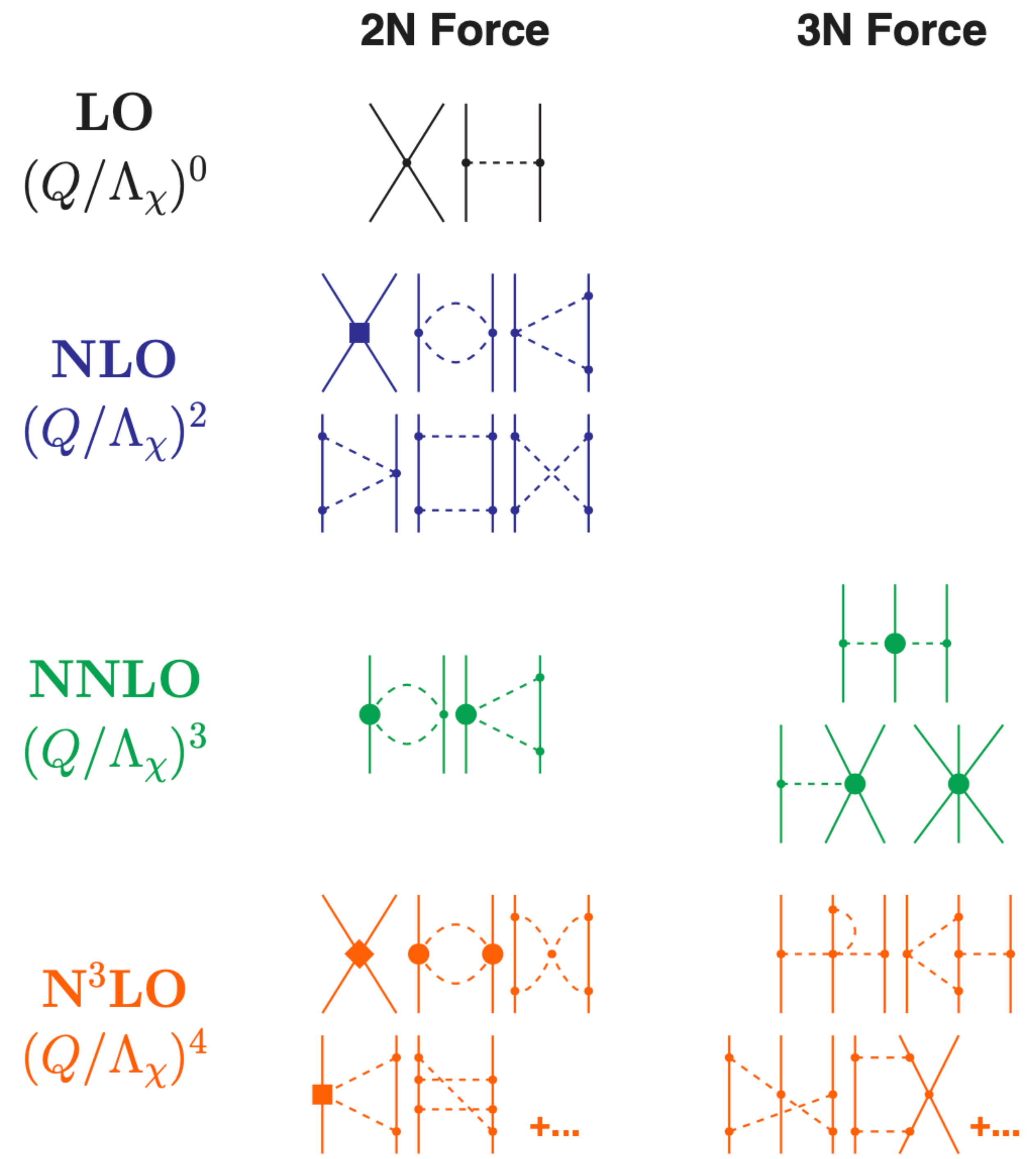

Option 1: Exact solutions have factorial or exponential scaling **e*ⁿ*** → limited to light nuclei

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

CPU-scalable to **heavy masses**?

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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○ 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**

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

→ *cf. energy density functionals*

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Dynamic correlations

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

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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

Self-consistent Green's functions (SCGF)

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

Symmetry restoration missing

Dynamical correlations on top

"Simple" symmetry-breaking reference state

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Projected Generator Coordinate Method (PGCM)

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Dynamical correlations not shown here

Sophisticated reference state (linear combination of projected dHFB states)

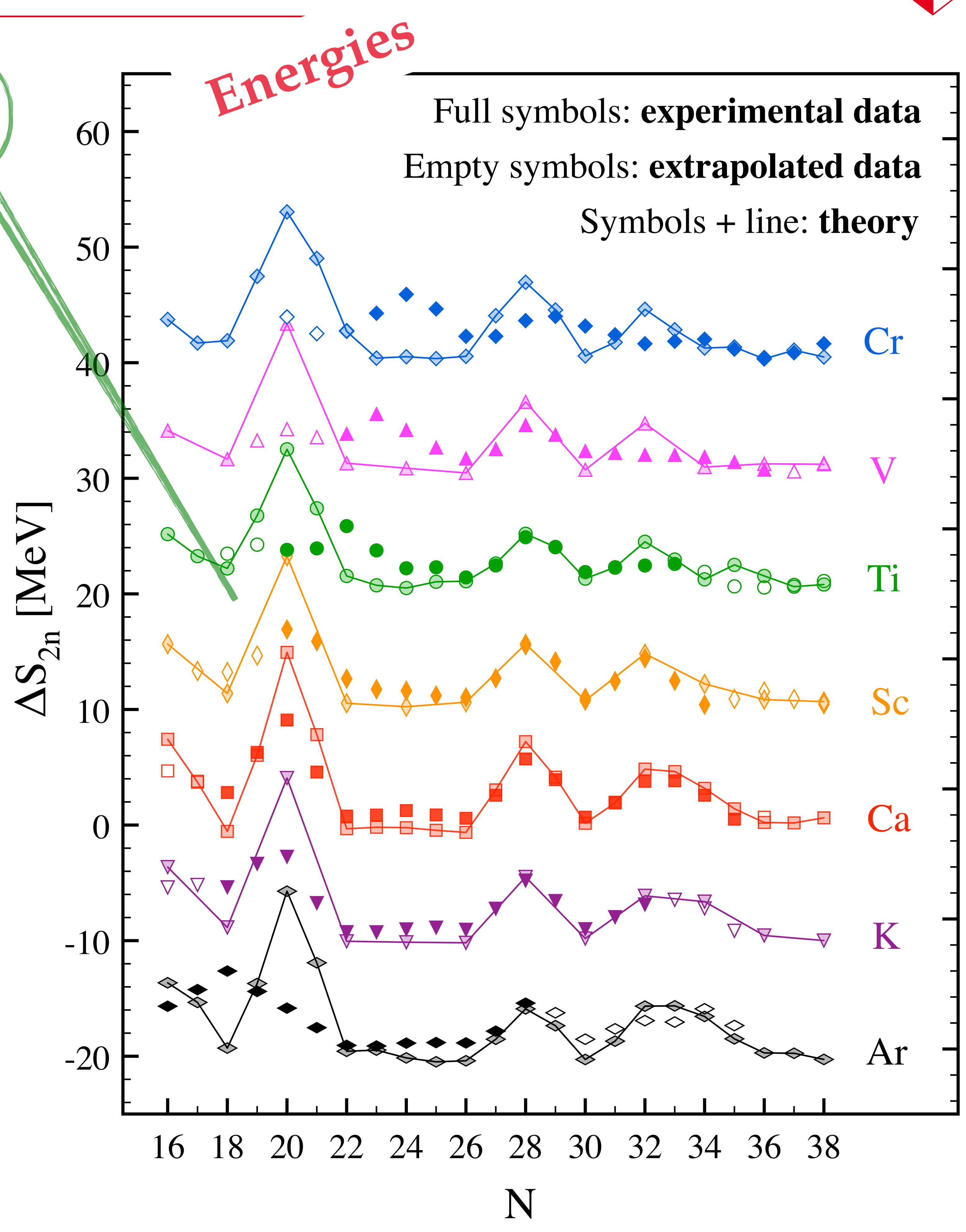
Superfluid self-consistent Green's functions

○ 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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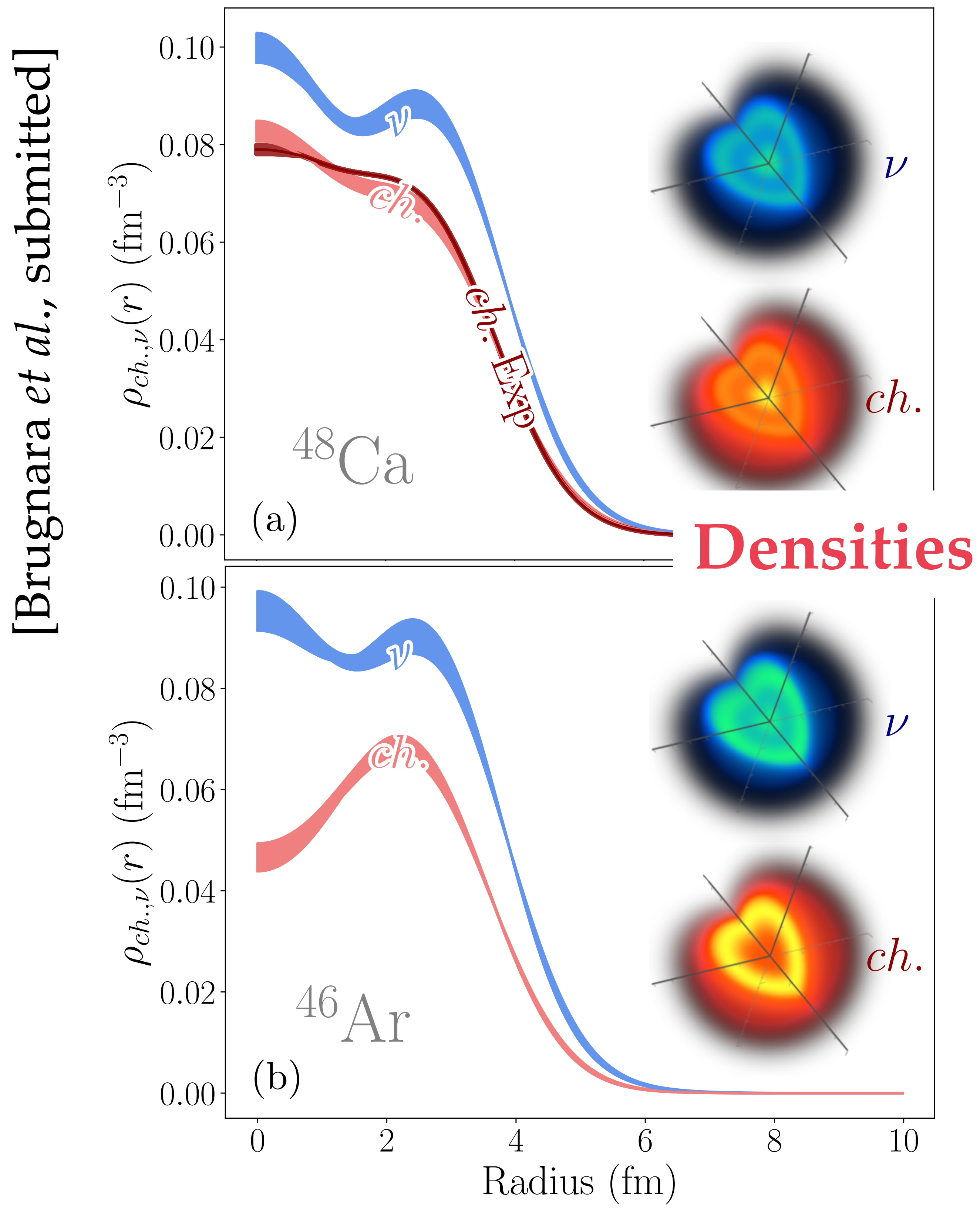

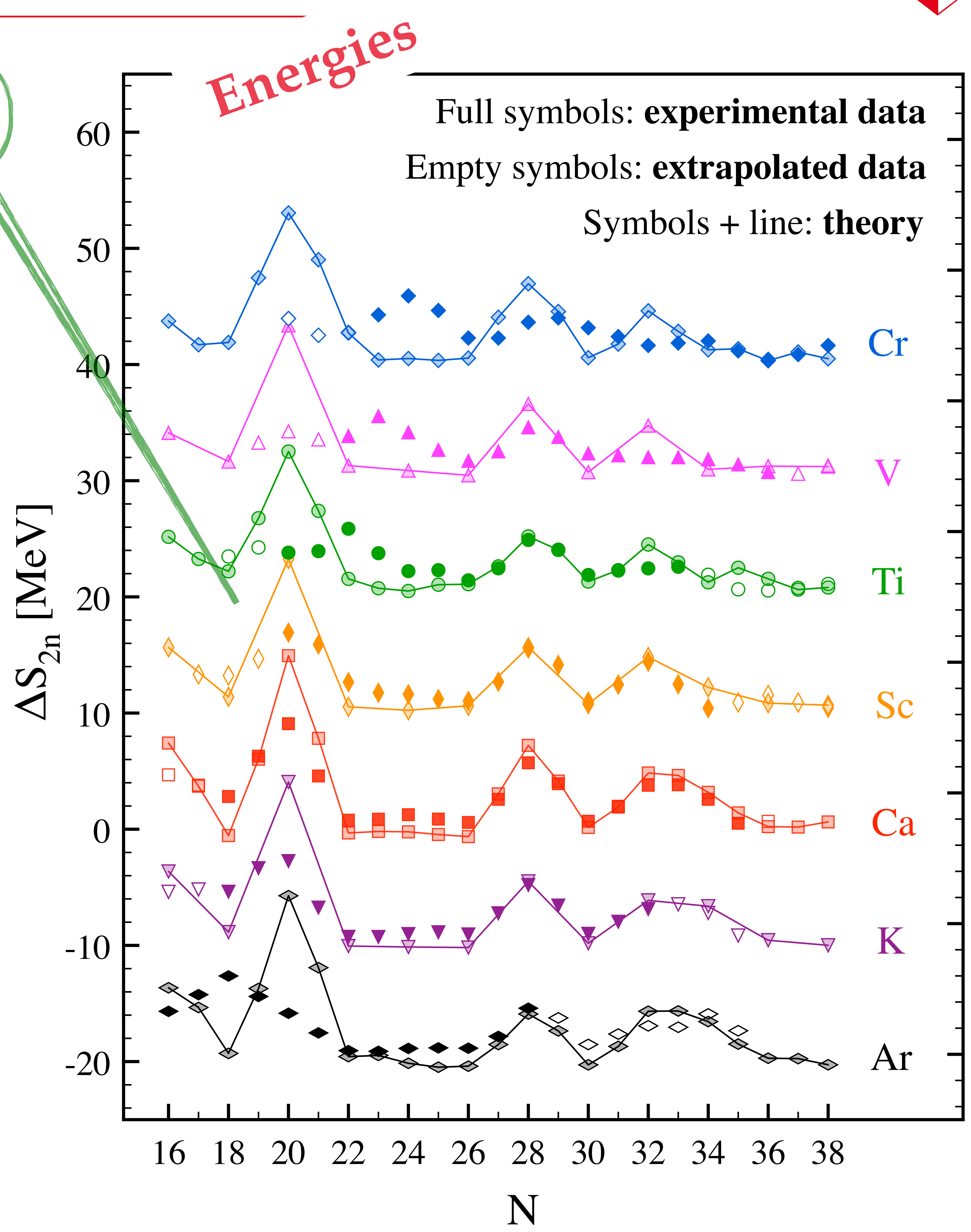

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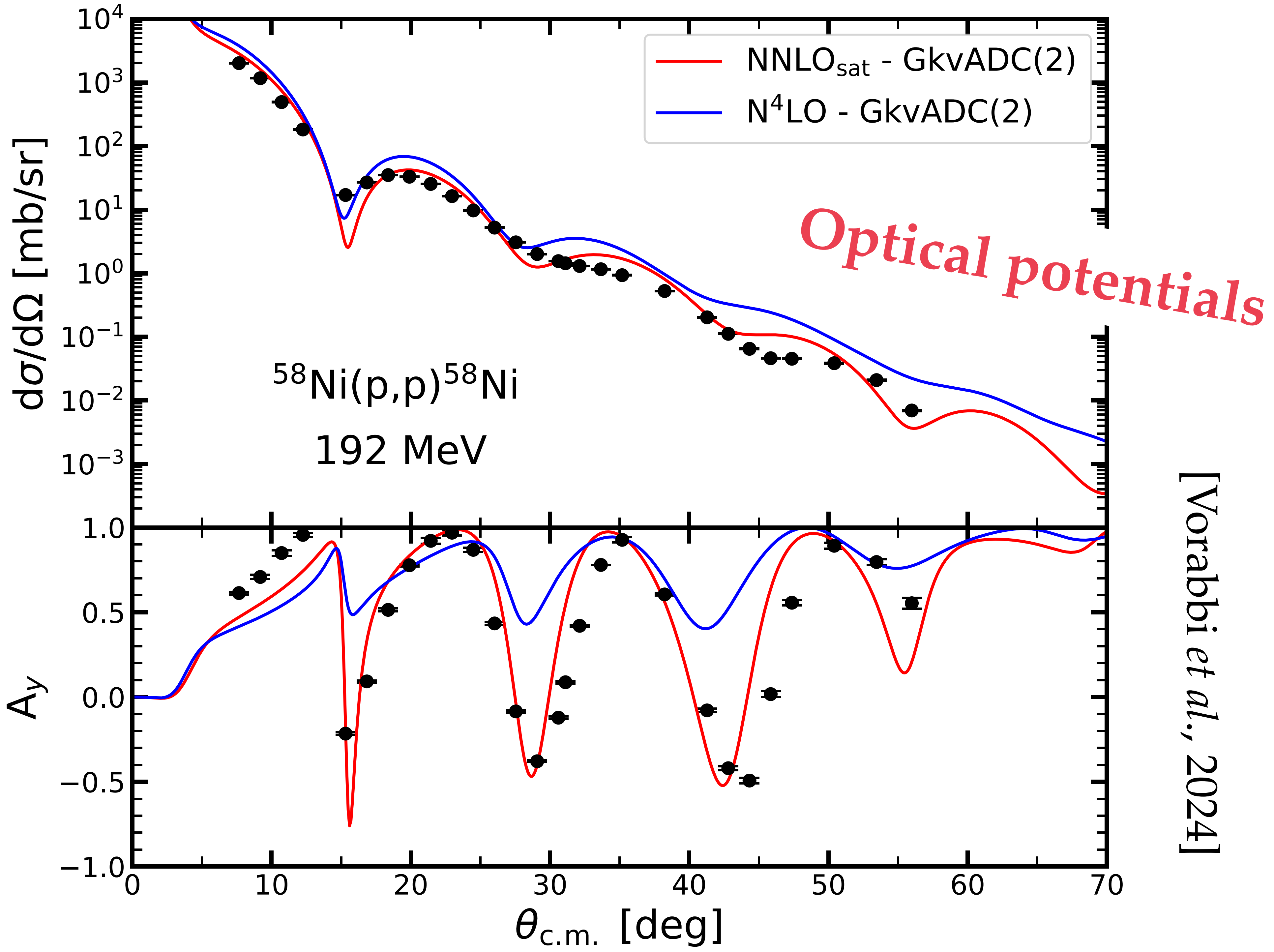

[Vorabbi *et al.*, 2024]

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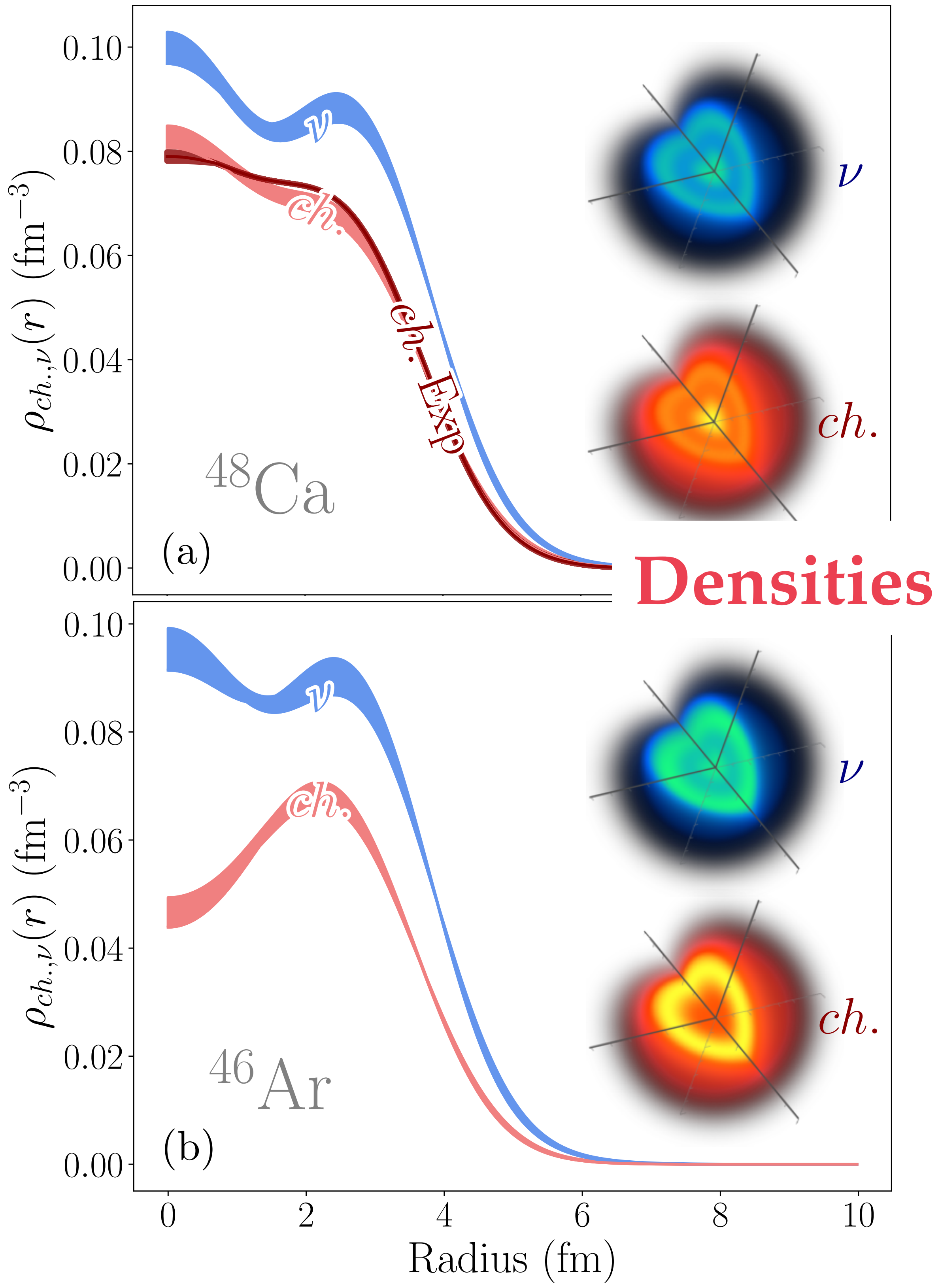
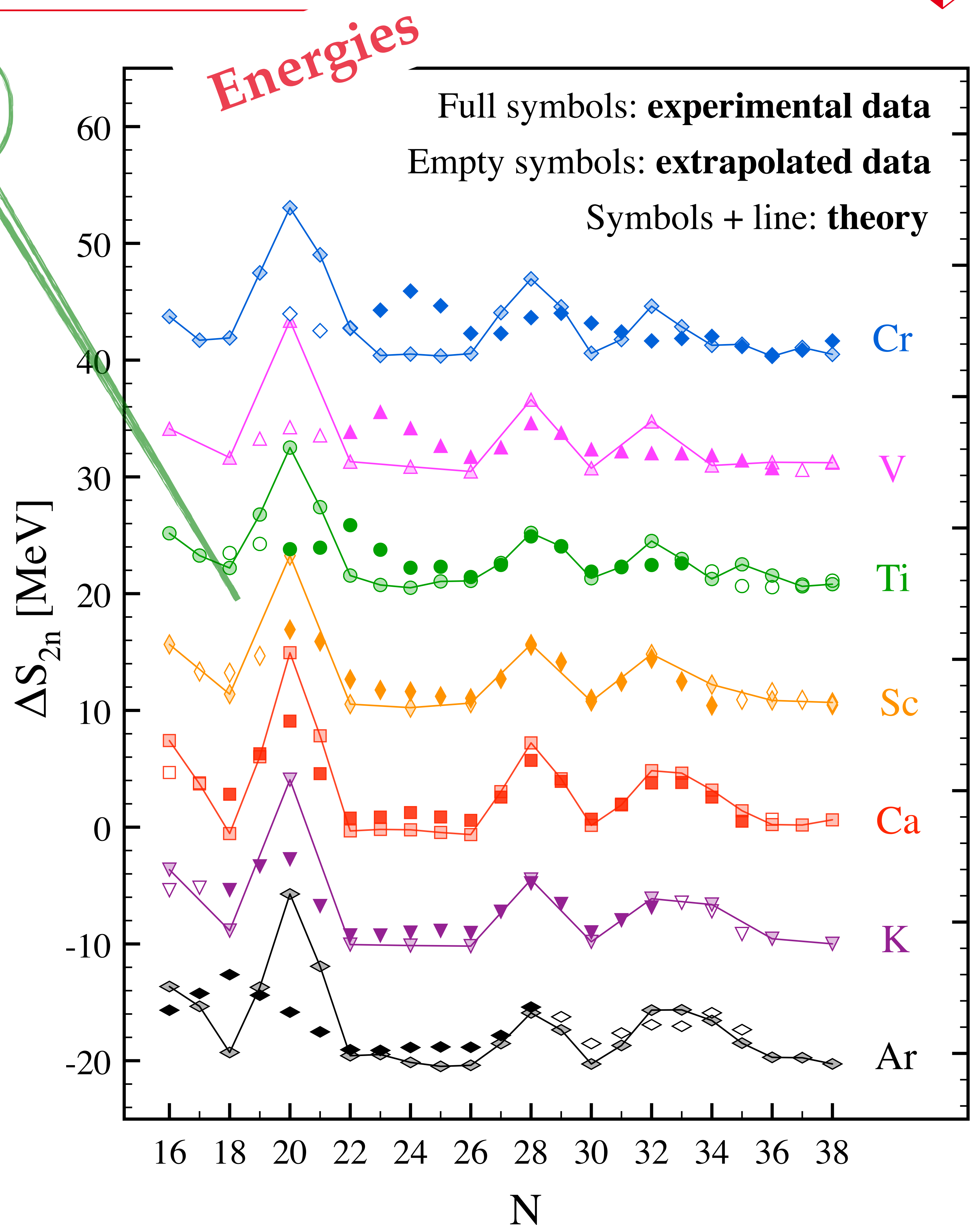
[Brugnara *et al.*, submitted]





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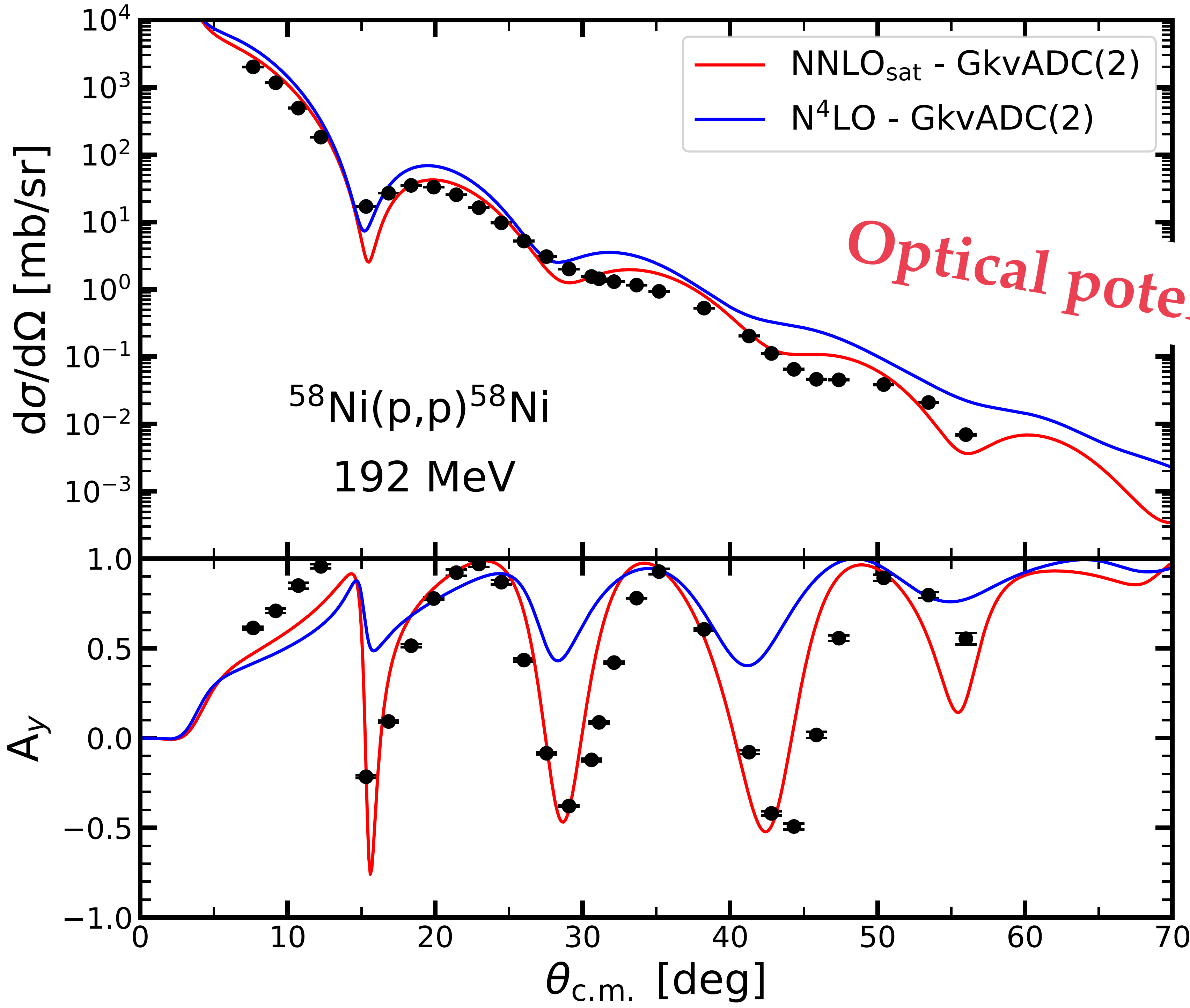
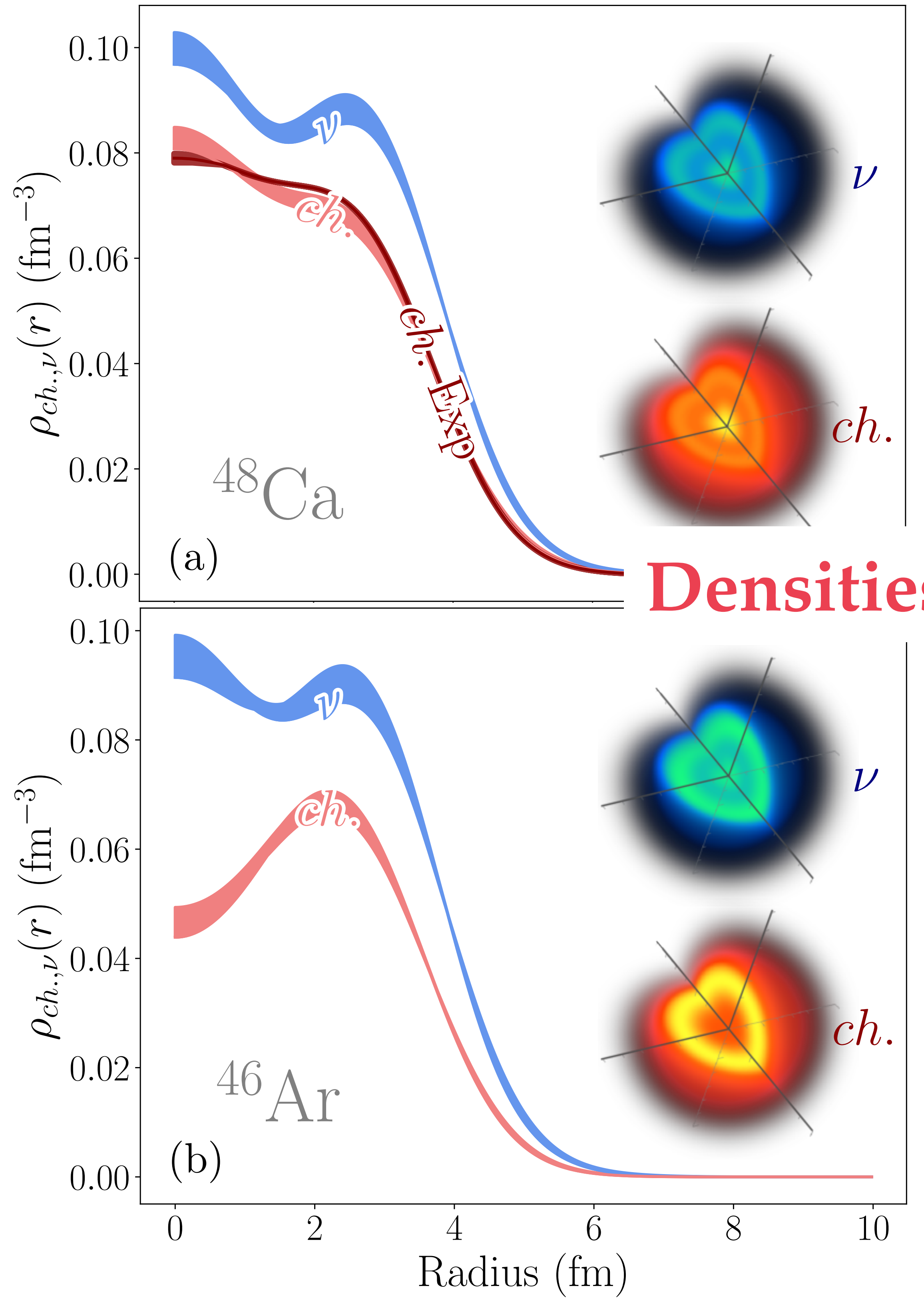


Optical potentials

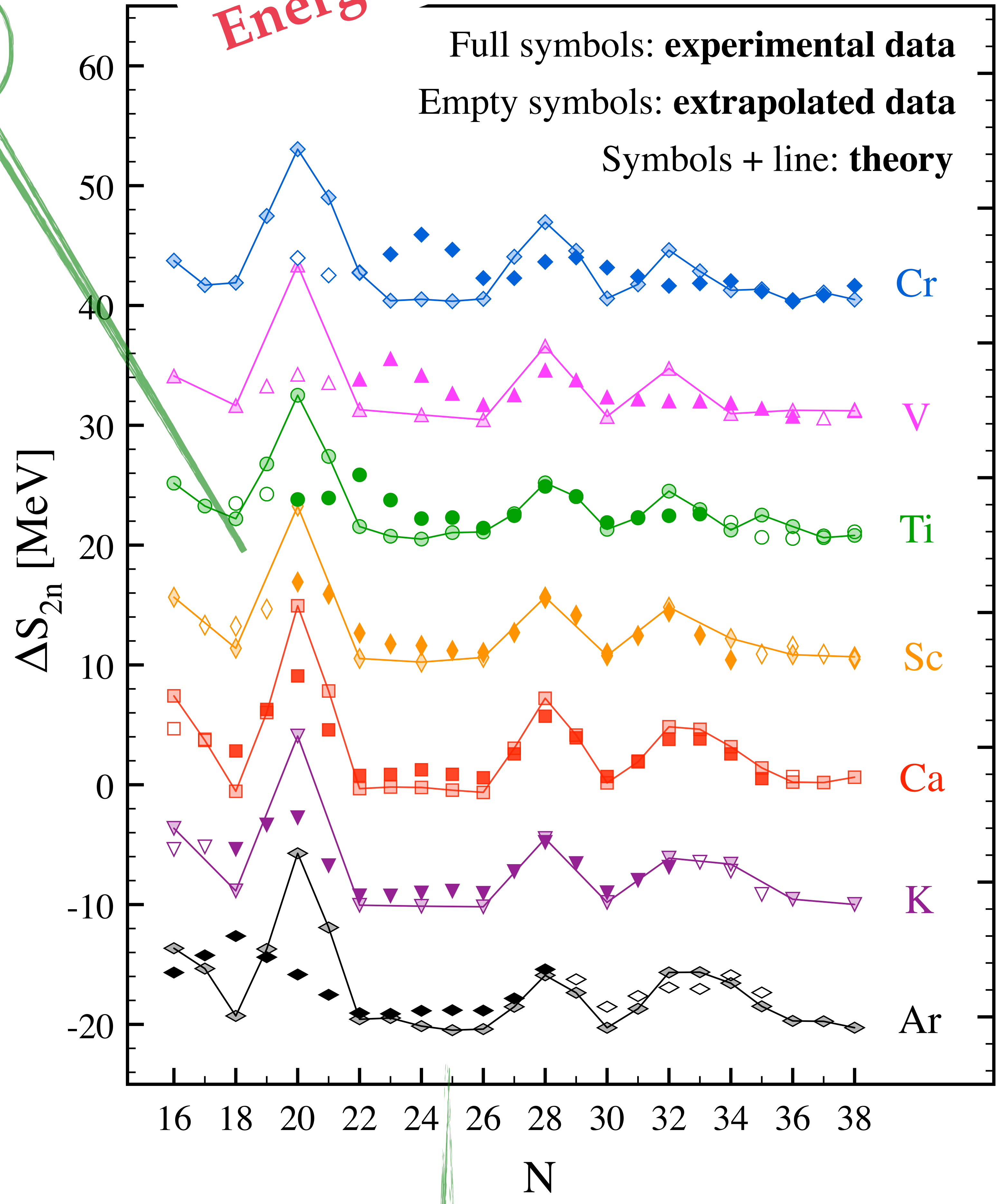
[Vorabbi *et al.*, 2024]



Densities

[Brugnara *et al.*, submitted]

Energies



[Somà *et al.*, 2021]

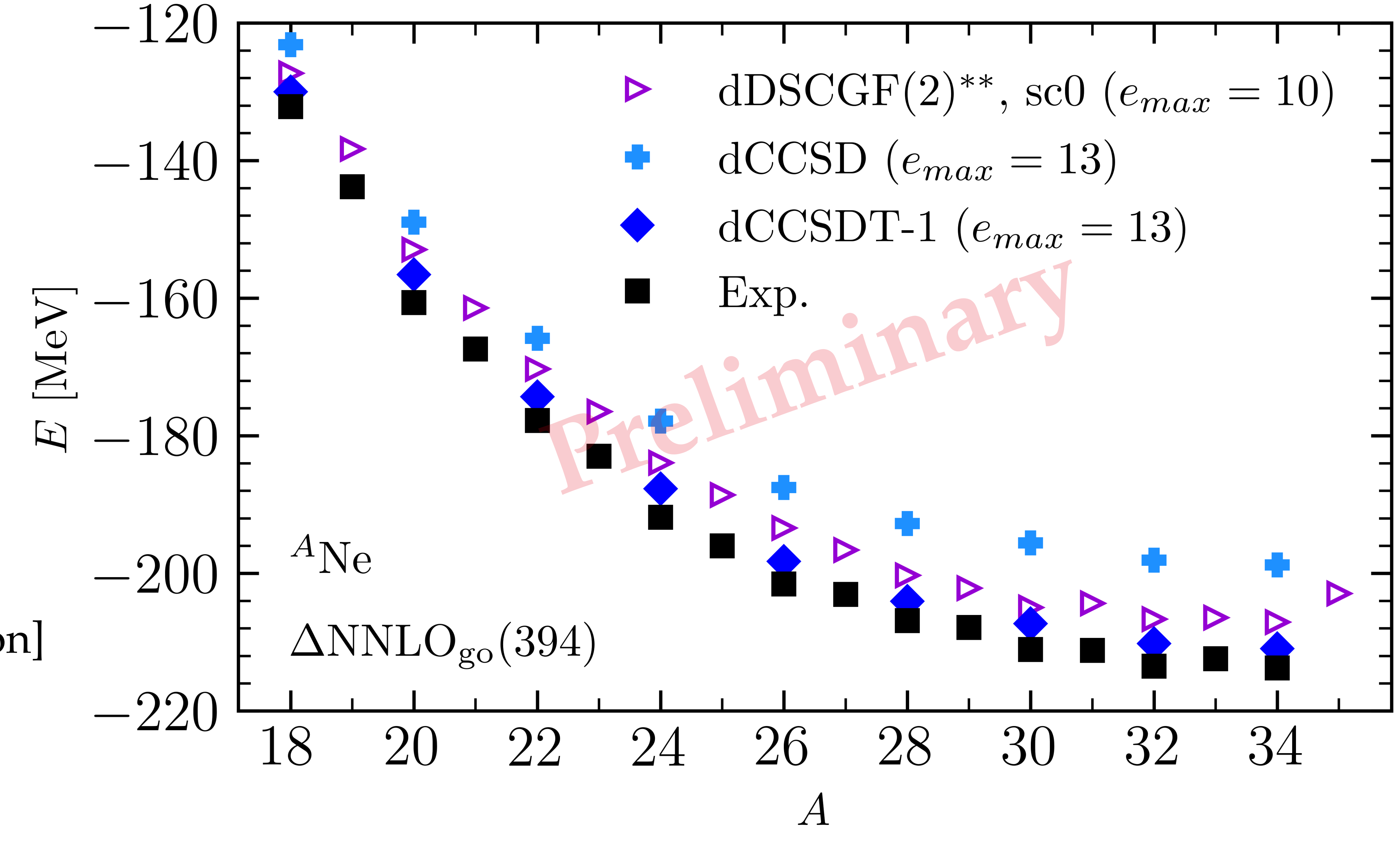
- ○ Accuracy degrades away from semi-magic Ca
- ○ Correlation with nuclear deformation
- → Calls for **explicit inclusion of deformation**

Deformed self-consistent Green's functions

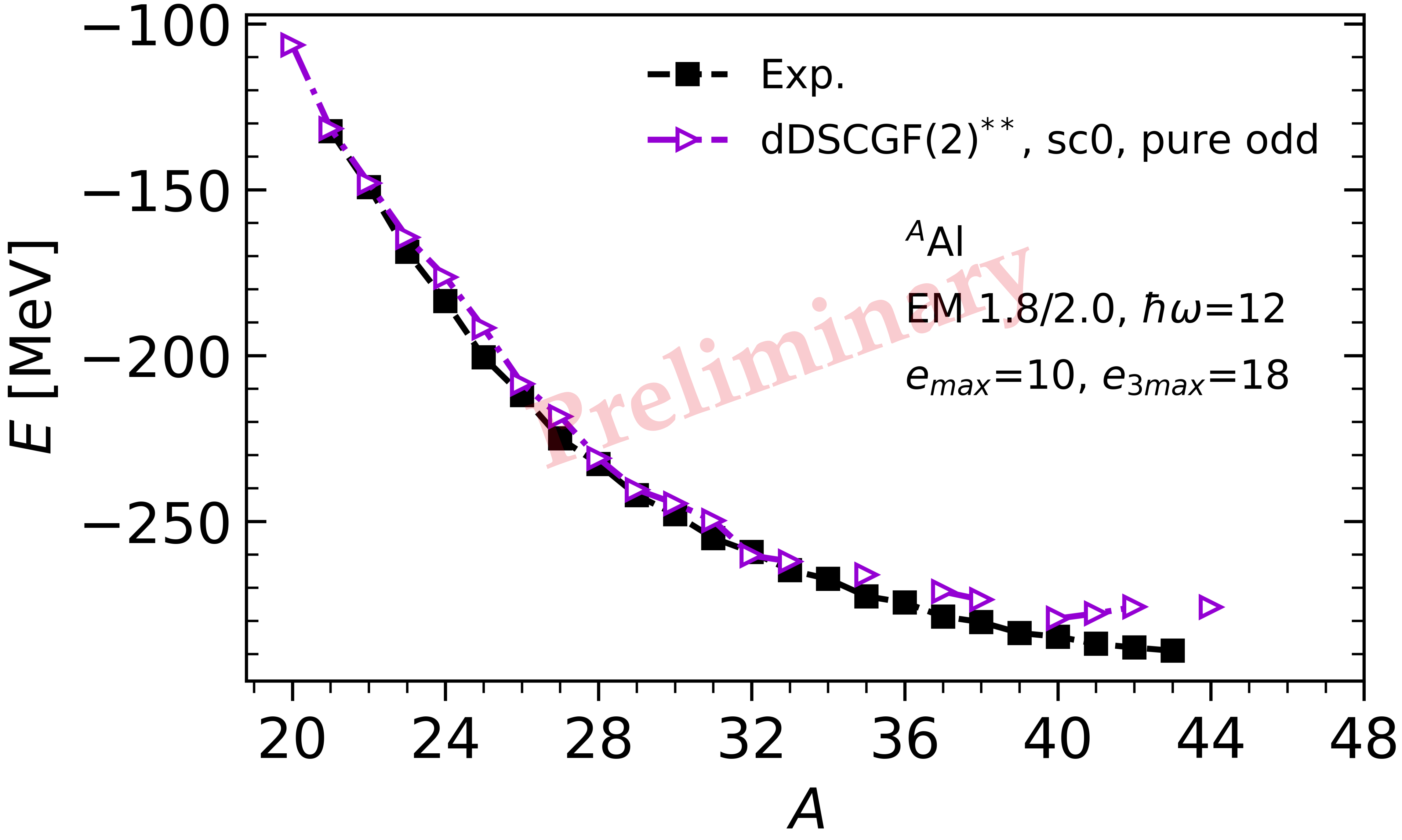
○ Symmetry breaking: rotational invariance

○ Dynamical correlations at 2nd order

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



[Scalesi *et al*. in preparation]



○ Trend consistent with CC results

○ Successful benchmark in odd-even isotopes

○ Preliminary test in odd-Z chain promising

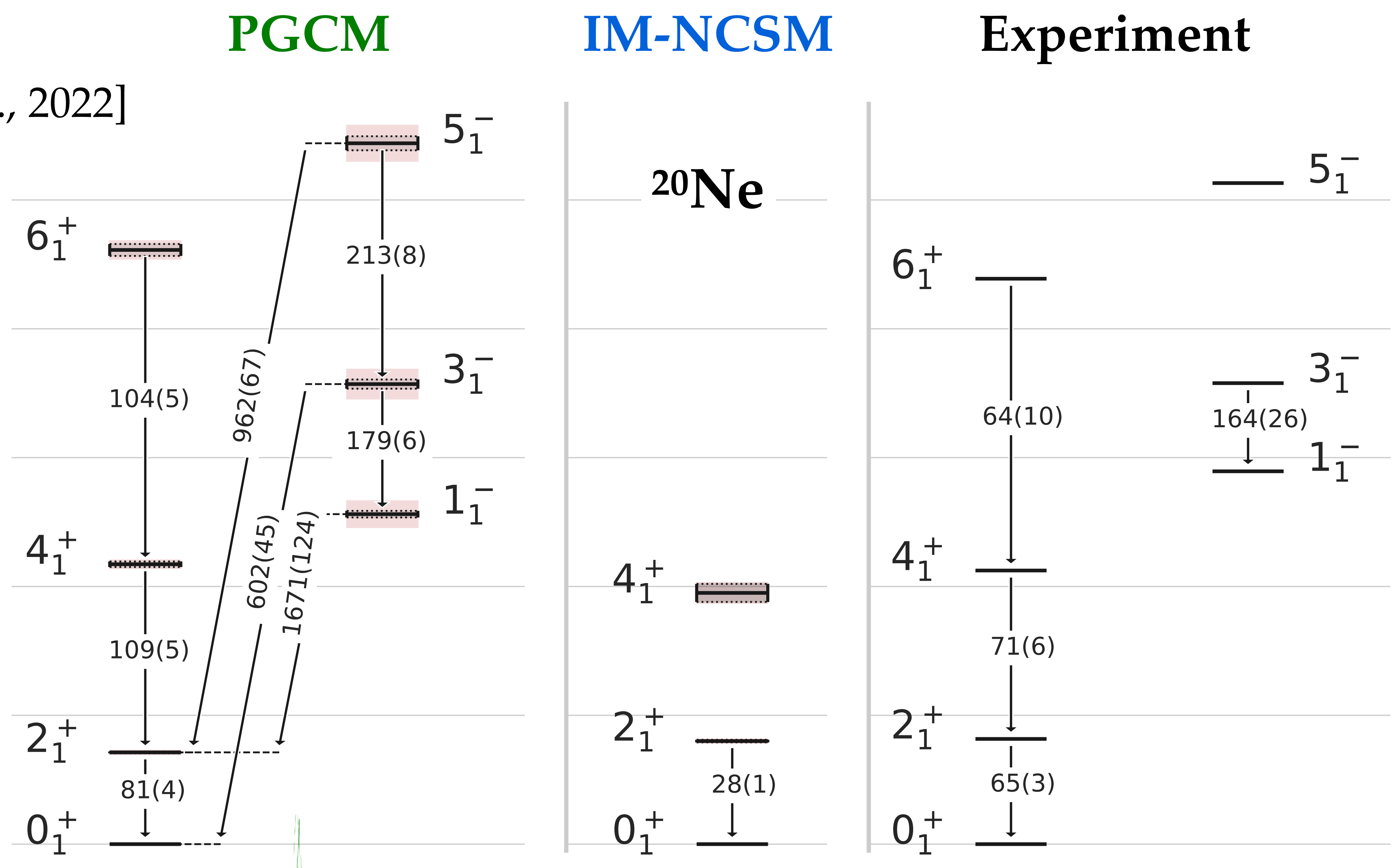
→ **First odd-odd calculations** with expansion methods

Projected generator coordinate method

- ○ Symmetry breaking & restoration
  - → particle number
  - → rotational invariance (axial)
  - → parity
- ○ No dynamical correlations

→ **Excitation spectra & collective properties**

[Frosini *et al.*, 2022]



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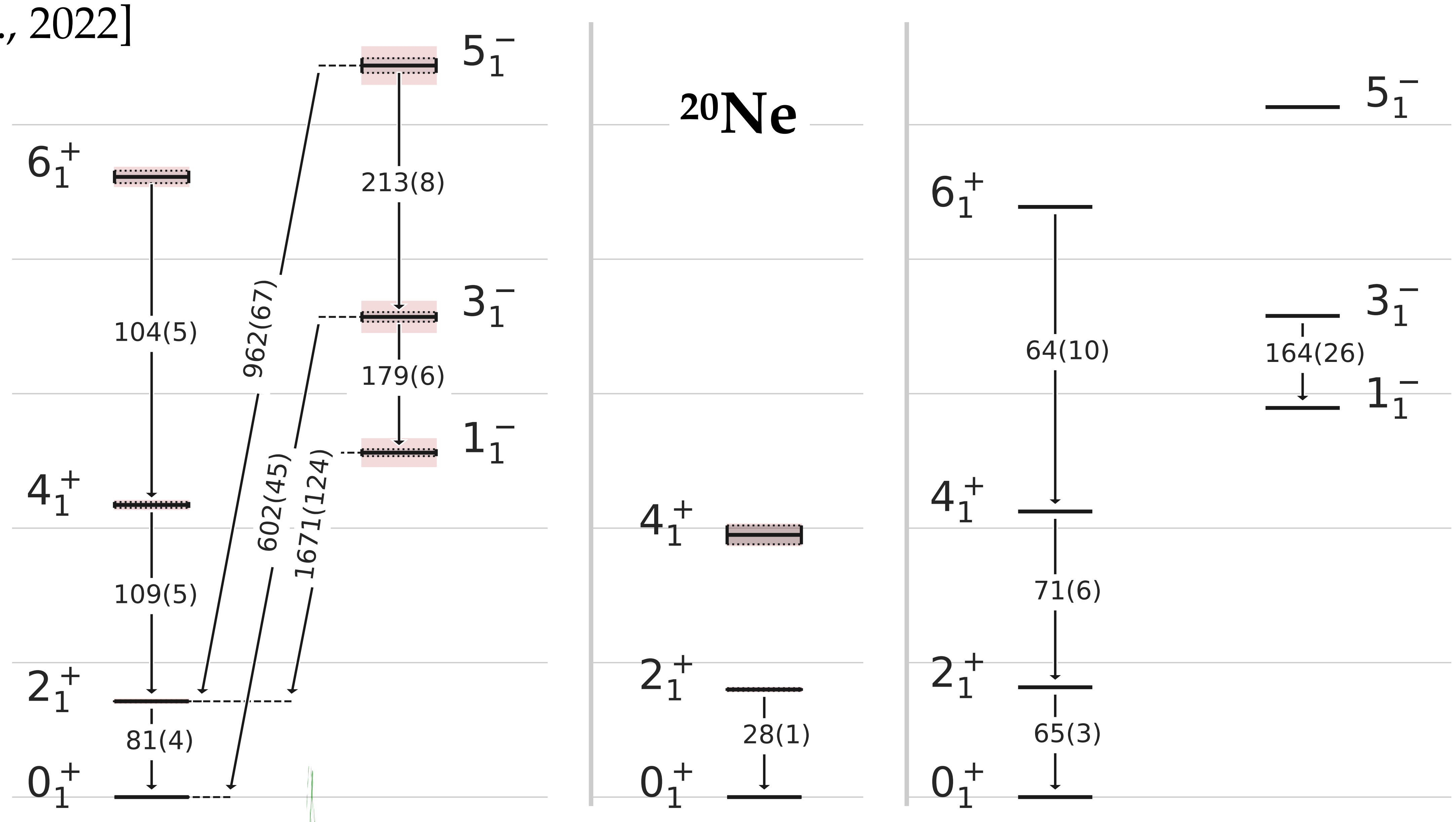

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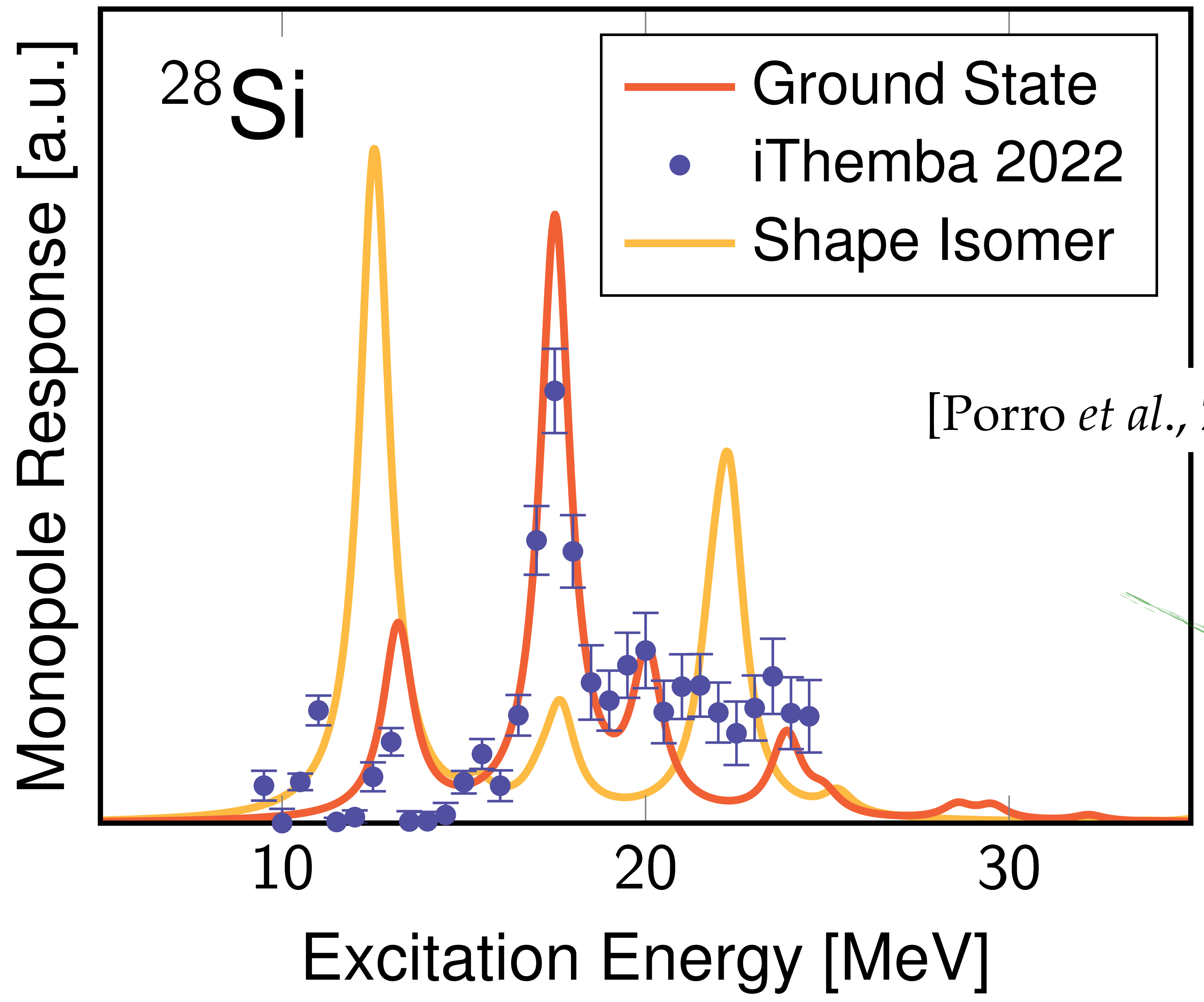


[Porro *et al.*, 2024]

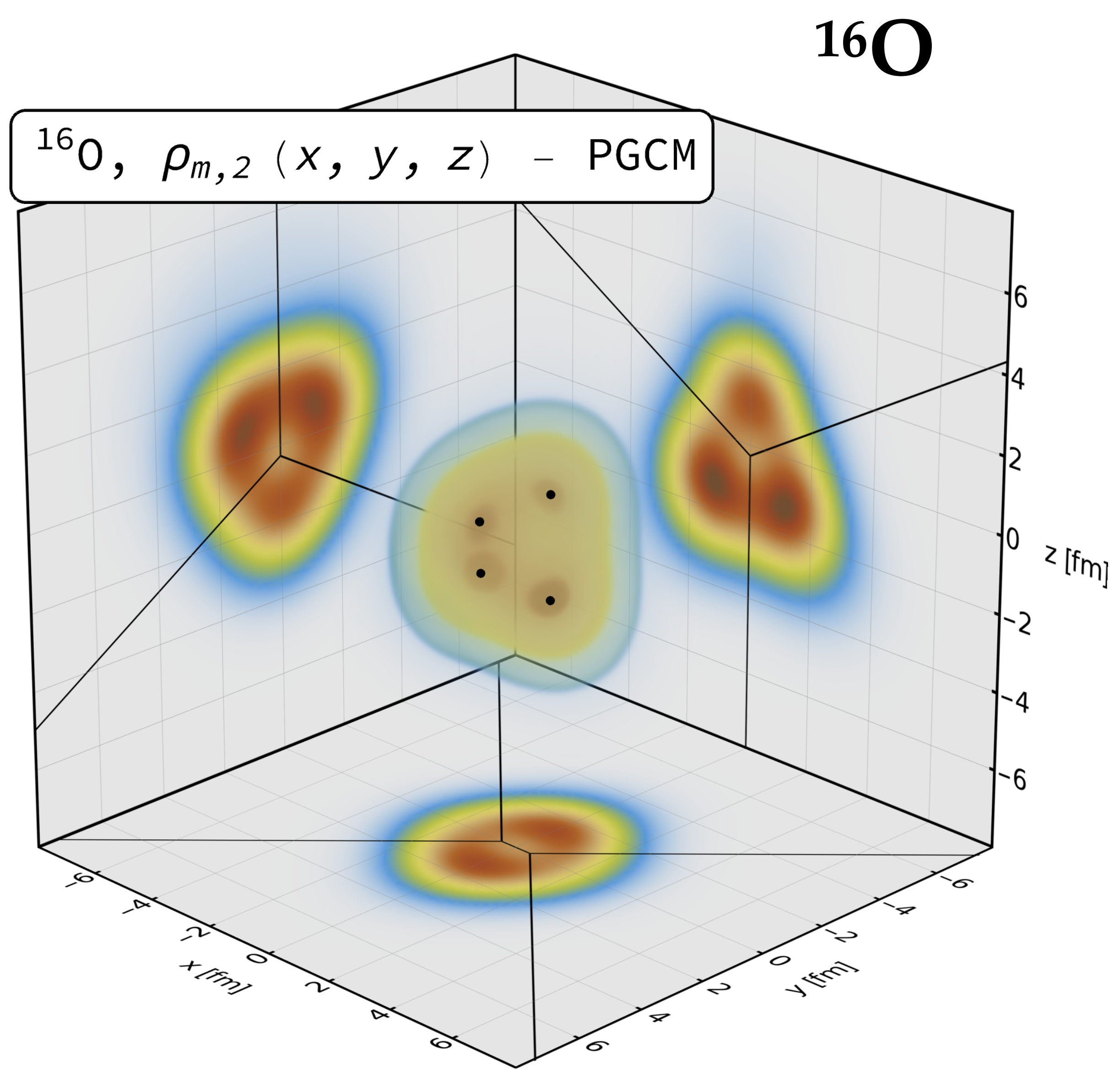
- ○ Oblate ground state & low-lying prolate isomer
  - → Shape coexistence (but weak mixing)

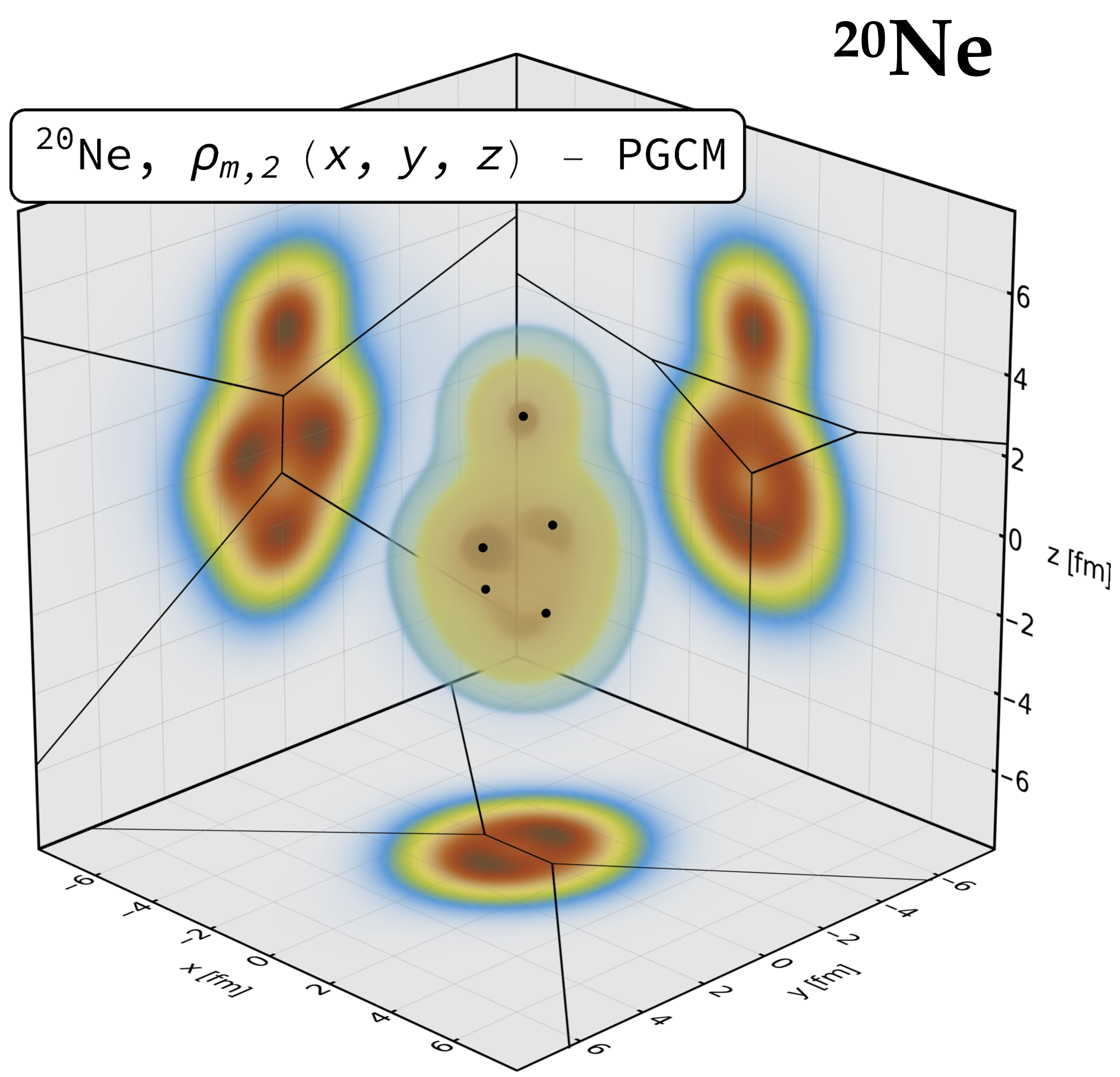
Nuclear structure & relativistic ion collisions

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

→ Test of the hydrodynamic QGP paradigm for small systems

→ New observables to test nuclear structure models





[Calculations by B. Bally]

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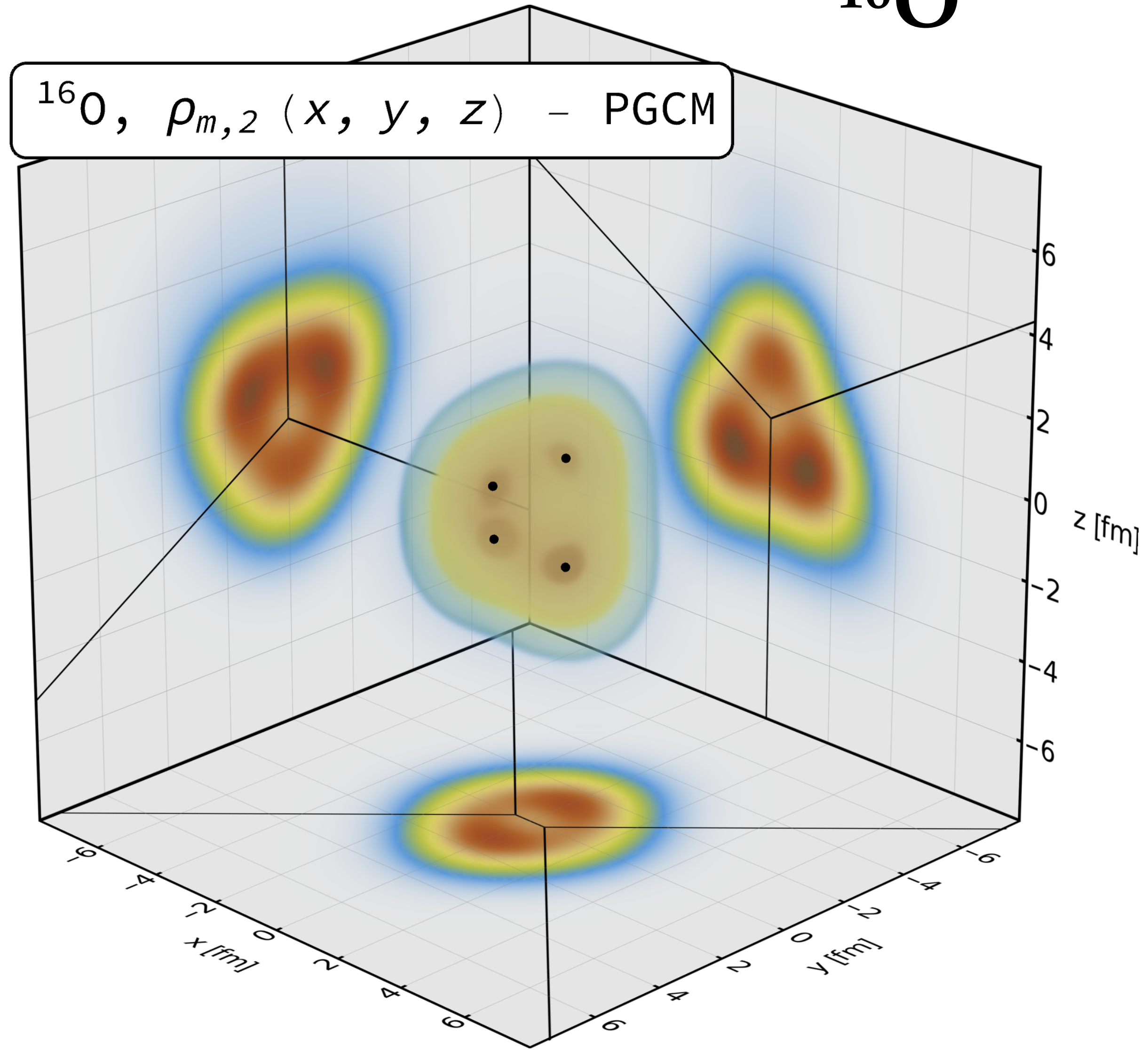
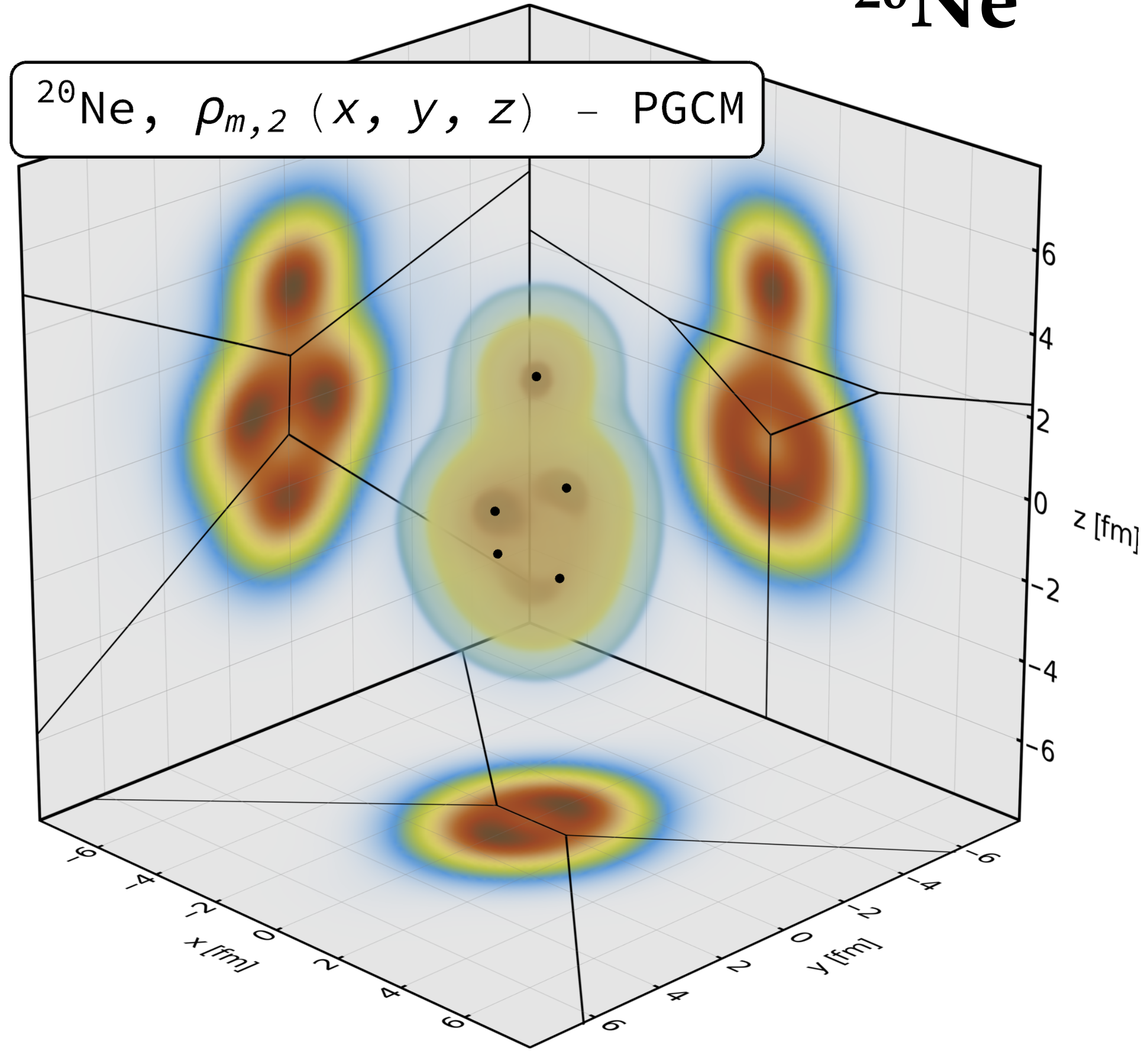
^{16}O



^{20}Ne

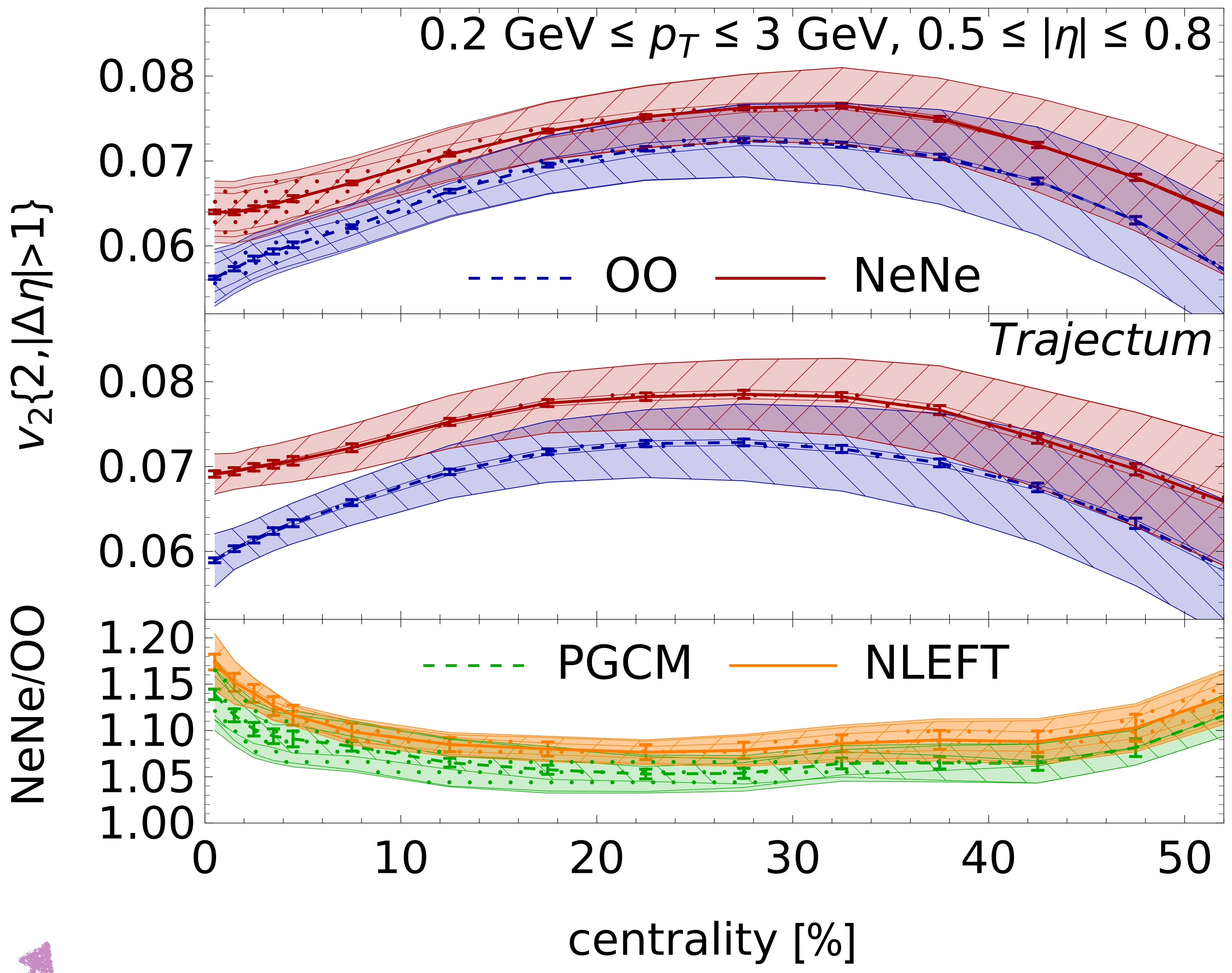


[Calculations by B. Bally]

Elliptic flow

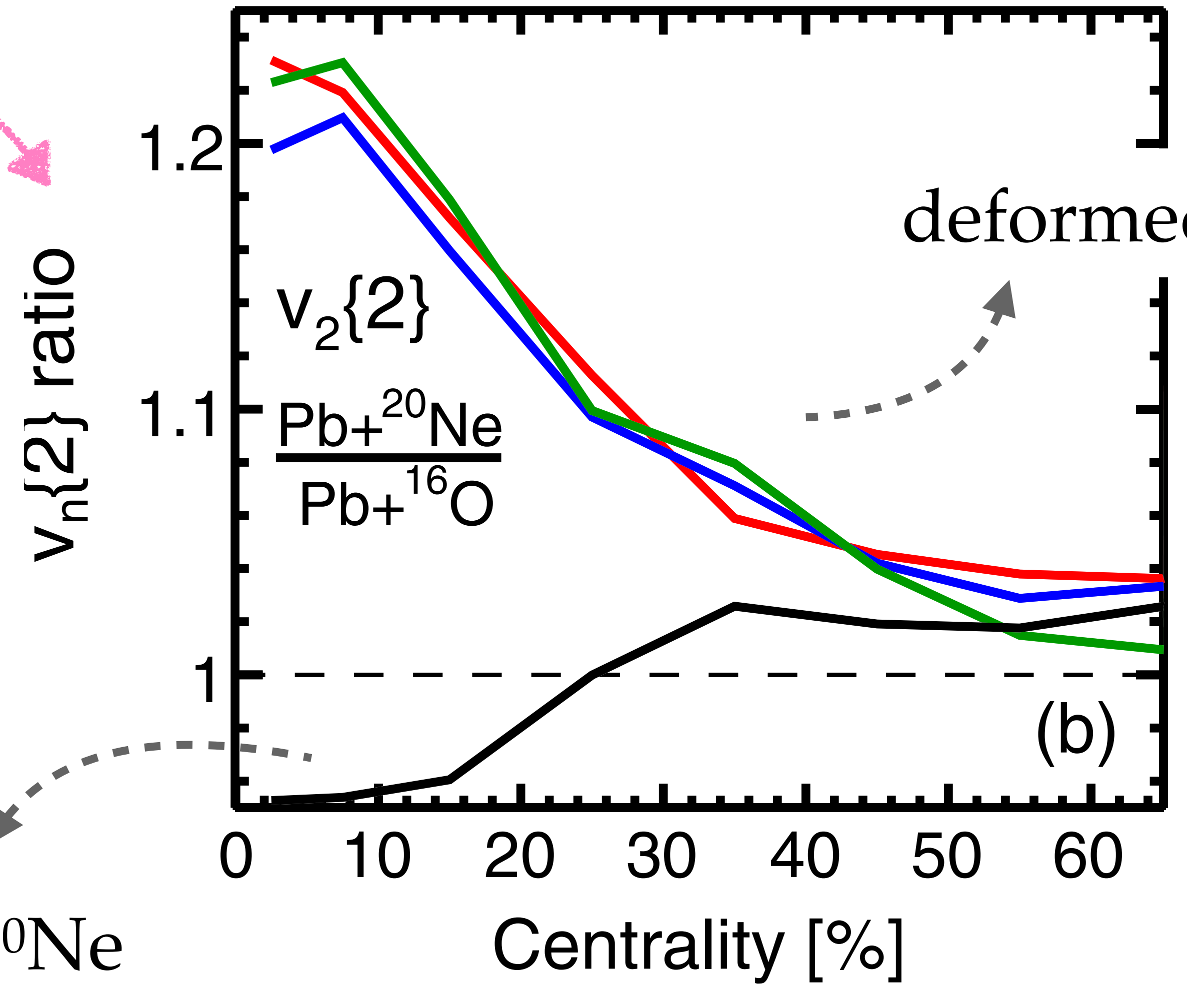
[Giacalone *et al.*, submitted]

^{20}Ne-^{20}Ne



Pb-^{20}Ne

[Giacalone *et al.*, 2025]



deformed ^{20}Ne

spherical ^{20}Ne

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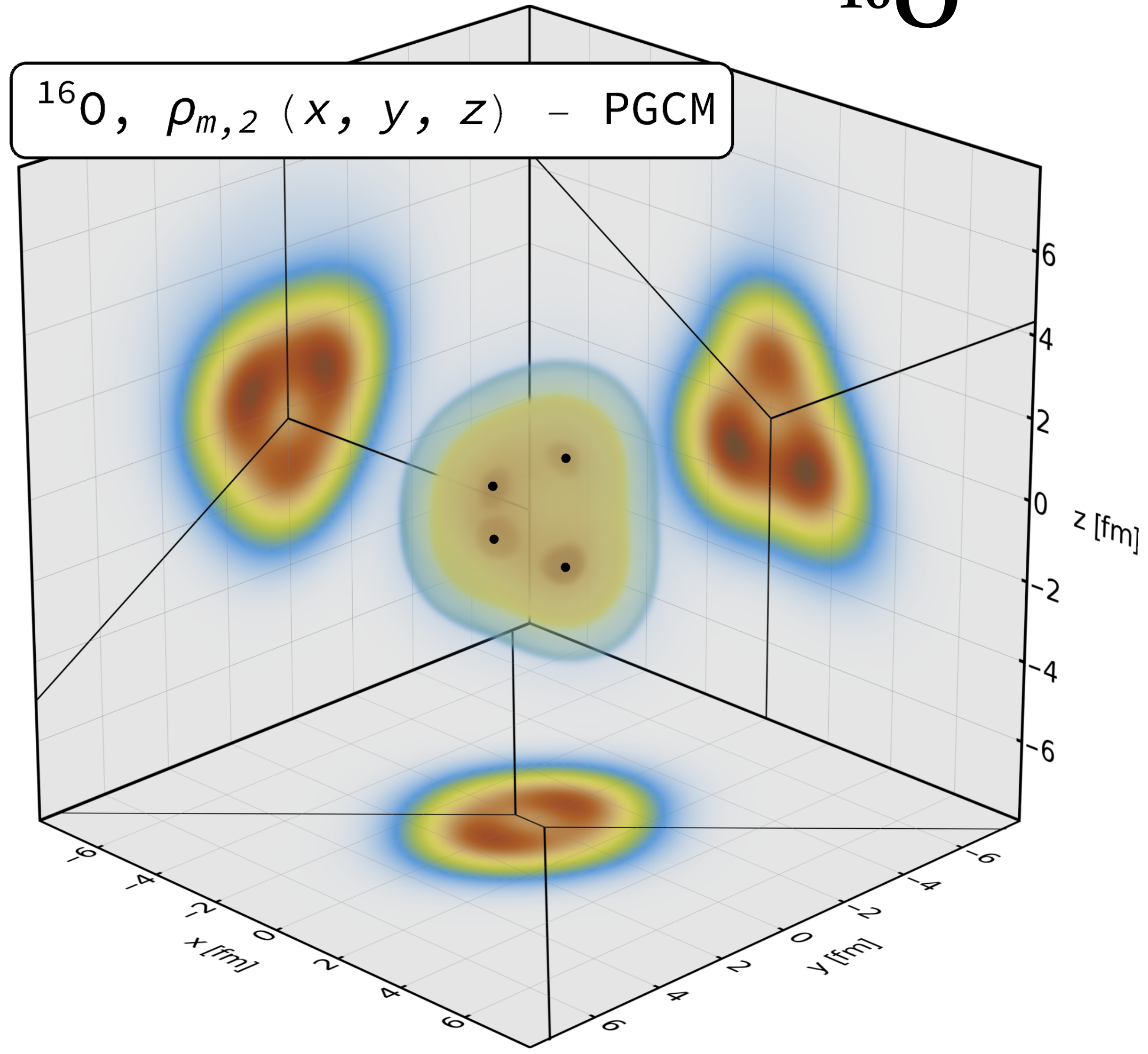

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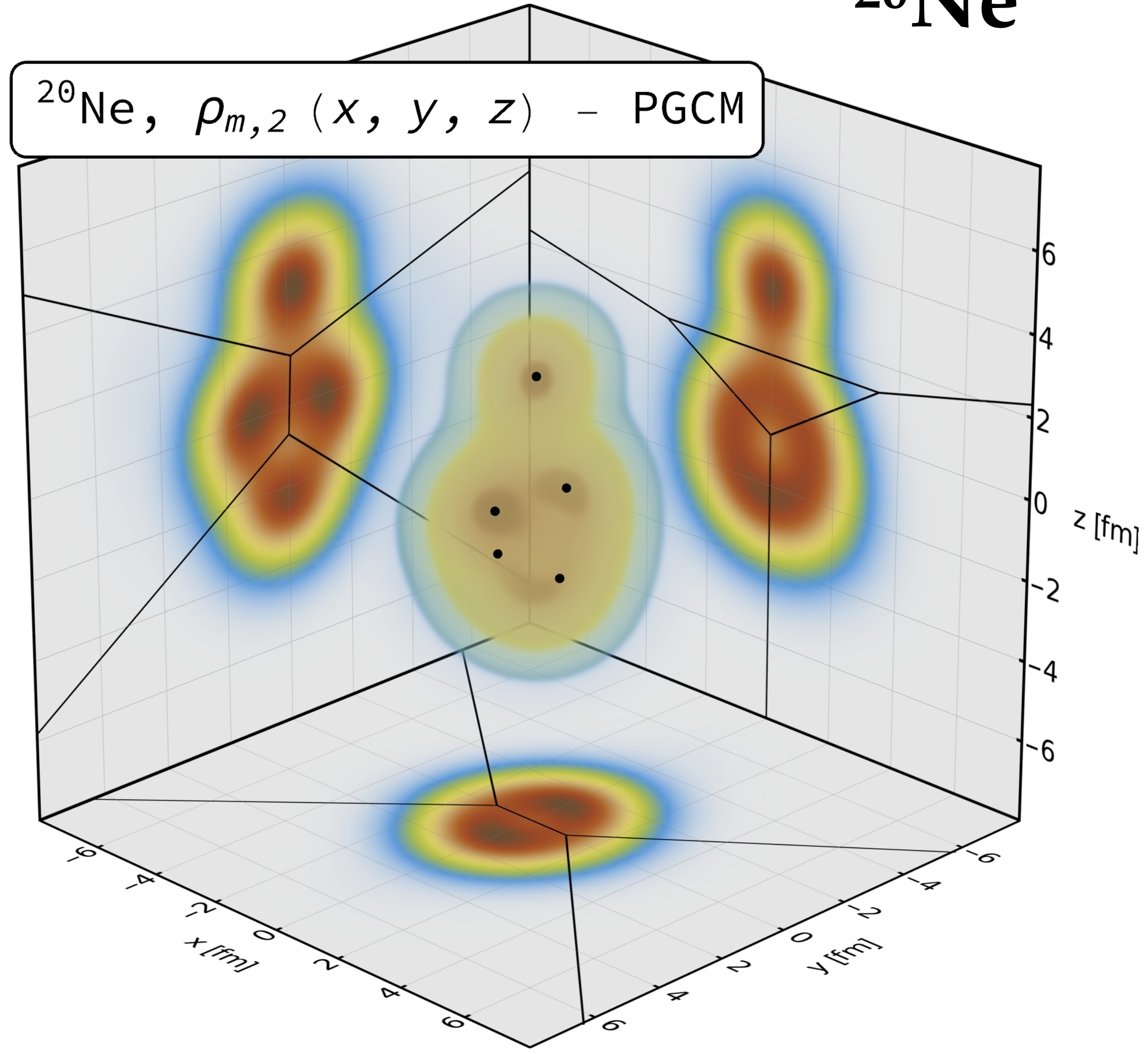

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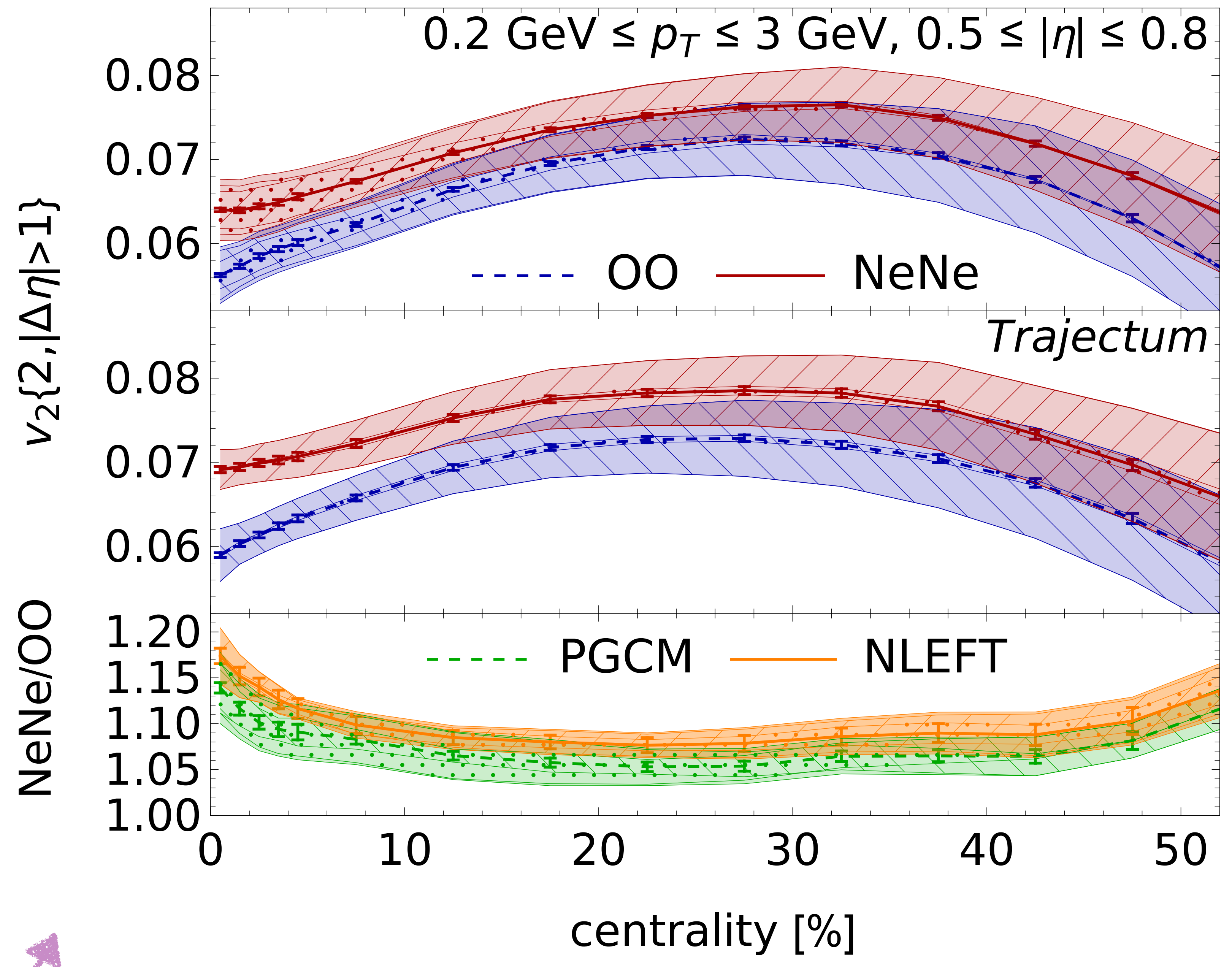

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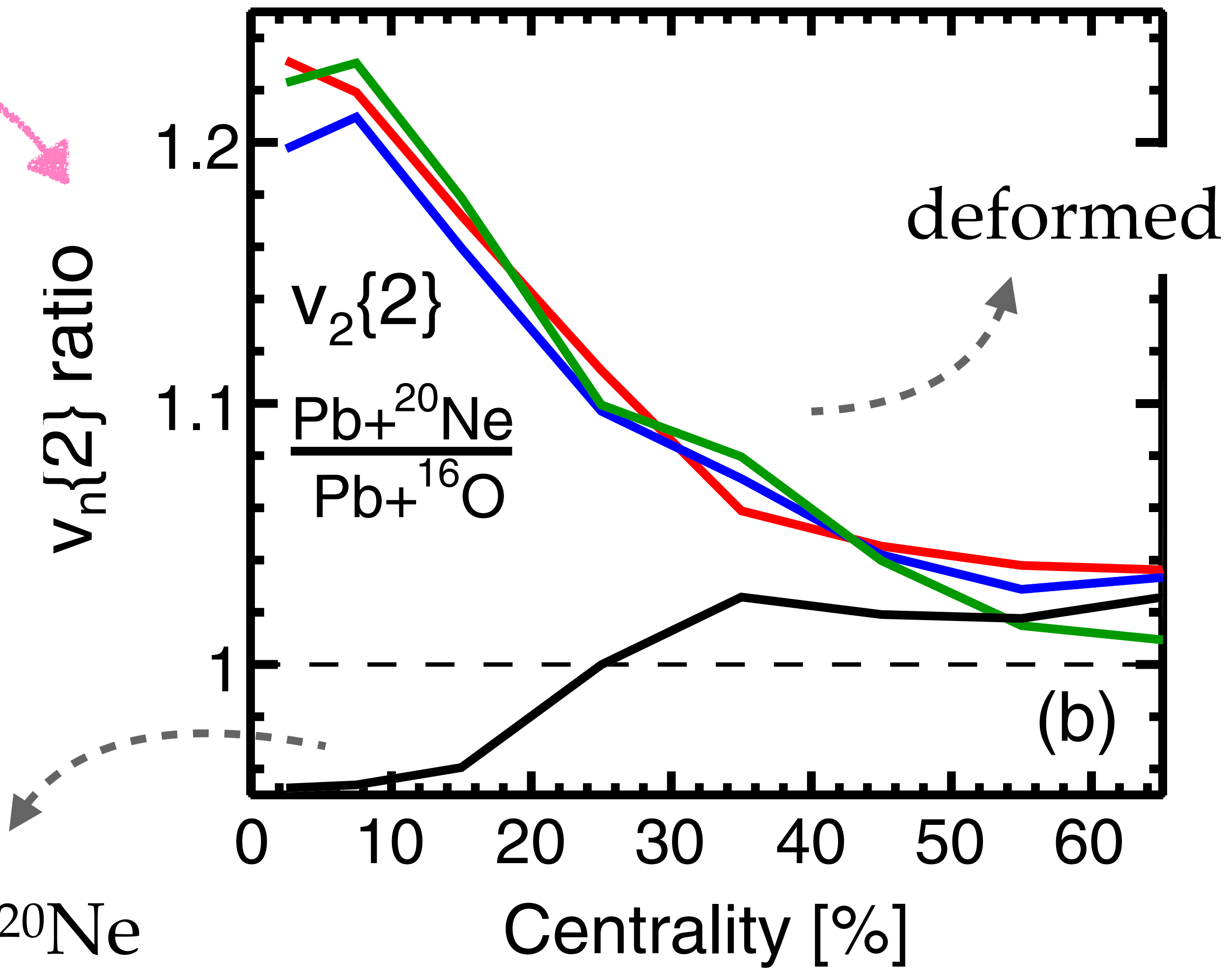


deformed ^{20}Ne

spherical ^{20}Ne

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

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

Perspectives

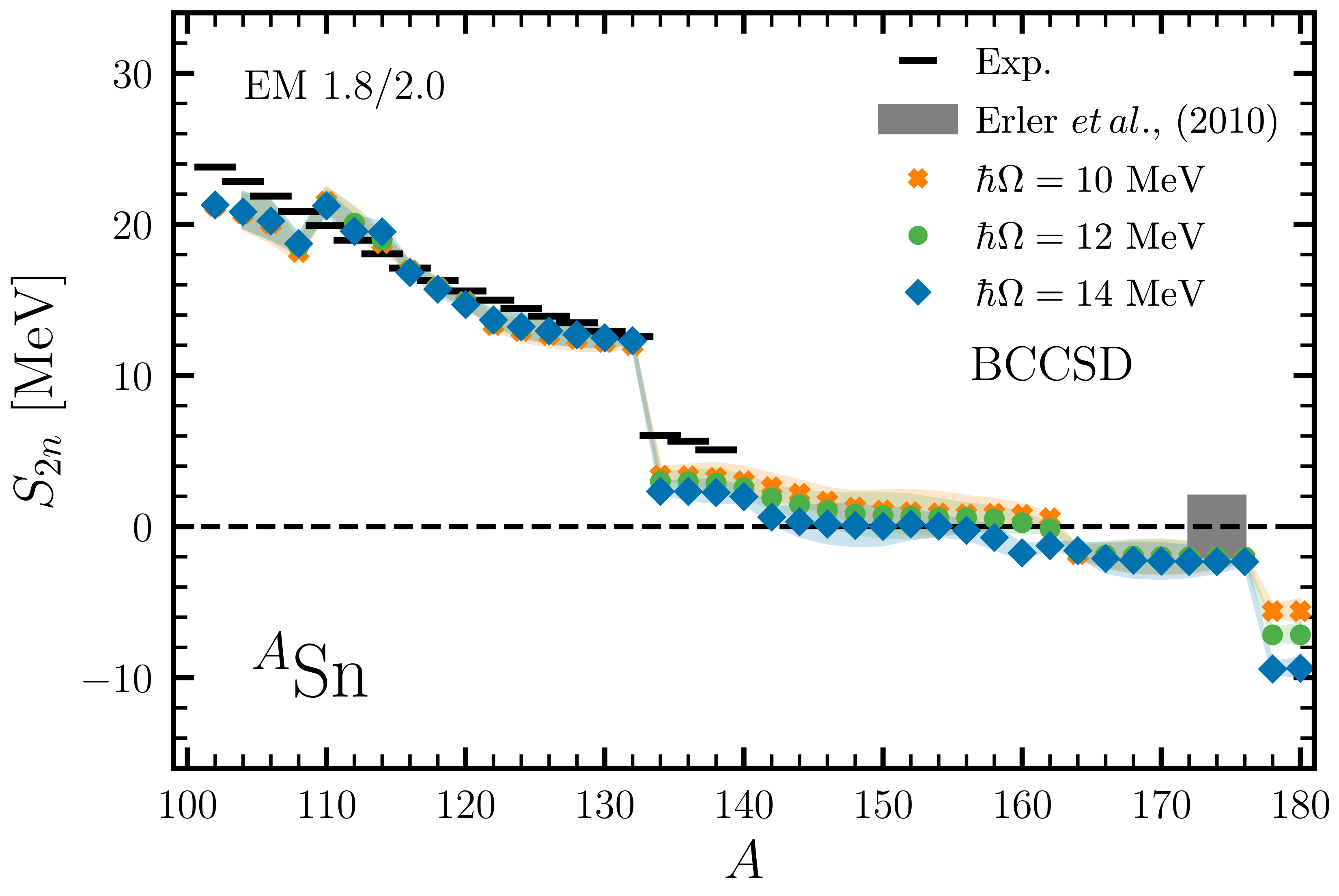
○ **How to extend such calculations to heavy systems?**

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., 2024]

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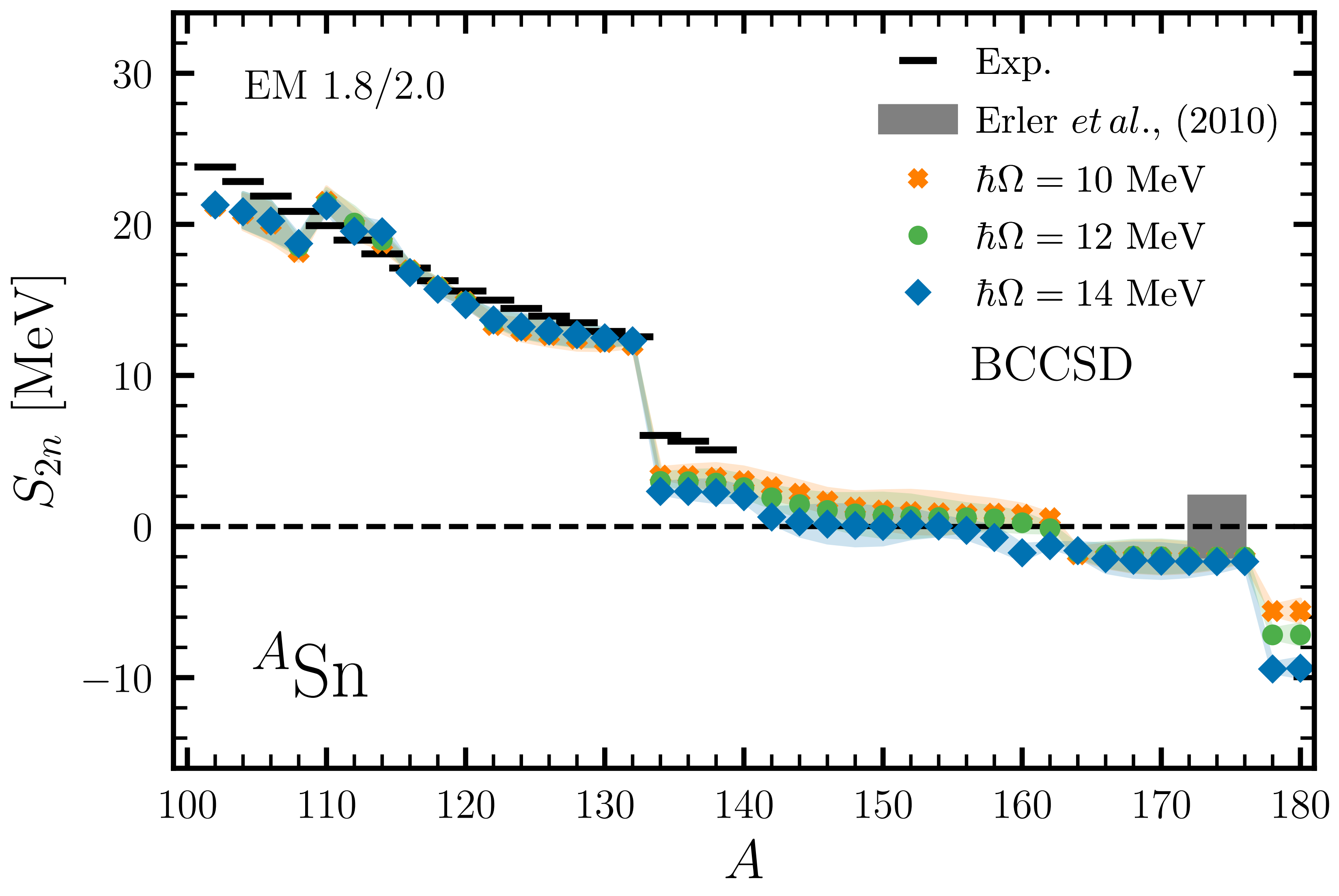
○ **Future requirement**: reduce **computational costs**

→ Development of dimensionality-reduction techniques

Importance truncation, natural orbitals, tensor factorisation

→ Use of emulators to produce statistically-relevant samples



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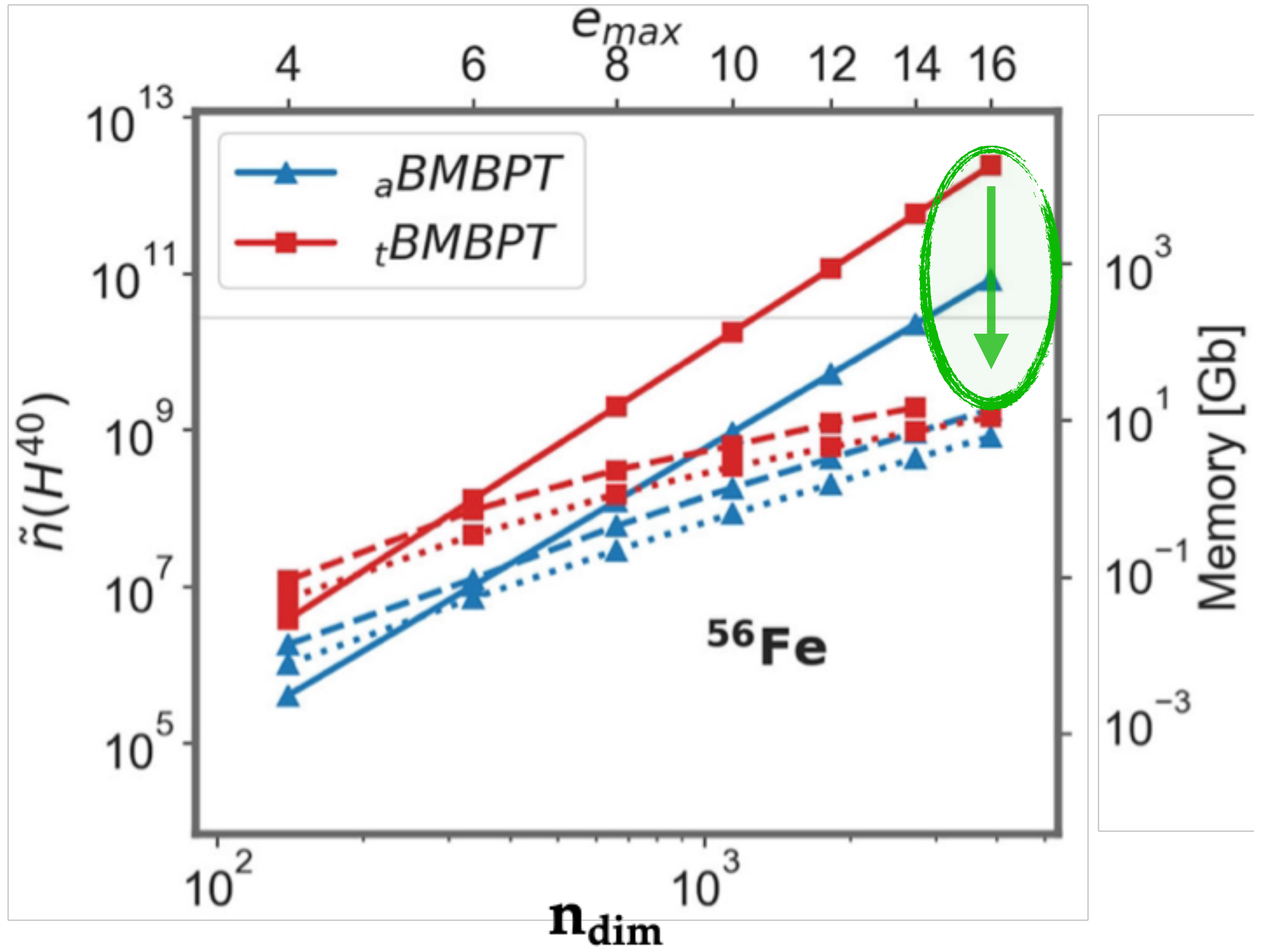

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