Many-body techniques for systematic calculations of closed- and open-shell nuclei

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INT program “*Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond*”

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Set-up

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

- View from a **many-body practitioner**
  - ***Level 1:*** Hamiltonians simply as input
  - ***Level 2:*** Interplay between many-body methods and nuclear interactions (feedback loop)
  - ***Level 3:*** Hamiltonian and many-body approach can not be disentangled → ”Chiral EFT in the A-body sector”

[Drissi, Duguet, Somà 2020]

- **Objectives of this talk**
  - Present recent progress and current limitations of some many-body techniques
  - Many-body calculations as a diagnostic tool for nuclear Hamiltonians
  - Discuss many-body uncertainties

- **Disclaimer**
  - UQ of the Hamiltonian absent

Ab initio Segrè chart

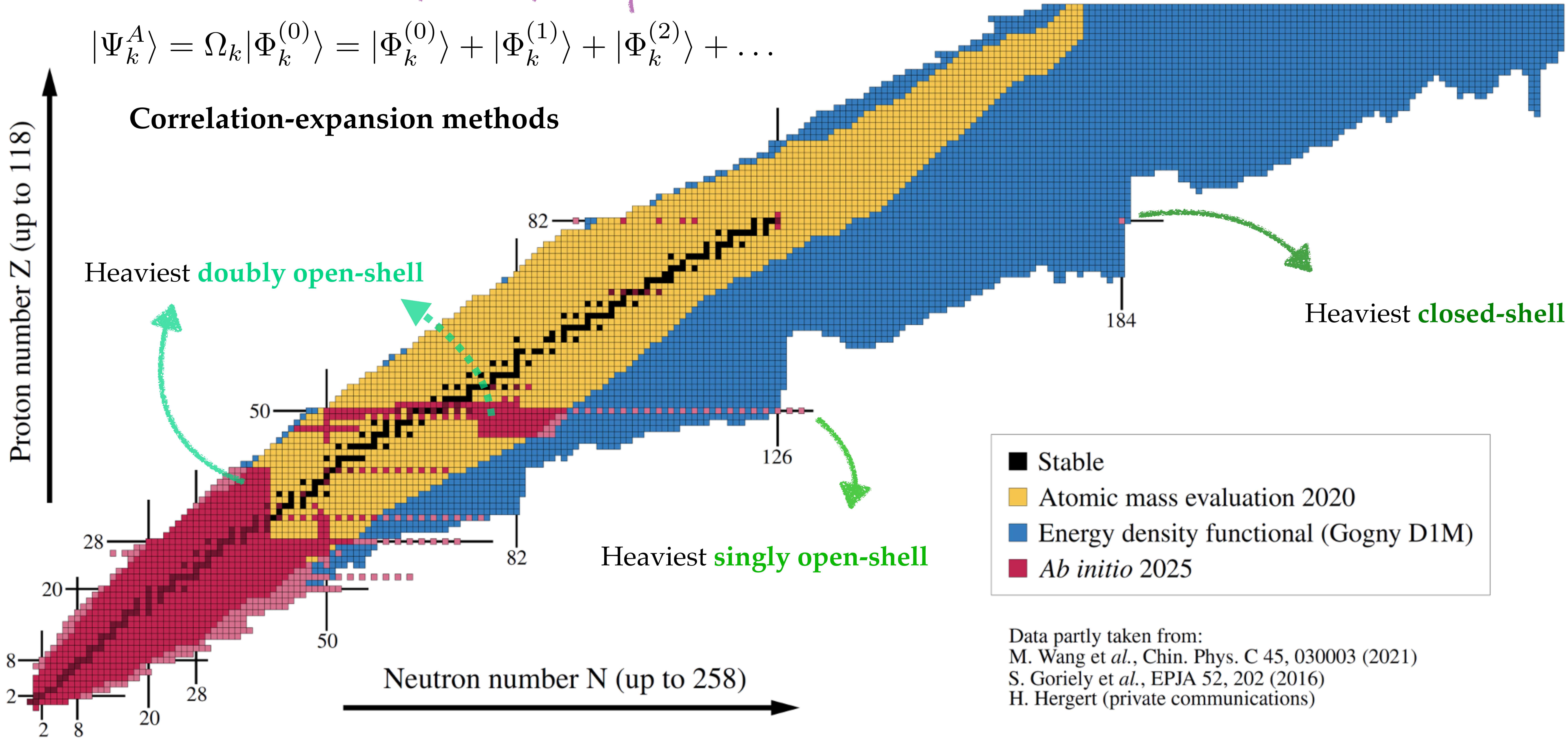
scaling n^4

scaling n^α with $\alpha > 4$

[Figure: B. Bally]

$$|\Psi^A_k\rangle = \Omega_k|\Phi^{(0)}_k\rangle = |\Phi^{(0)}_k\rangle + |\Phi^{(1)}_k\rangle + |\Phi^{(2)}_k\rangle + \dots$$

Correlation-expansion methods



Heaviest **doubly open-shell**

Heaviest **closed-shell**

Heaviest **singly open-shell**

- ■ Stable
- 🟨 Atomic mass evaluation 2020
- 🟦 Energy density functional (Gogny D1M)
- 🟥 *Ab initio* 2025

Data partly taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
S. Goriely et *al.*, EPJA 52, 202 (2016)
H. Hergert (private communications)

Correlation-expansion strategies

- ⦿ Correlation expansion performed in terms of particle-hole excitations

$$|\Psi^A_k\rangle = \Omega_k|\Phi^{(0)}_k\rangle = |\Phi^{(0)}_k\rangle + |\Phi^{(1)}_k\rangle + |\Phi^{(2)}_k\rangle + \ldots$$

Static correlations

Dynamical correlations

U(1)$_N$ x U(1)$_Z$ → Superfluidity

SU(2) → Deformation

- ○ Problem: expansion **breaks down in open-shell systems**
- ○ Solution: start from a **symmetry-breaking reference state** → At some point, necessary to **restore symmetries**
- ○ Price to pay: more involved formalism & **higher computational costs** (quasiparticles, lack of rotational invariance, …)

Different strategies

(1) Expand, then restore →
- ○ Many-body perturbation theory (**MBPT**)
- ○ Coupled-cluster (**CC**)
- ○ Self-consistent Green's functions* (**SCGF**)

(2) Restore, then expand →
- ○ In-medium SRG (**IMSRG**)
- ○ Projected generator coordinate method + perturbation theory (**PGCM-PT**)

→ Most efficient strategy depends on **observable, required accuracy, Hamiltonian, …**

→ Very important to develop **different complementary** approaches

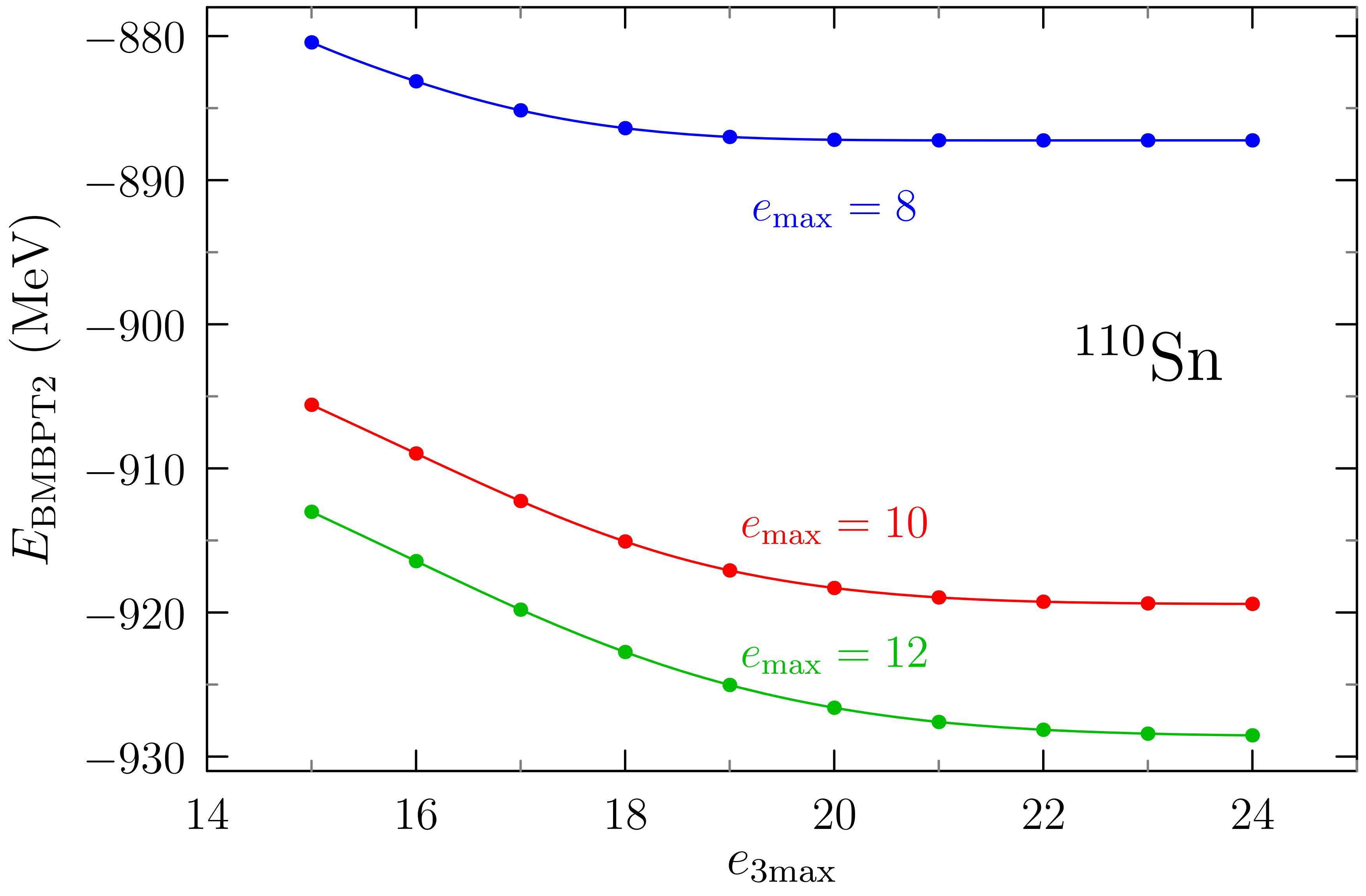
Hamiltonian menu

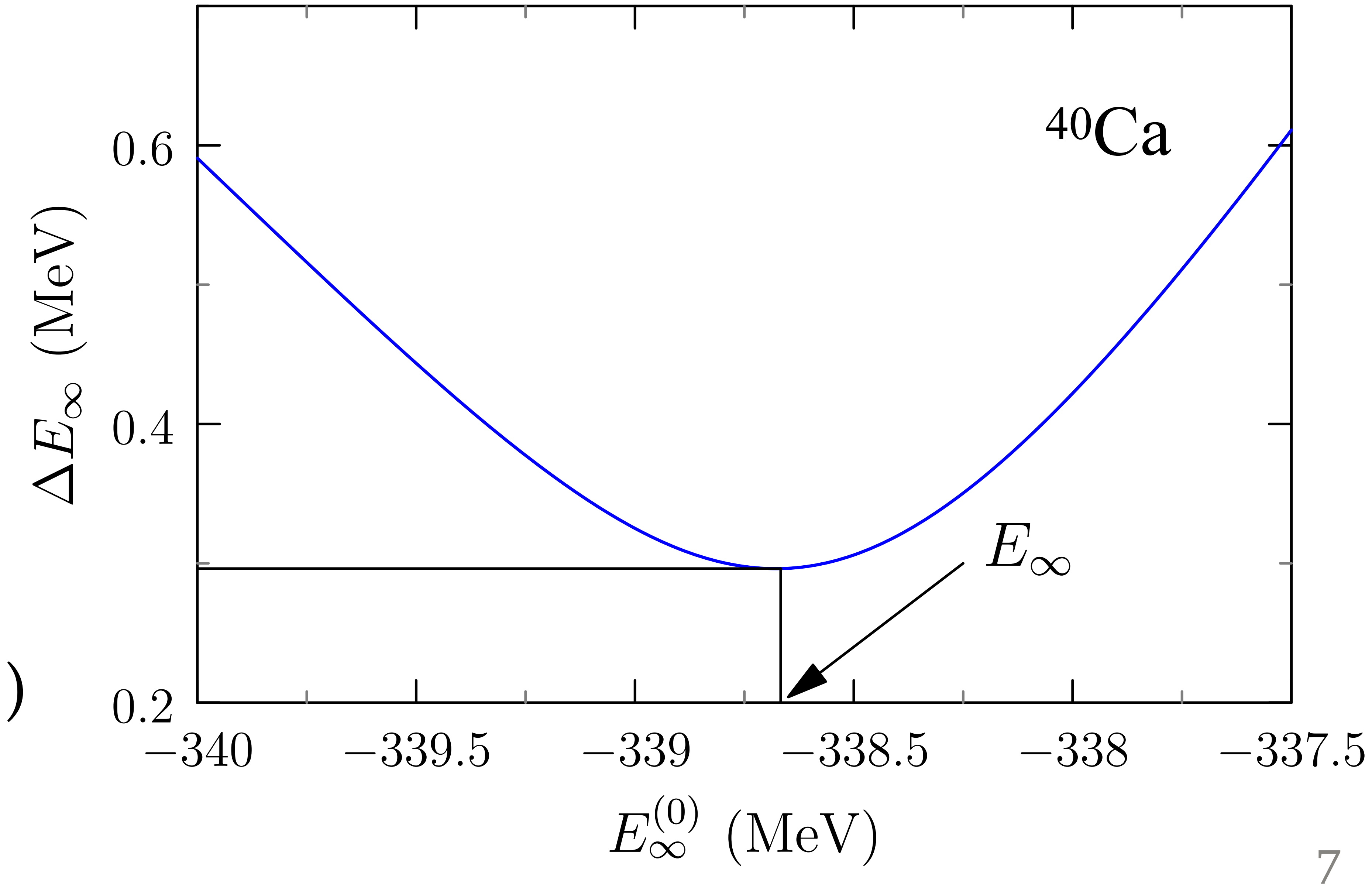
EM 1.8/2.0	○ N^{3}LO 2N + N^{2}LO 3N, SRG only on 2N ○ 3N Adjusted on A=3,4	2011	[Hebeler *et al.*]
N^{2}LO$_{\text{sat}}$	○ N^{2}LO 2N+3N, no SRG ○ Adjusted also on C and O data (energies and radii)	2015	[Ekström *et al.*]
NN+3N(lnl)	○ N^{3}LO 2N + N^{2}LO 3N, SRG consistently on 2N+3N ○ Combination of local and non-local 3N regulators	2020	[Somà *et al.*]
N^{3}LO$_{\text{TUD}}$	○ N^{3}LO 2N + 3N, three cutoffs available (450, 500, 550 MeV) ○ ^{16}O energy used to fix 3N contact	2020	[Hüther *et al.*]
ΔN^{2}LO$_{\text{GO}}$(394)	○ Explicit Δ-isobar degrees of freedom, no SRG ○ Includes constraints from saturation point & symmetry energy	2020	[Jiang *et al.*]
N^{3}LO$_{\text{Texas}}$	○ N^{3}LO 2N + N^{2}LO 3N, no SRG ○ Emulator-accelerated fits including ^{16}O data	2025	[Hu *et al.*]

1. MBPT

BMBPT large-scale calculations

- Bogolyubov (deformed) many-body perturbation theory (**BMBPT**)
  - **Reference state** → **deformed HFB** calculation (axial symmetry)
  - Dynamical correlations computed on top of global HFB minimum
- Hamiltonian → EM 1.8/2.0
- **All even-even nuclei with $2 \leq Z \leq 50$** at **BMBPT2** level → ~ 520 isotopes
- Model space → $e_{max} = 6\text{-}10$, $e_{3max} = 15\text{-}24$
  - e_{3max} extrapolation not necessary
  - e_{max} extrapolation via formula of More *et al.* 2013
    - → Independently for different $\hbar\omega$ + adding a value at $e_{max} = \infty$
    - → $E_\infty^{(0)}$ used as a parameter to minimise errors for various $\hbar\omega$
- **Evaluation of other uncertainties** ongoing (BMBPT3, symmetry breaking, …)

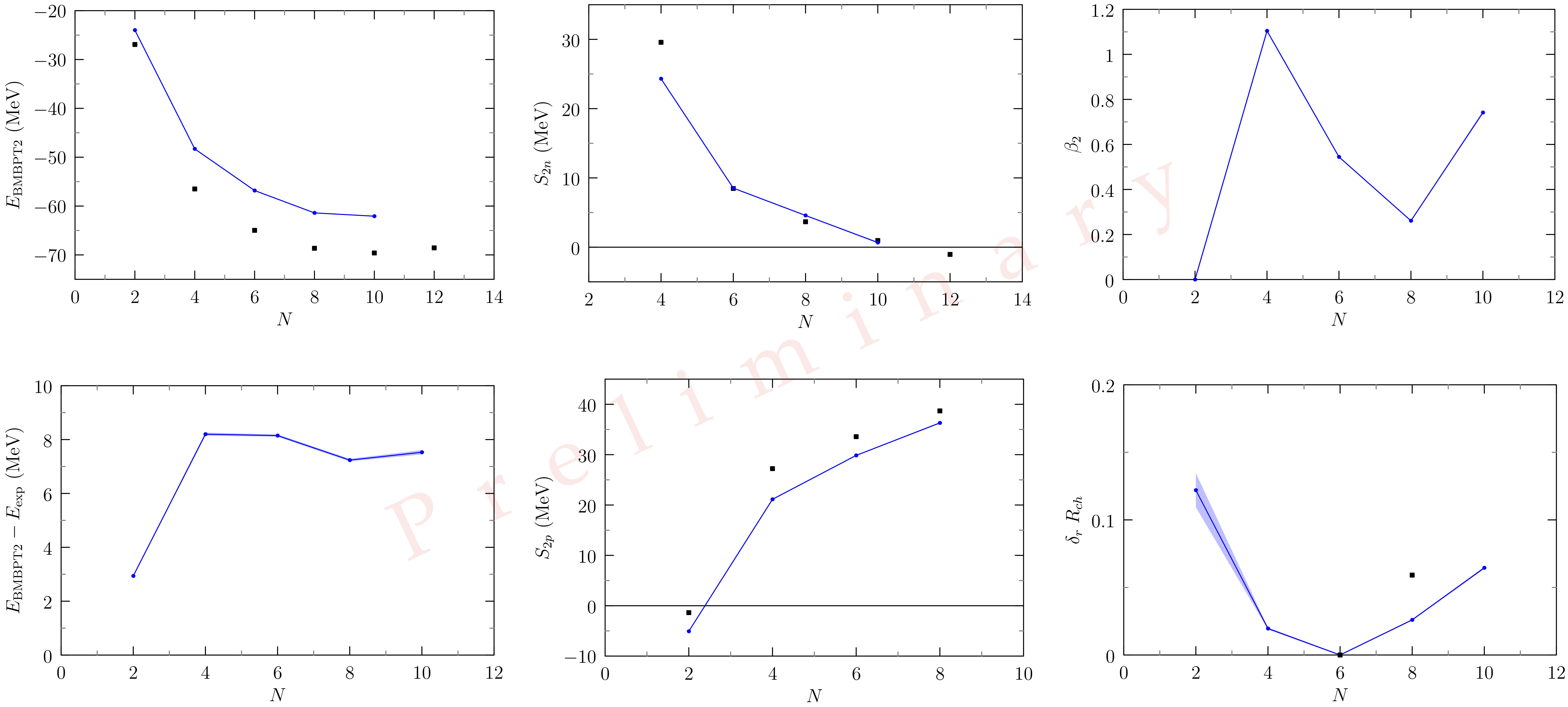




[Durel *et al.*, in preparation]

BMBPT2 systematics — Beryllium (Z=4)

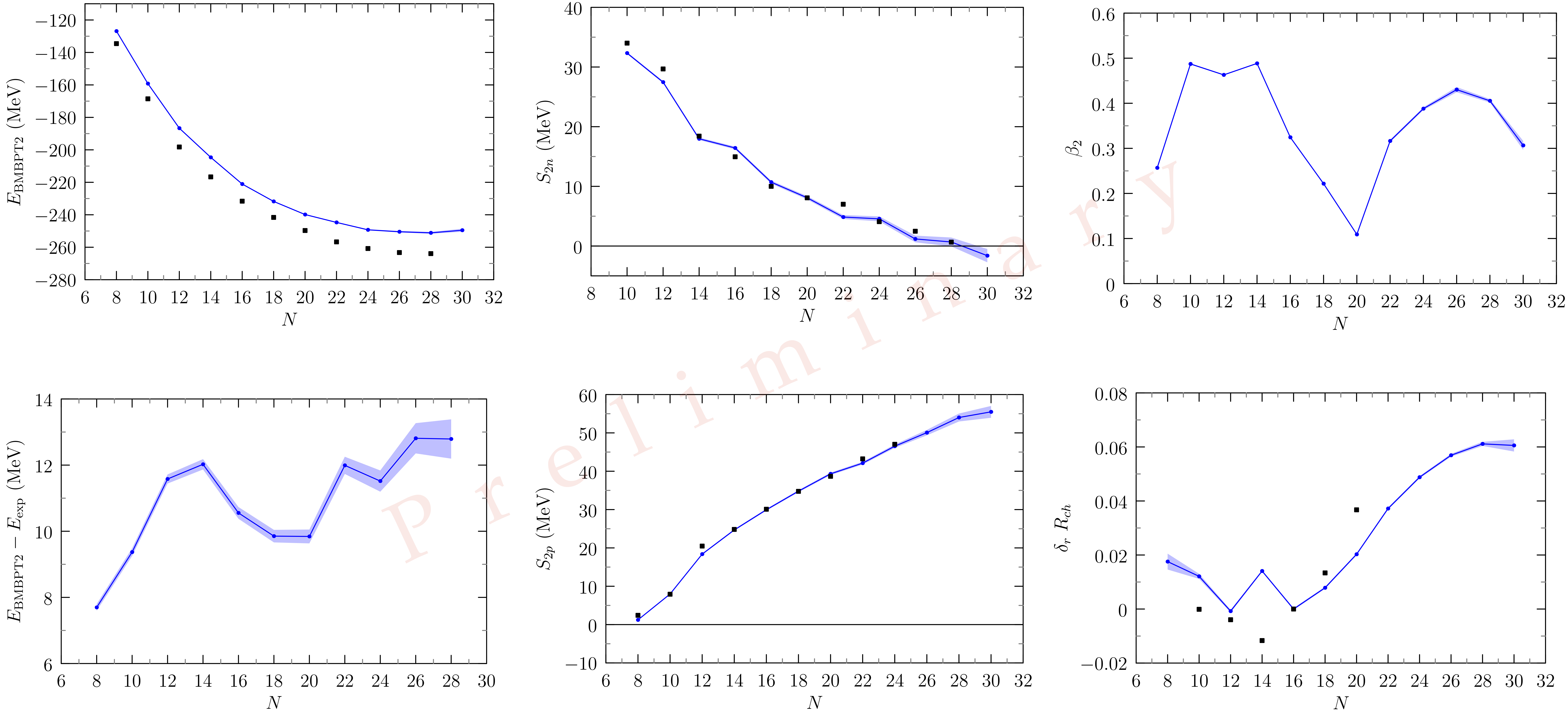
[Durel *et al.*, in preparation]



Preliminary

BMBPT2 systematics — Magnesium (Z=12)

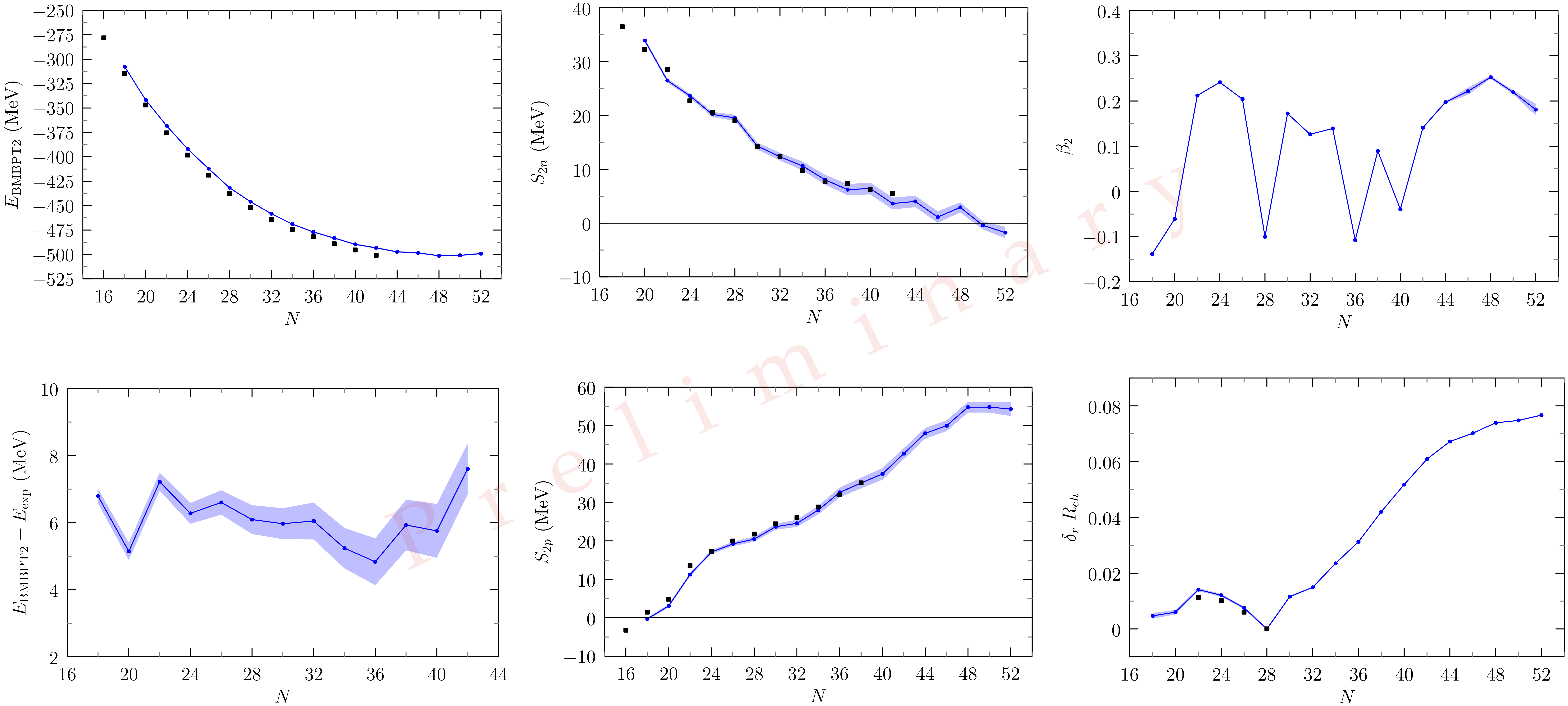
[Durel *et al.*, in preparation]



preliminary

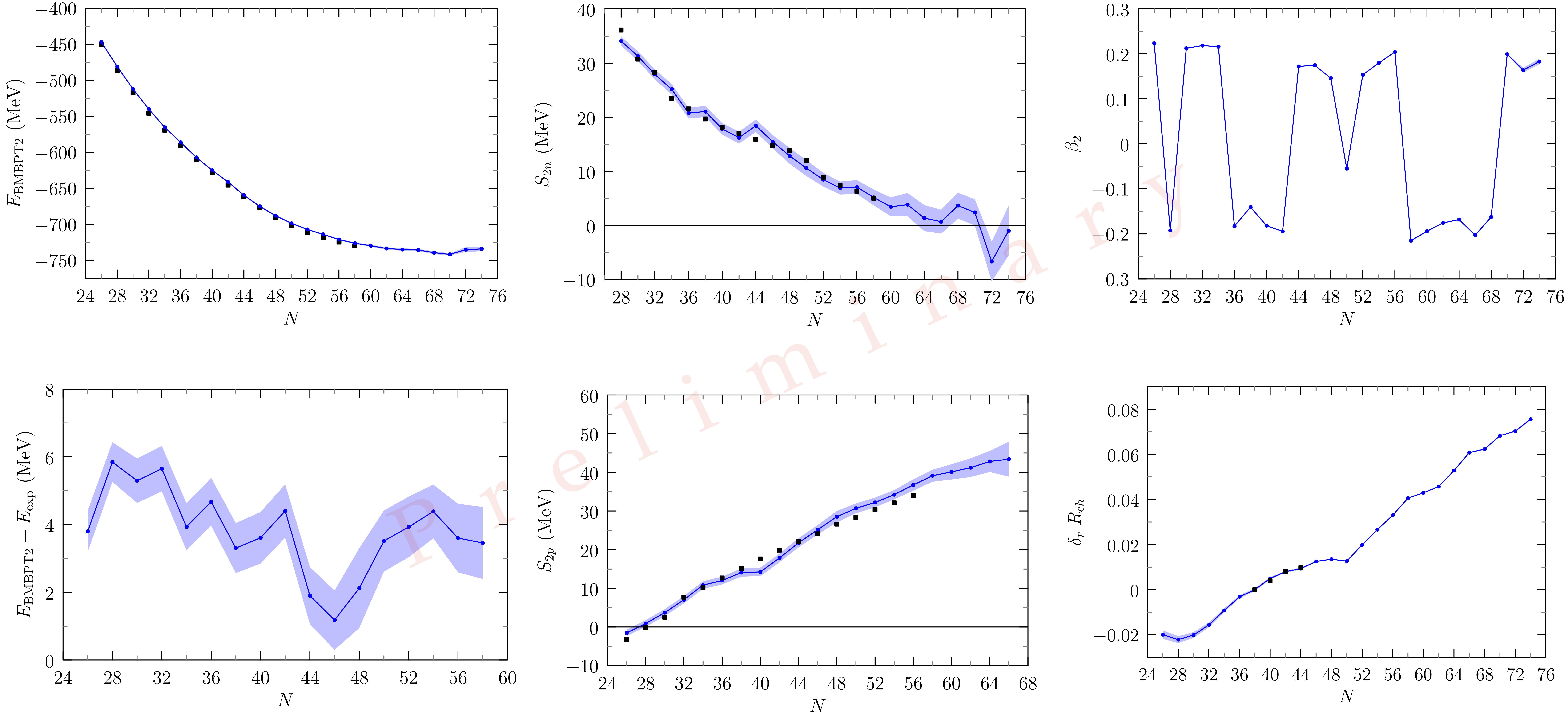
BMBPT2 systematics — Titanium (Z=22)

[Durel *et al.*, in preparation]



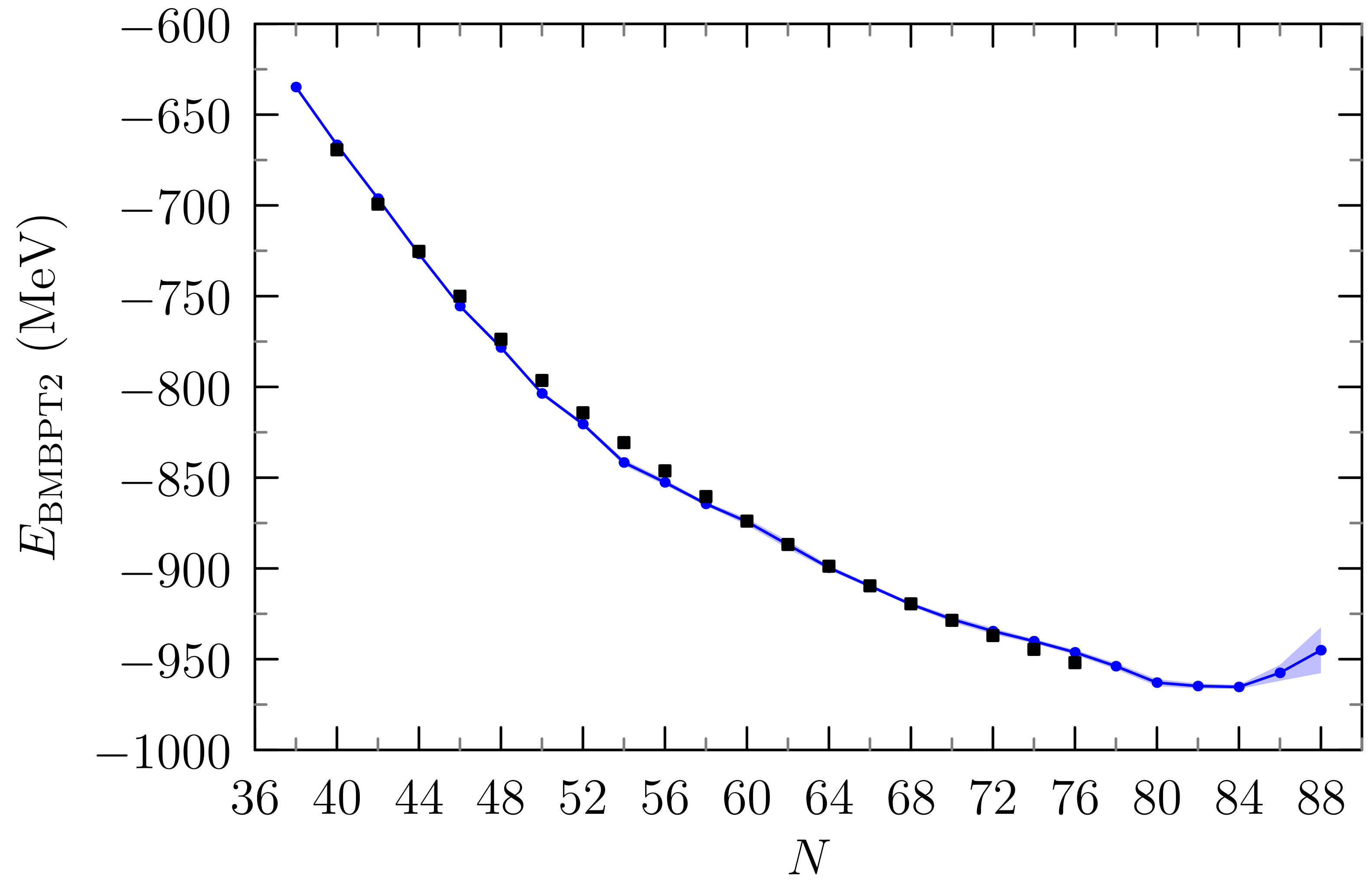
BMBPT2 systematics — Germanium (Z=32)

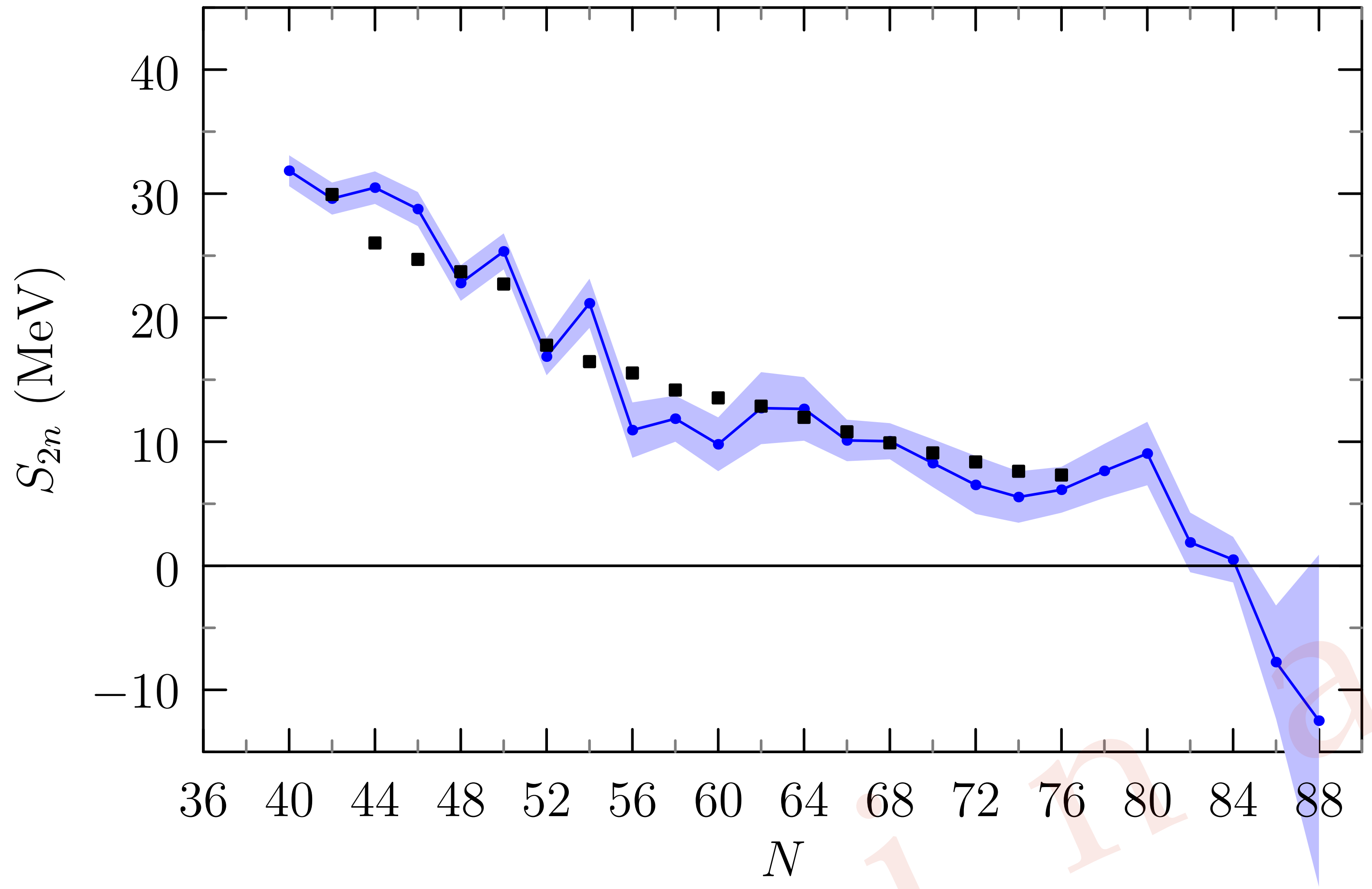
[Durel *et al.*, in preparation]

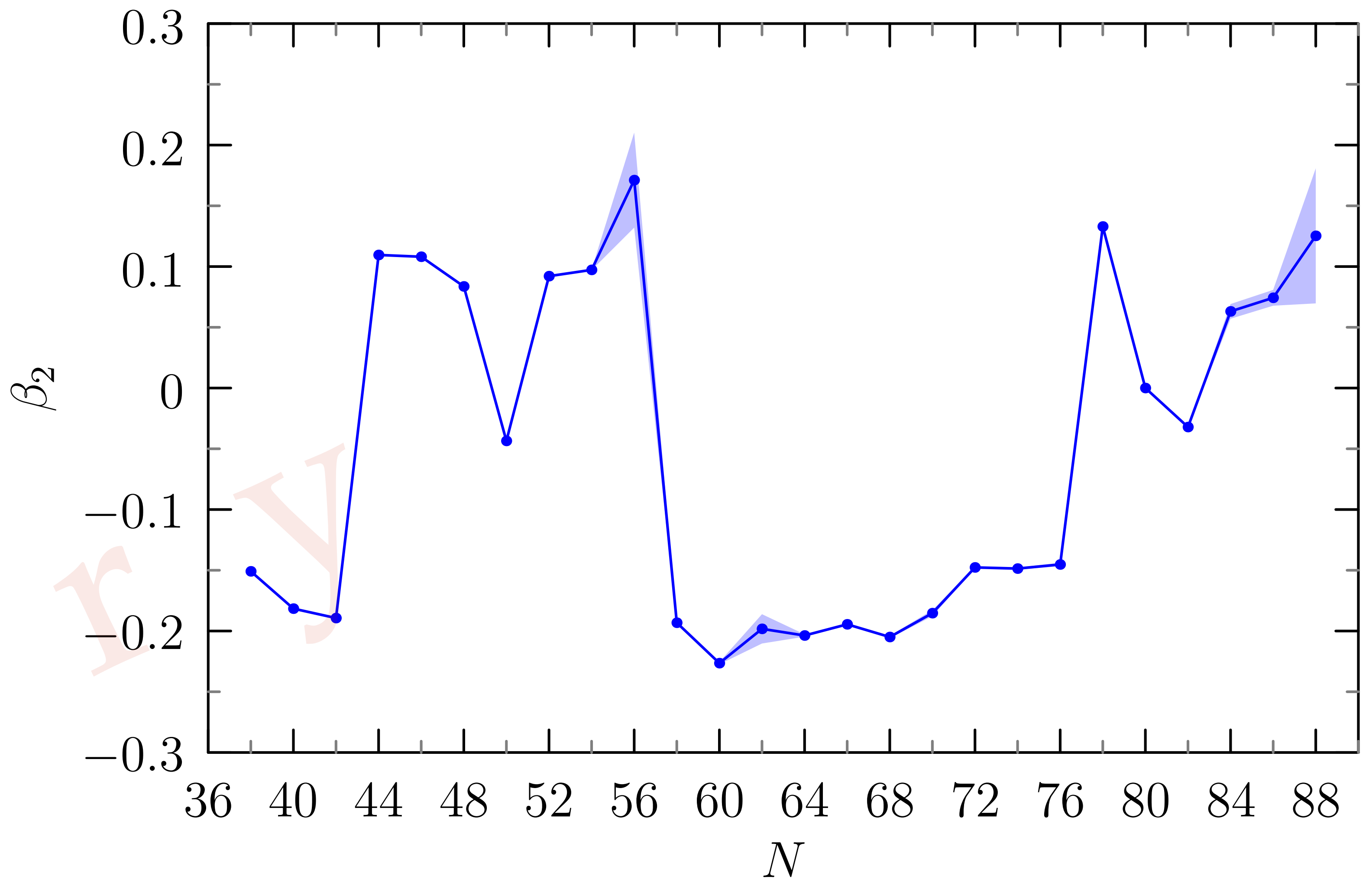


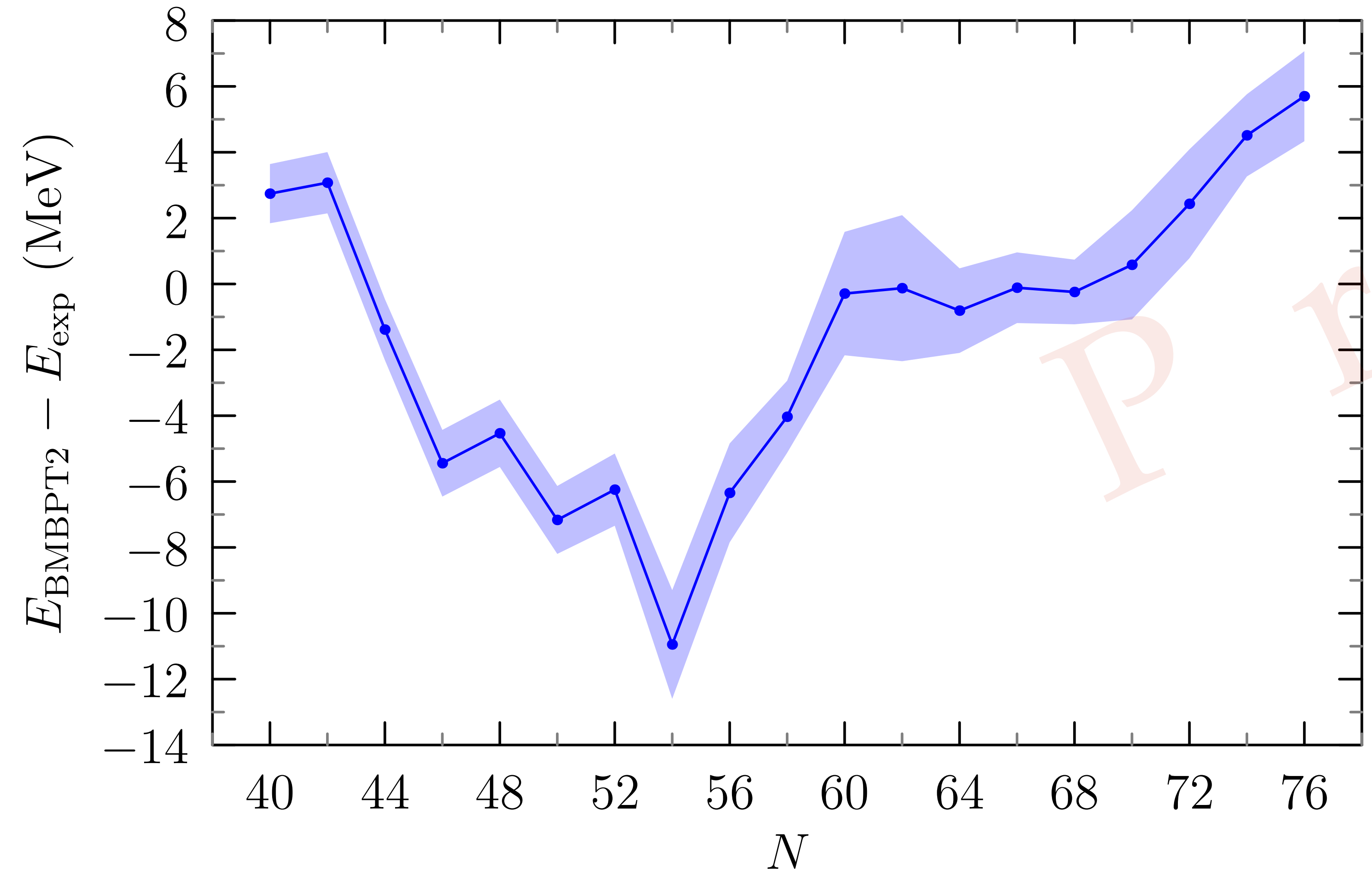
BMBPT2 systematics — Molybdenum (Z=42)

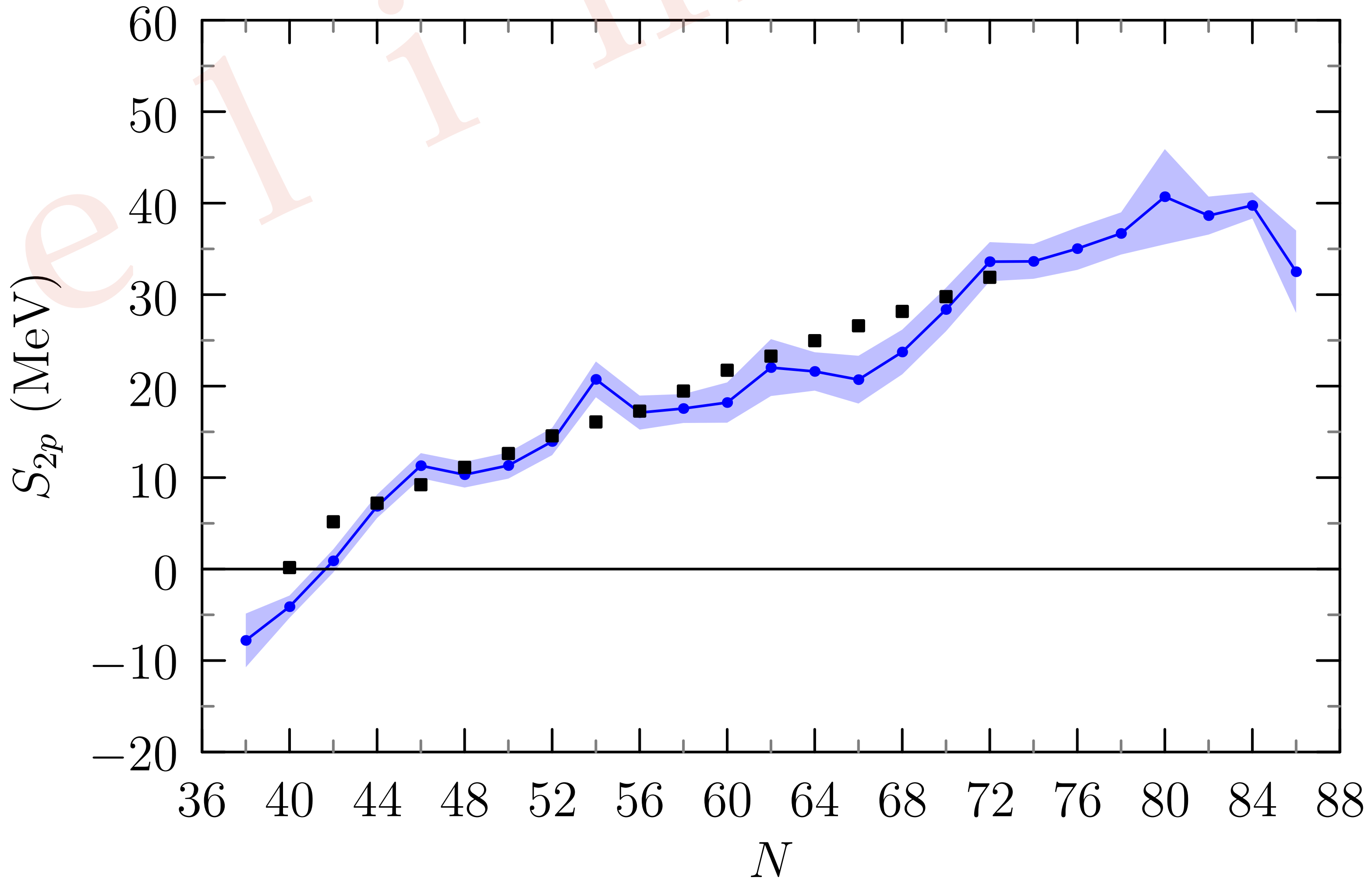
[Durel *et al.*, in preparation]

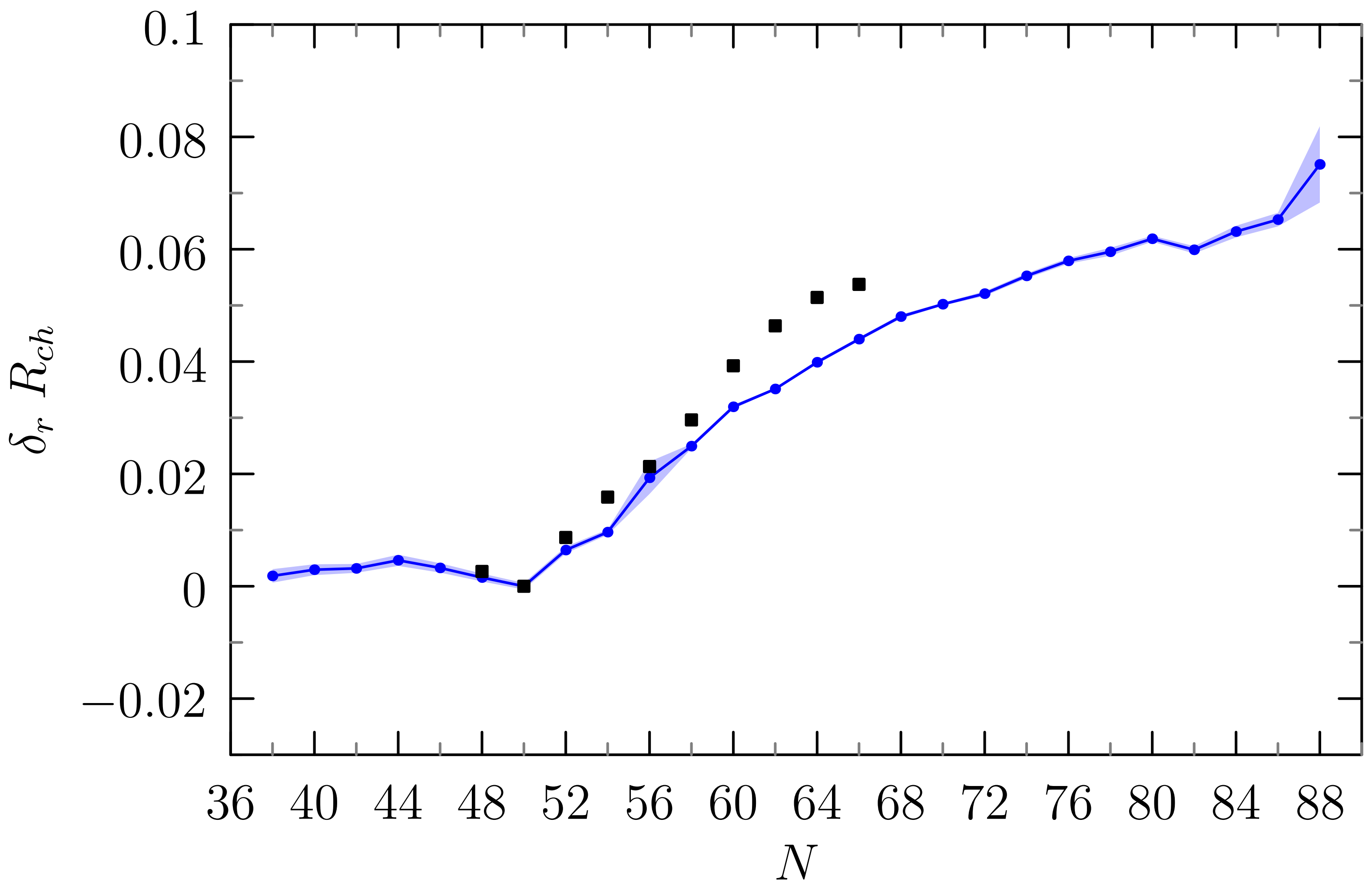






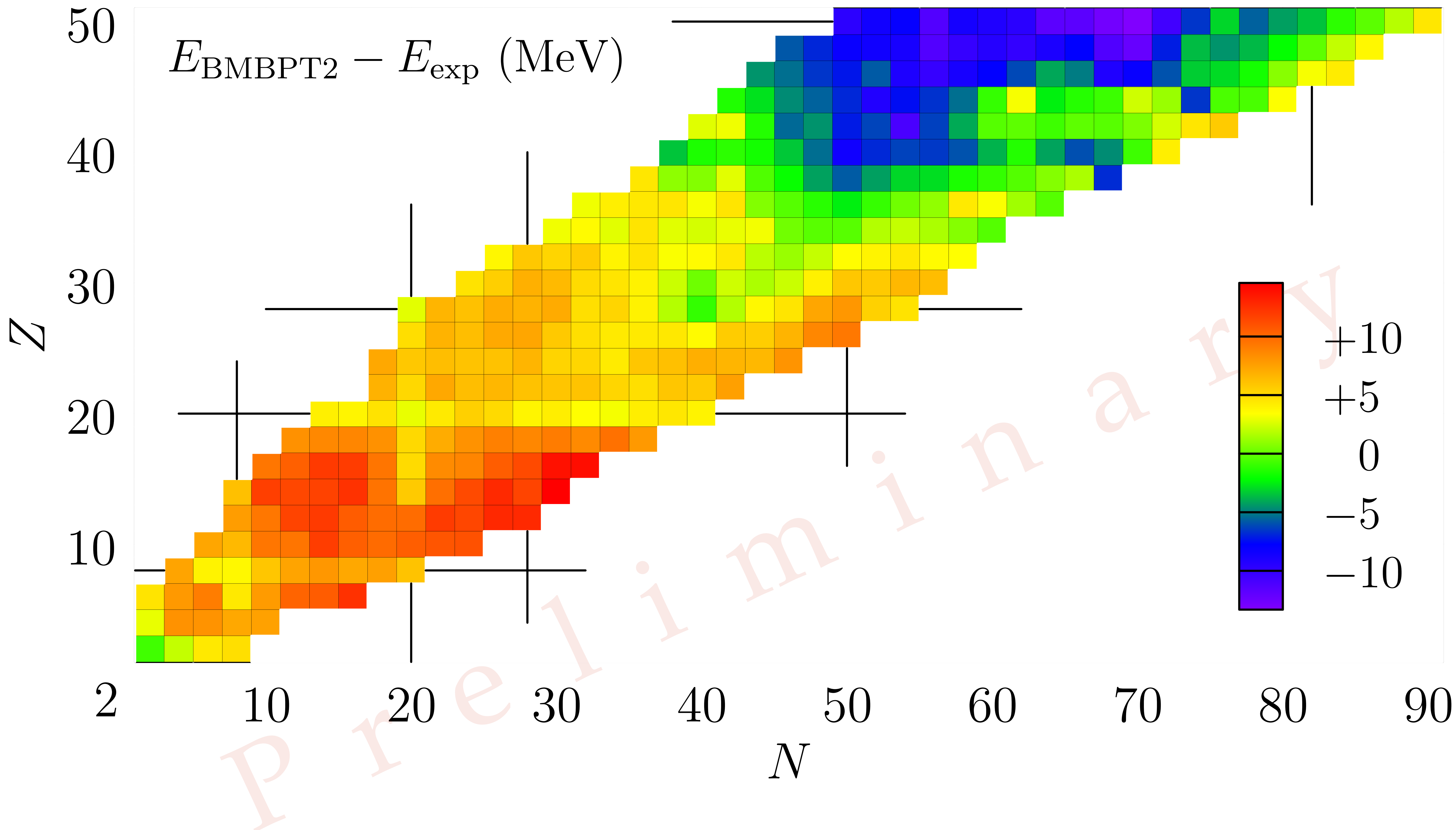






Preliminary

BMBPT2 systematics — Deviation to data

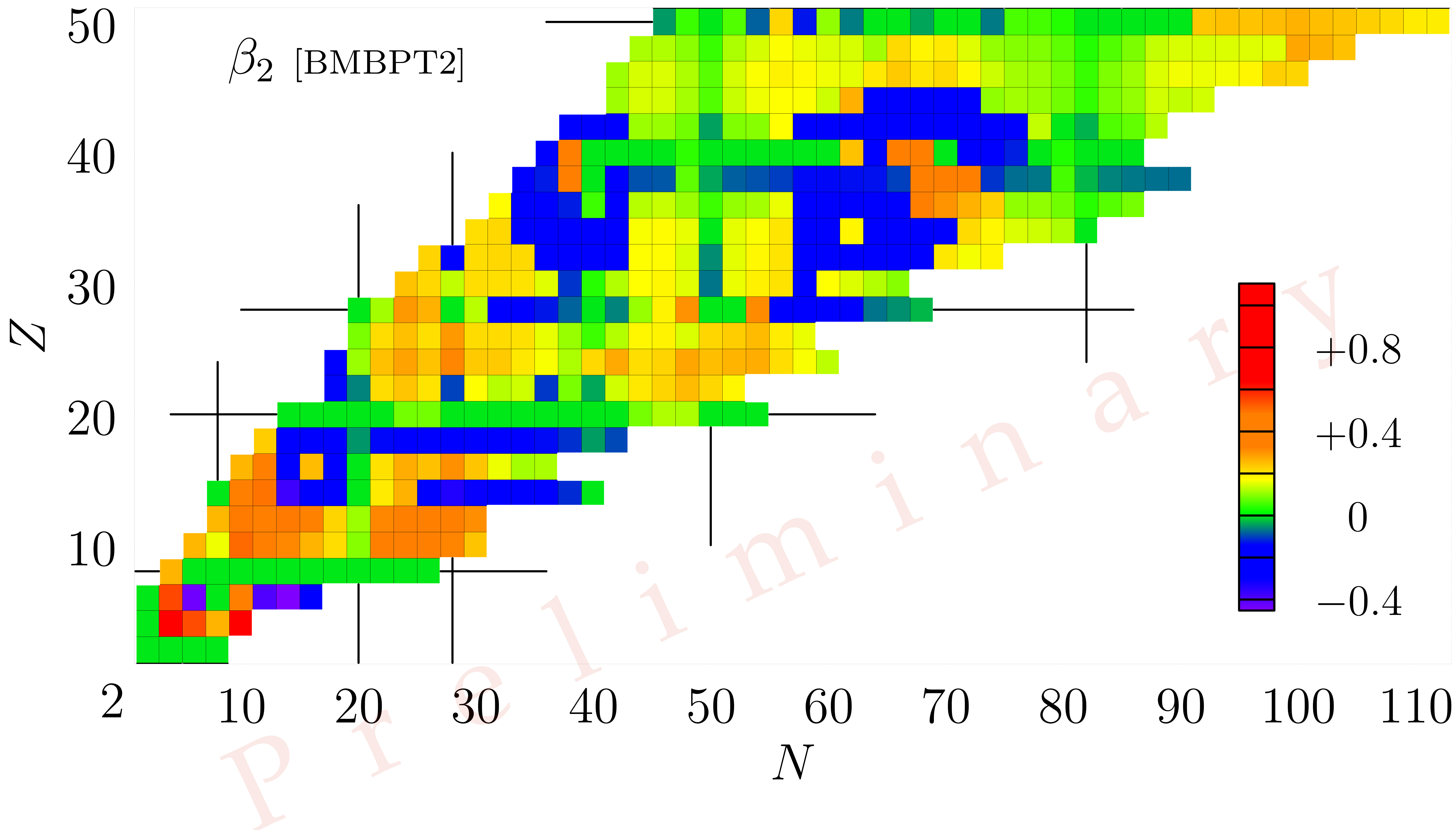


Preliminary

[Durel *et al.*, in preparation]

- ○ BMBPT2 **more bound** w.r.t. data as A increases → consistent with previous studies (e.g. Arthuis *et al.* 2024)
- ○ For large Z, BMBPT2 **less bound** w.r.t. data for neutron-rich isotopes → cf. Hu *et al.* 2025
- ○ Semi-magic chains systematically more bound by few MeV → **missing angular-momentum projection**?

BMBPT2 systematics — Deformation map



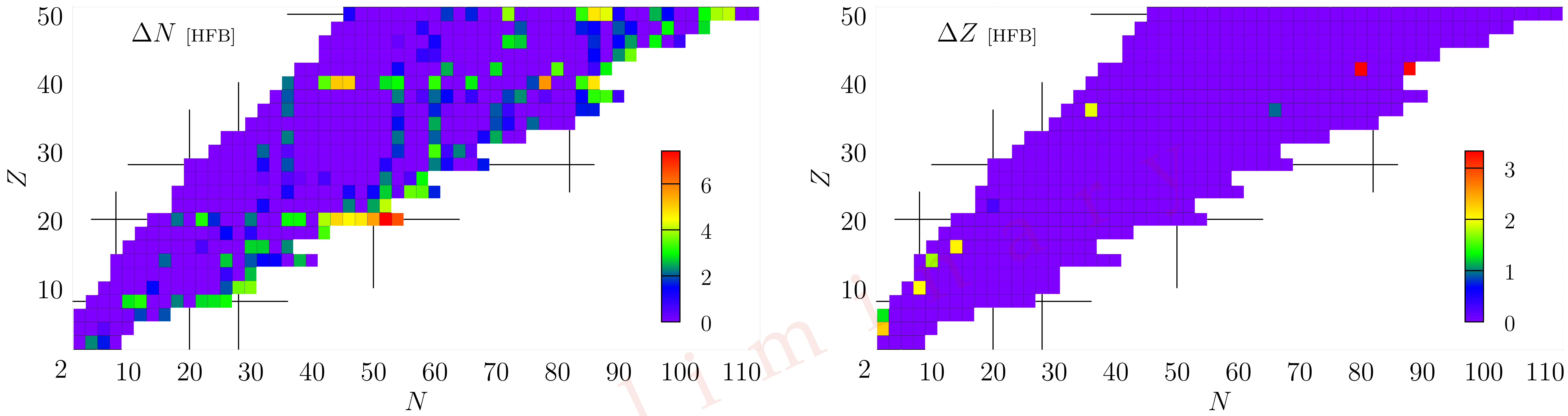
Preliminary

[Durel *et al.*, in preparation]

- ○ Spherical solutions around **shell closures**
- ○ **Known region of deformation** visible (e.g. “islands of inversion”)
- ○ Qualitatively consistent with EDF systematics (e.g. Bender *et al.* 2006)

BMBPT2 systematics — Pairing map

[Durel *et al.*, in preparation]



preliminary

- **Deformation dominates** over pairing
- Confirms earlier indications that **ab initio Hamiltonians generate little pairing**
- **Neutron** pairing active mainly along some isotopic/isotonic chains
- **Proton** pairing almost absent

2. SCGF

Self-consistent Green's function approach

Green's functions

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle \Psi^A_0 | \mathcal{T}[a_\alpha(t_\alpha) a^\dagger_\beta(t_\beta)] | \Psi^A_0 \rangle$$

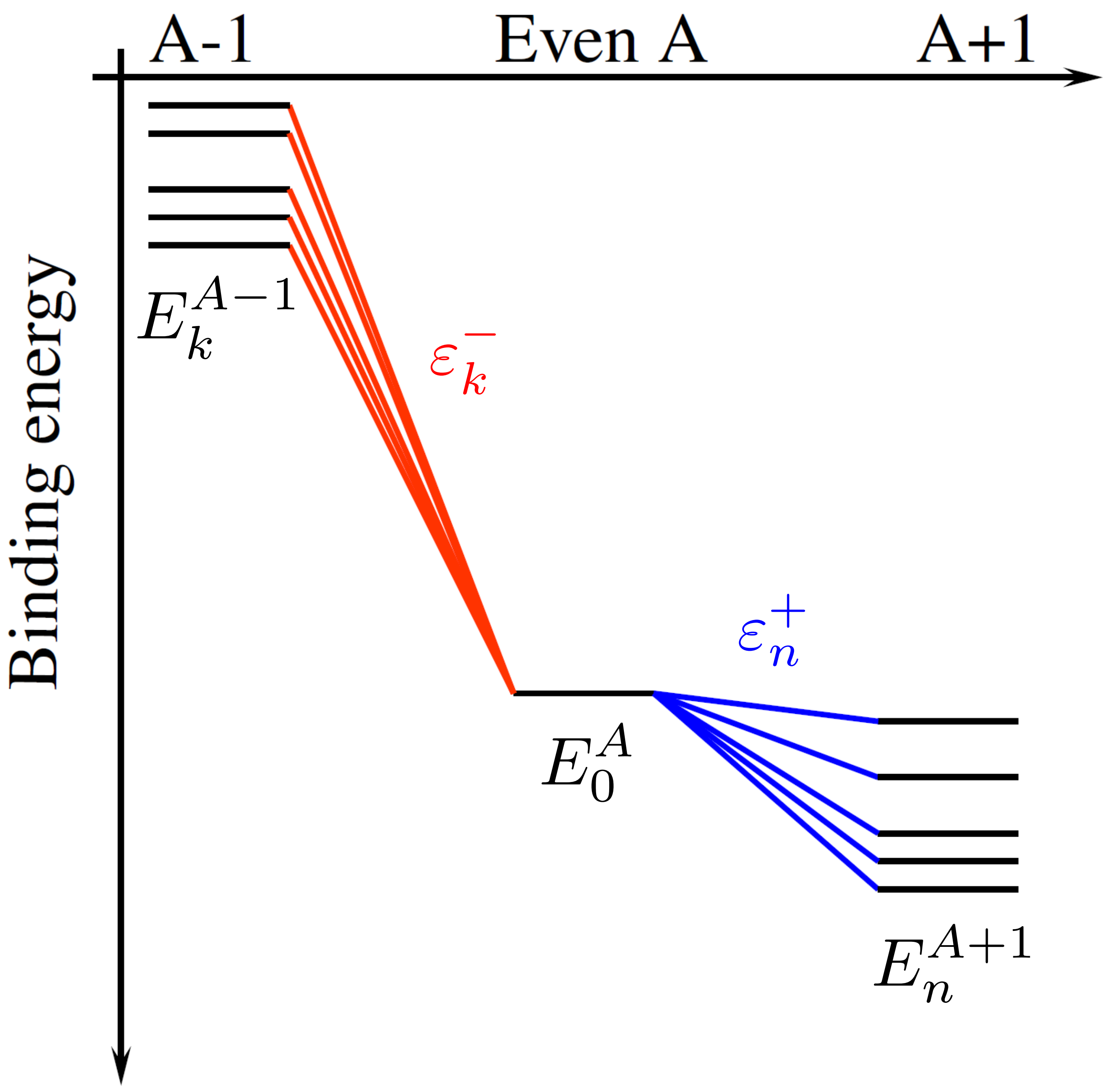
$$\mathrm{i}\, g^{4-\mathrm{pt}}_{\alpha\gamma\beta\delta}(t_\alpha, t_\gamma, t_\beta, t_\delta) \equiv \langle \Psi^A_0 | \mathcal{T}[a_\gamma(t_\gamma) a_\alpha(t_\alpha) a^\dagger_\beta(t_\beta) a^\dagger_\delta(t_\delta)] | \Psi^A_0 \rangle$$

$$\dots$$

Dyson equation

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) + \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, \Sigma^\star_{\gamma\delta}(\omega)\, g_{\delta\beta}(\omega)$$

Self-energy expansion → Many-body approximations



$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}^n_\alpha)^* \mathcal{X}^n_\beta}{\omega - \varepsilon^+_n + i\eta} + \sum_k \frac{\mathcal{Y}^k_\alpha (\mathcal{Y}^k_\beta)^*}{\omega - \varepsilon^-_k - i\eta}$$

Separation energies

$$\varepsilon^+_n = E^{A+1}_n - E^A_0$$

$$\varepsilon^-_k = E^A_0 - E^{A-1}_k$$

Transition amplitudes

$$\mathcal{X}^n_\alpha = \langle \Psi^{\text{A+1}}_n | a^\dagger_\alpha | \Psi^{\text{A}}_0 \rangle$$

$$\mathcal{Y}^k_\alpha = \langle \Psi^{\text{A-1}}_k | a_\alpha | \Psi^{\text{A}}_0 \rangle$$

Kallén-Lehmann spectral representation

Three different implementations

- Spherical Dyson (**sDSCGF**)
- Spherical Gorkov (**sGSCGF**)
- Deformed Dyson (**dDSCGF**)

→ Symmetry restoration still missing

Self-energy expansion

- Exact self-energy can be expanded and decomposed as

Static self-energy

$$\Sigma^{*}_{\alpha\beta}(\omega) = \Sigma^{(n=1)}_{\alpha\beta}(\omega) + \Sigma^{(n>1)}_{\alpha\beta}(\omega) \equiv \Sigma^{(\infty)}_{\alpha\beta} + \tilde{\Sigma}_{\alpha\beta}(\omega)$$

Dynamic self-energy

- **Dynamic** (energy-dependent) self-energy also displays a spectral representation

$$\widetilde{\Sigma}_{\alpha\beta}(\omega) = \sum_{j} \frac{\mathcal{M}^{\dagger}_{\alpha j}\,\mathcal{M}_{j\beta}}{\omega - \mathcal{E}^{+}_{j} + i\eta} + \sum_{k} \frac{\mathcal{N}_{\alpha k}\,\mathcal{N}^{\dagger}_{k\beta}}{\omega - \mathcal{E}^{-}_{k} - i\eta} \xrightarrow{\textbf{Dyson eq. in matrix form}} \varepsilon_i \begin{pmatrix} \mathcal{Z}^{i}_{\alpha} \\ \mathcal{W}^{i}_{j} \\ \mathcal{W}^{i}_{k} \end{pmatrix} = \begin{pmatrix} h^{(0)}_{\alpha\delta} + \Sigma^{(\infty)}_{\alpha\delta} & \mathcal{M}^{\dagger}_{\alpha j} & \mathcal{N}_{\alpha k} \\ \mathcal{M}_{j\delta} & \mathcal{E}^{+}_{j} & 0 \\ \mathcal{N}^{\dagger}_{k\delta} & 0 & \mathcal{E}^{-}_{k} \end{pmatrix} \begin{pmatrix} \mathcal{Z}^{i}_{\delta} \\ \mathcal{W}^{i}_{j} \\ \mathcal{W}^{i}_{k} \end{pmatrix}$$

A+1 configurations

A-1 configurations

- Self-energy approximated via the **Algebraic Diagrammatic Construction** (ADC)

1. Rewrite exact self-energy as

$$\widetilde{\Sigma}^{(\mathrm{ADC})}_{\alpha\beta}(\omega) = \sum_{jj'} M^{\dagger}_{\alpha j} \left[\frac{1}{\omega\mathbb{1} - (E^{>} + C) + i\eta\mathbb{1}} \right]_{jj'} M_{j'\beta} + \sum_{kk'} N_{\alpha k} \left[\frac{1}{\omega\mathbb{1} - (E^{<} + D) - i\eta\mathbb{1}} \right]_{kk'} N^{\dagger}_{k'\beta}$$

Non-diagonal energy matrices

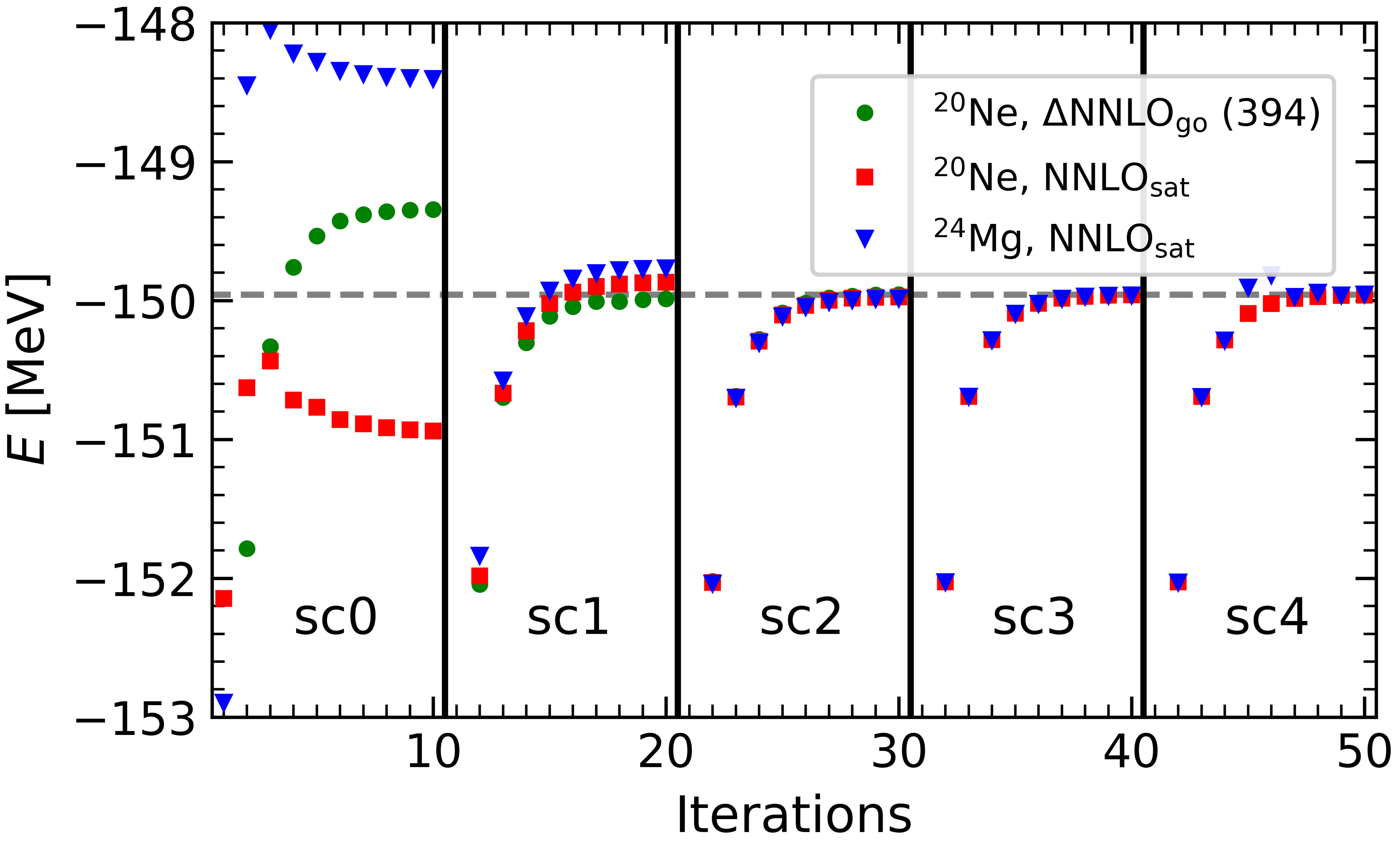
[Schirmer 1982]

2. Expand *M*, *N*, *C* & *D* in perturbation → Combine them to construct ADC at order *n*, i.e. **ADC(*n*)**
3. Determine *M*, *N*, *C* & *D* by requiring that ADC(*n*) contains standard **perturbative expansion up to order *n***

Self-energy expansion

Self-consistency

[Scalesi 2024]



Converged result independent of the reference state

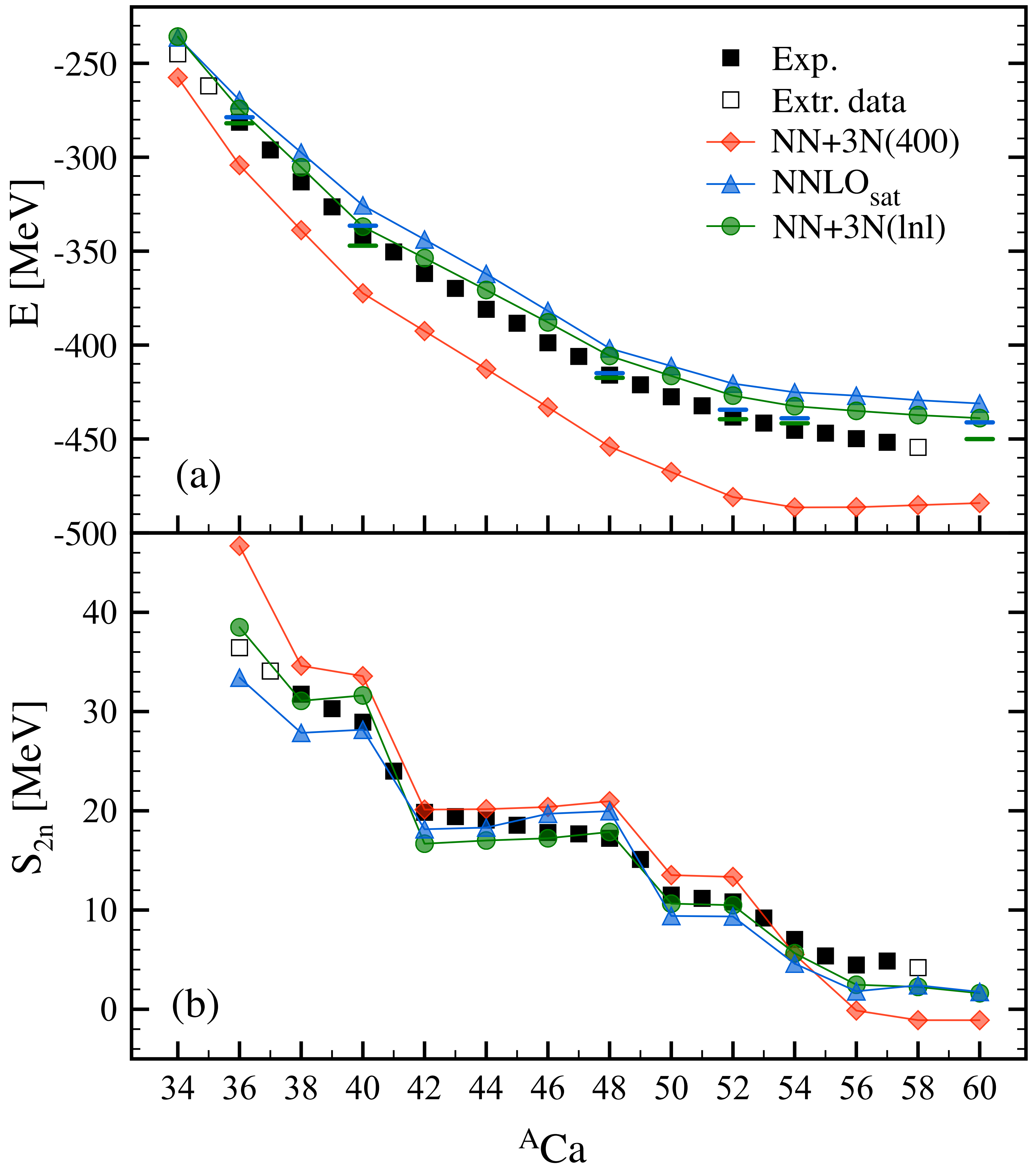
Available schemes

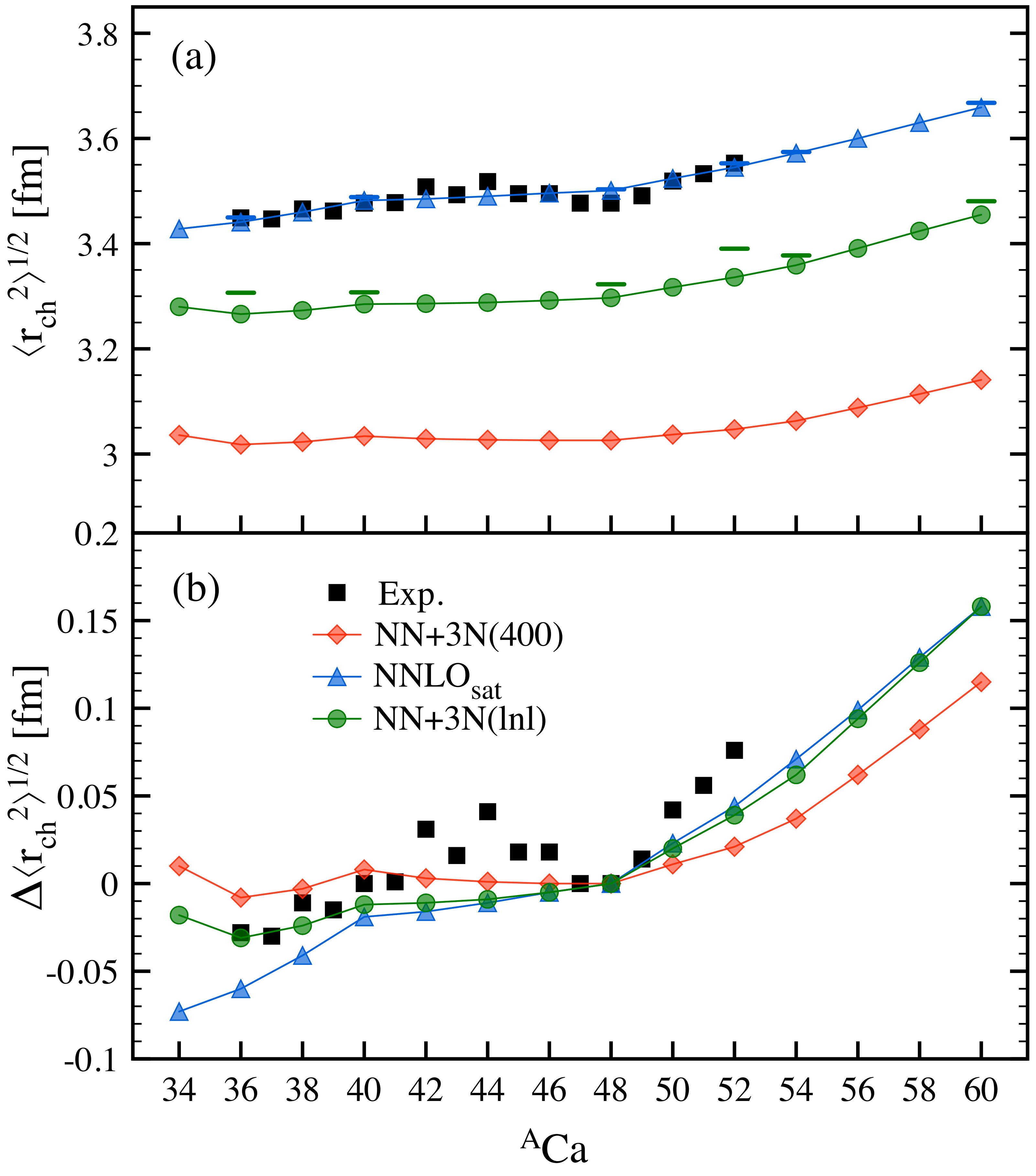
	ADC(2)	ADC(3)
sDCSGF	✓	✓
sGCSGF	✓	✗*
dDCSGF	✓	✓

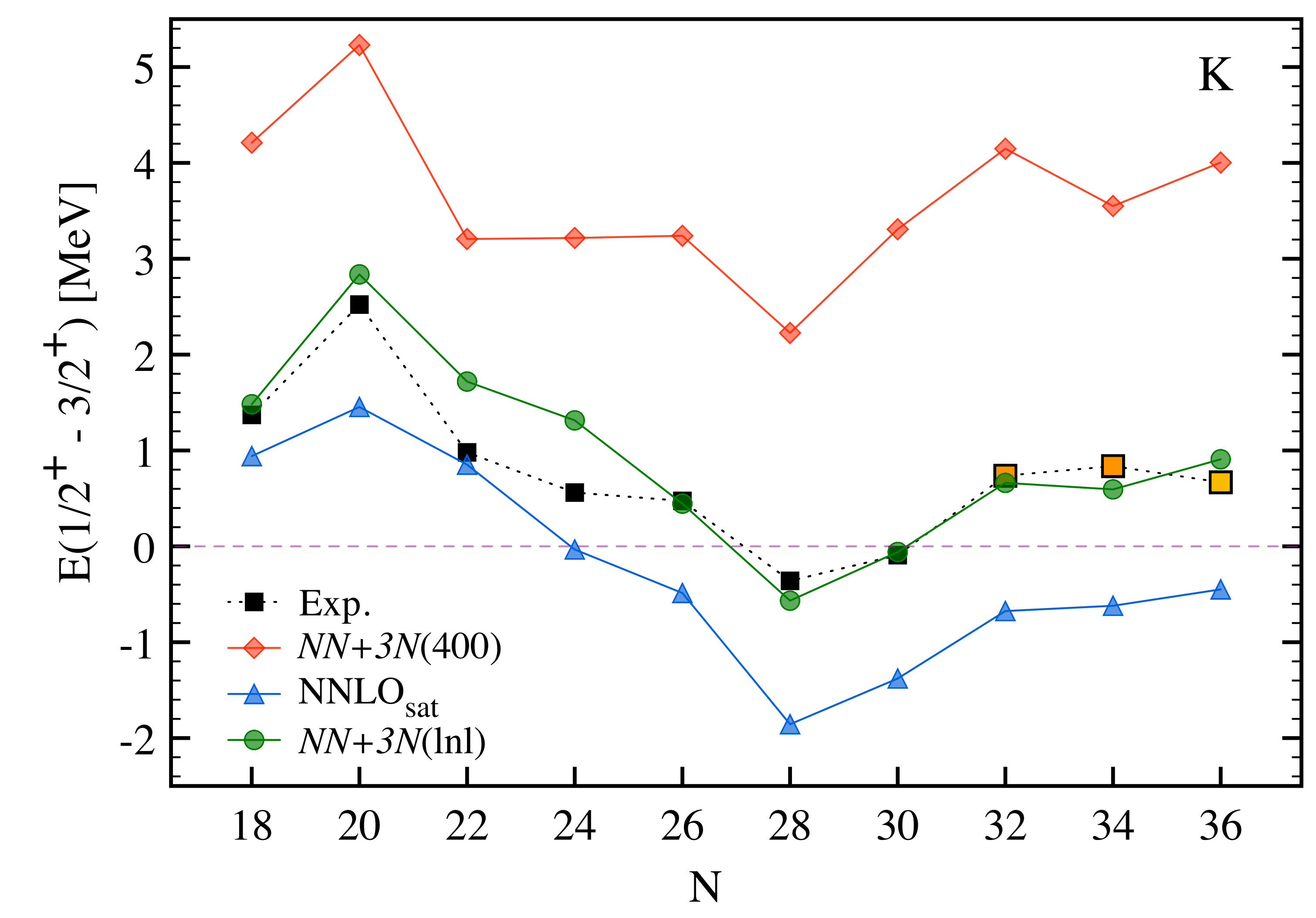
* Formally derived, but not implanted yet

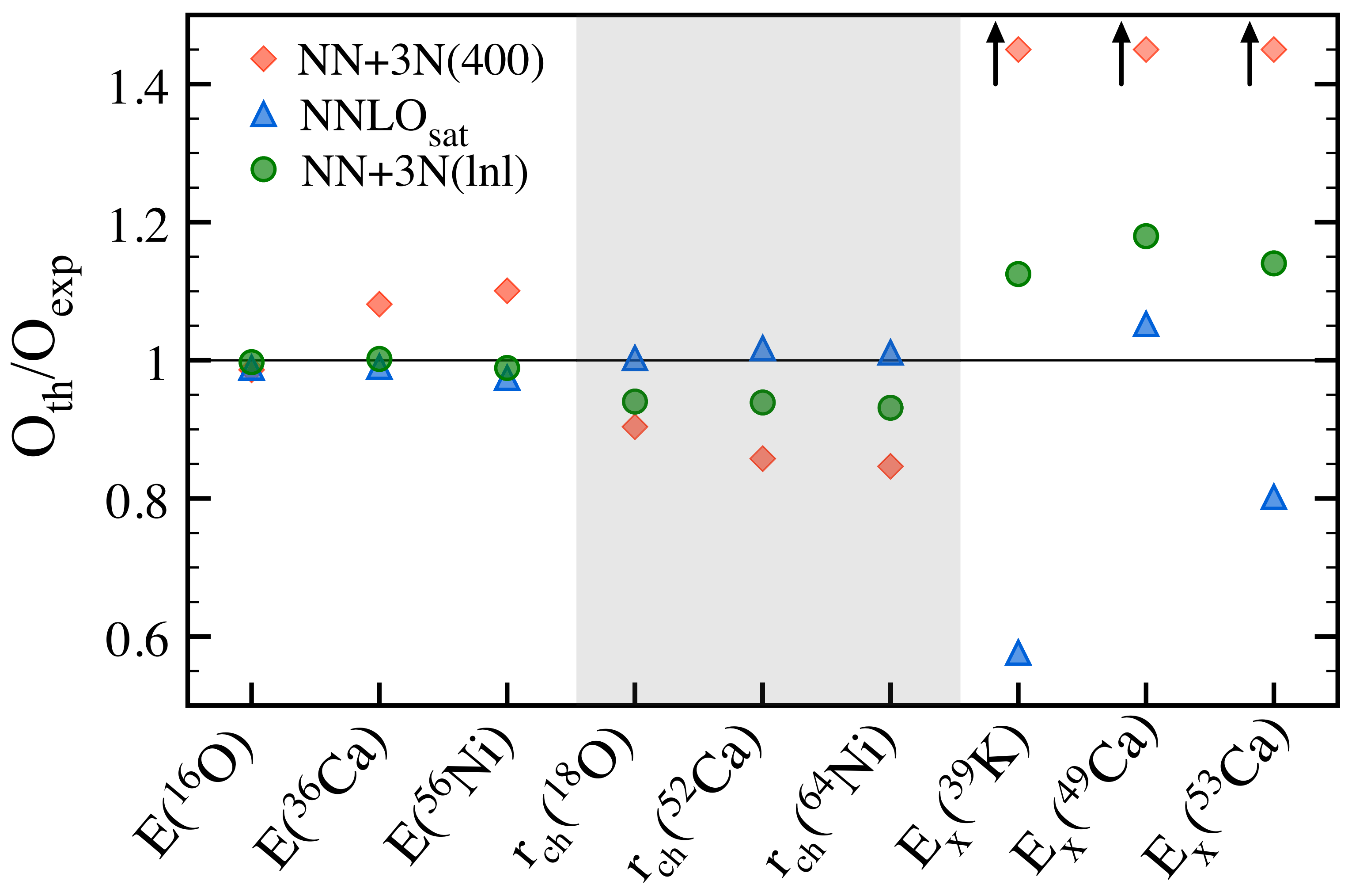
Testing Hamiltonians along semi-magic chains

[Somà *et al.*, 2020]







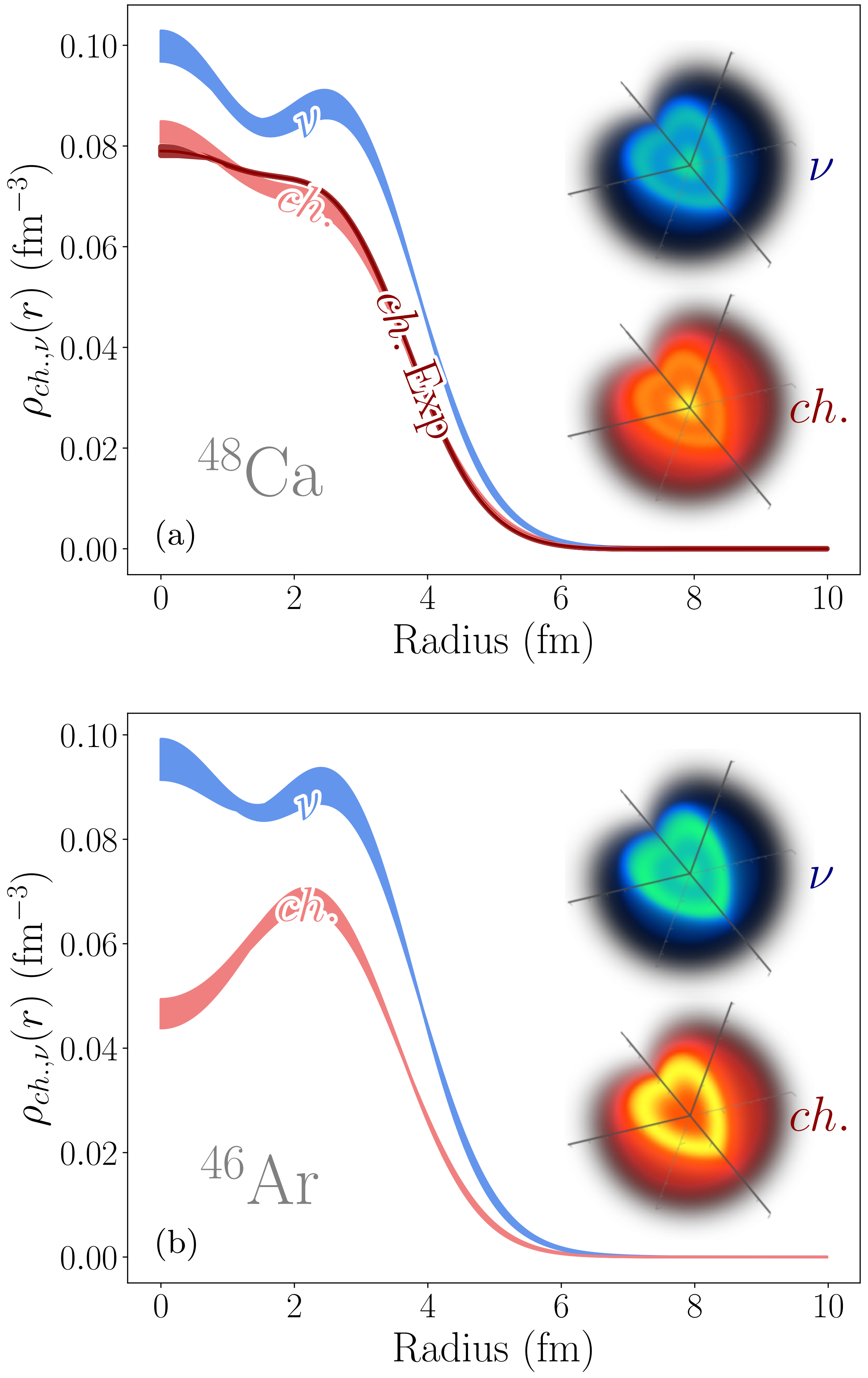


○ **No Hamiltonian** performs well for all observables

○ However, when one does, the description is consistent* along the chain

When radii are fine…

Charge density distributions

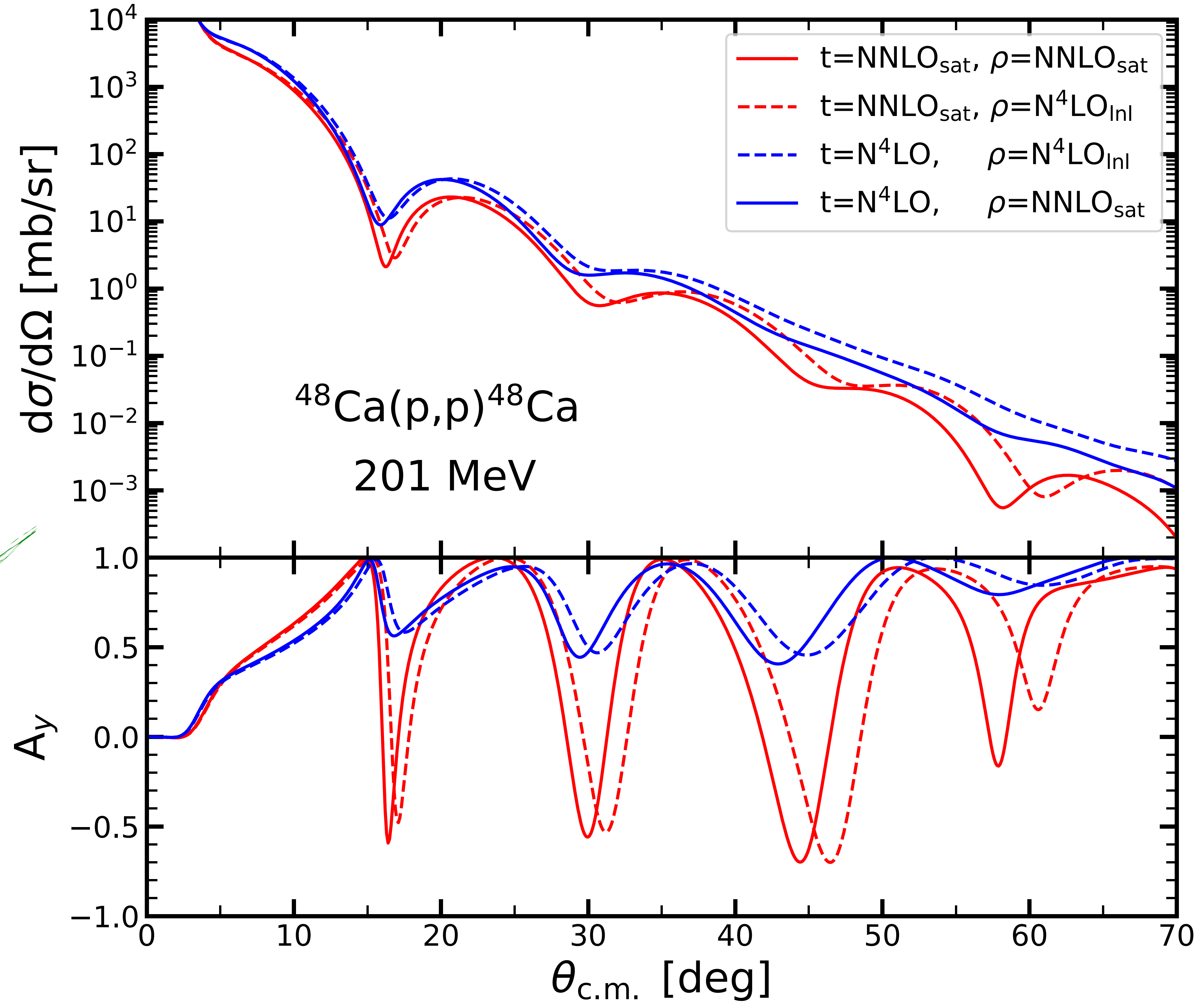


- ○ Good reproduction of ^{48}Ca
- ○ Prediction of a **central depletion** for ^{46}Ar
- ○ Consistent with proton-transfer on ^{46}Ar

[Brugnara *et al.*, 2025]

Optical potentials

[Vorabbi *et al.*, 2024]



- ○ Folding density with NN t-matrix
- ○ Sensitivity to input Hamiltonian
- ○ Data well described for E~50-250 MeV

When radii are fine…

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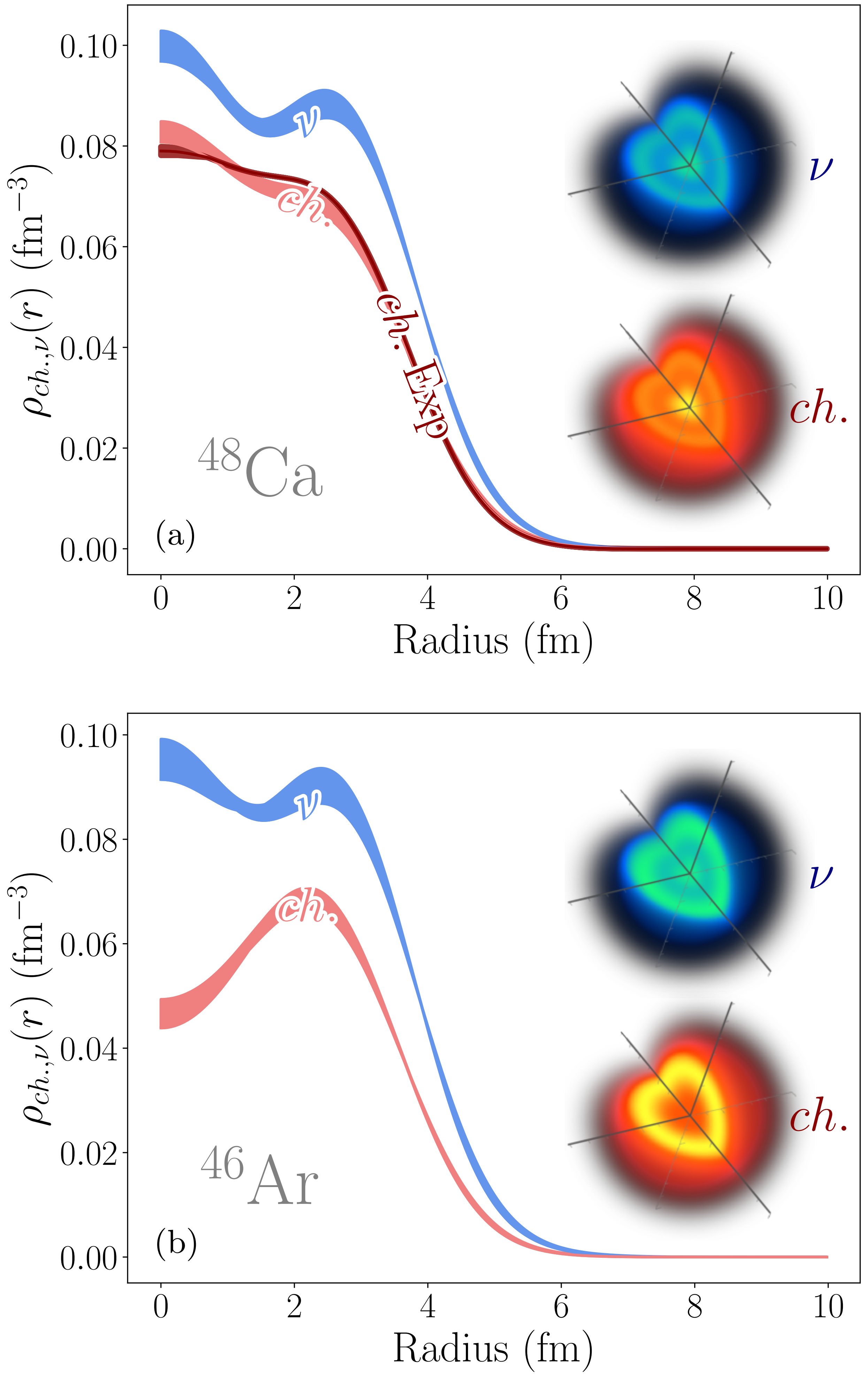

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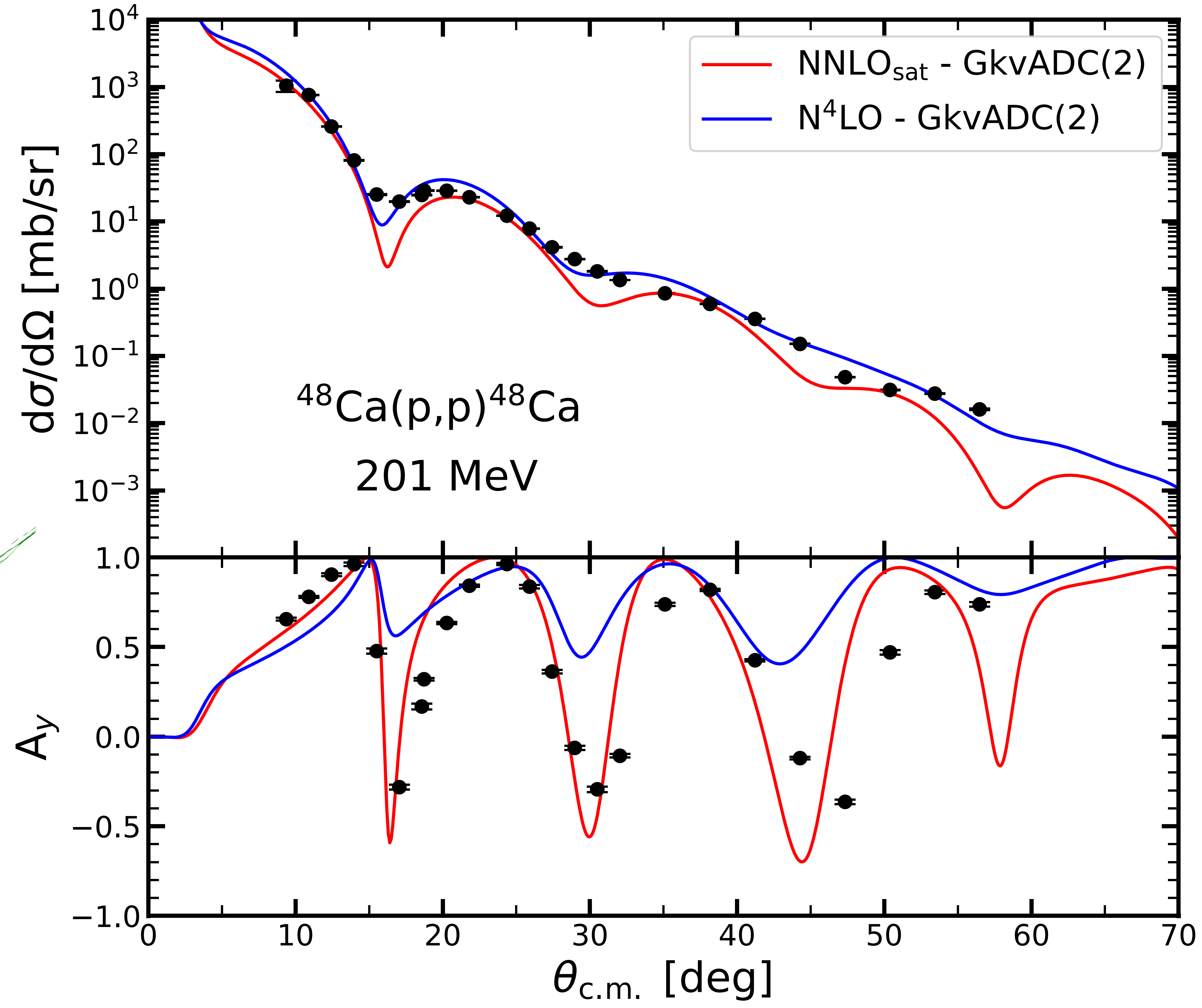

[Vorabbi *et al.*, 2024]

- ○ Folding density with NN t-matrix
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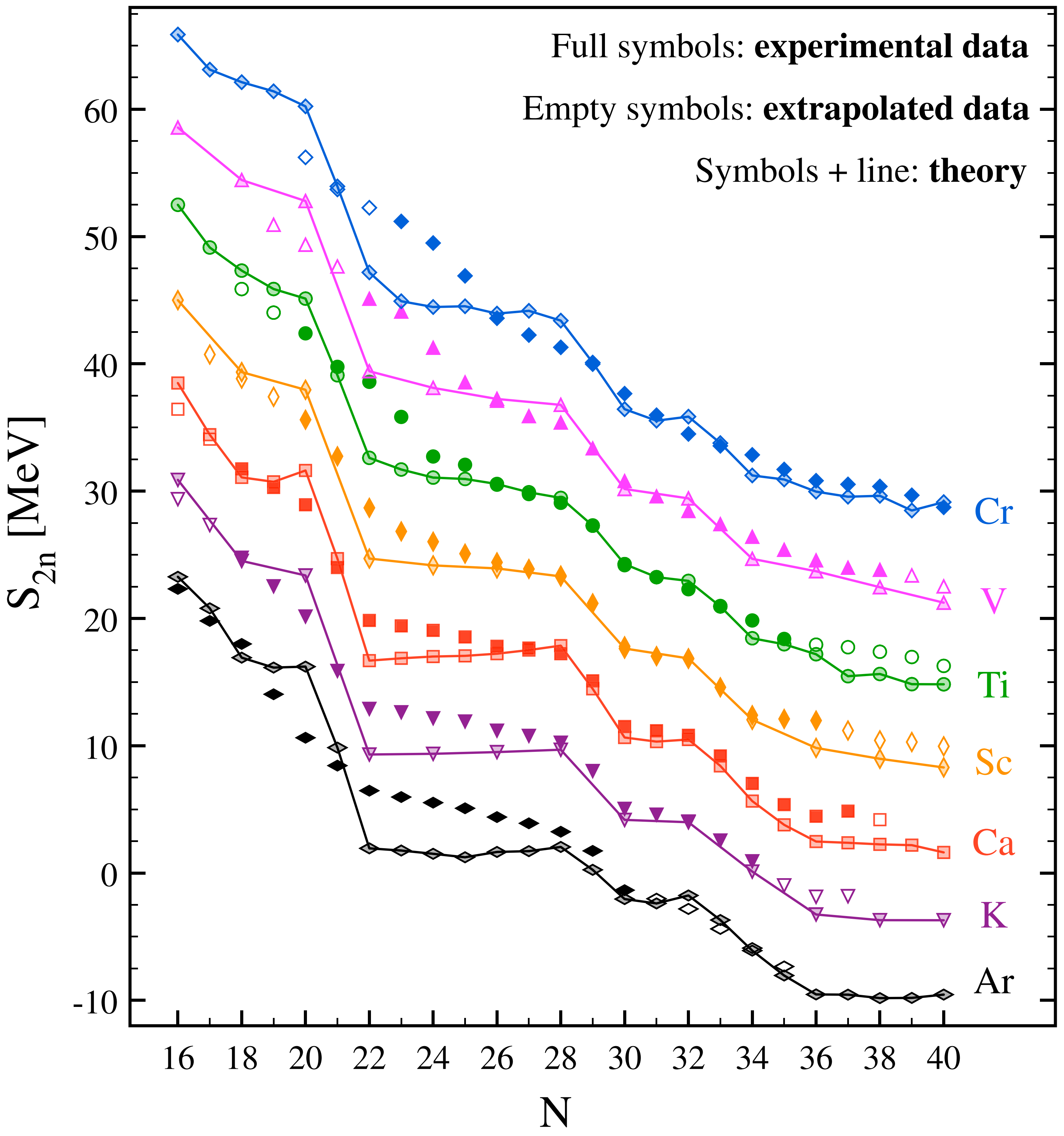
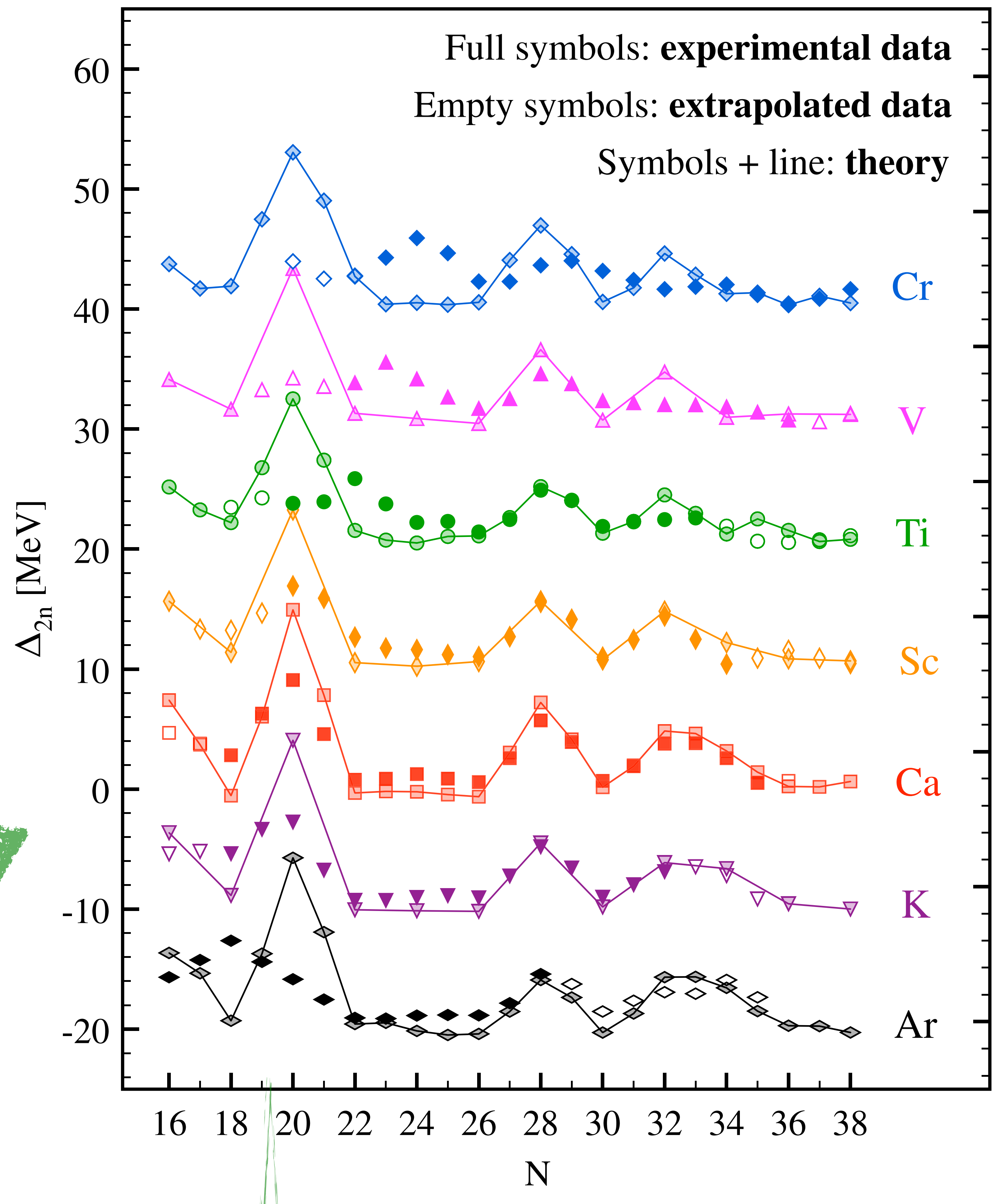
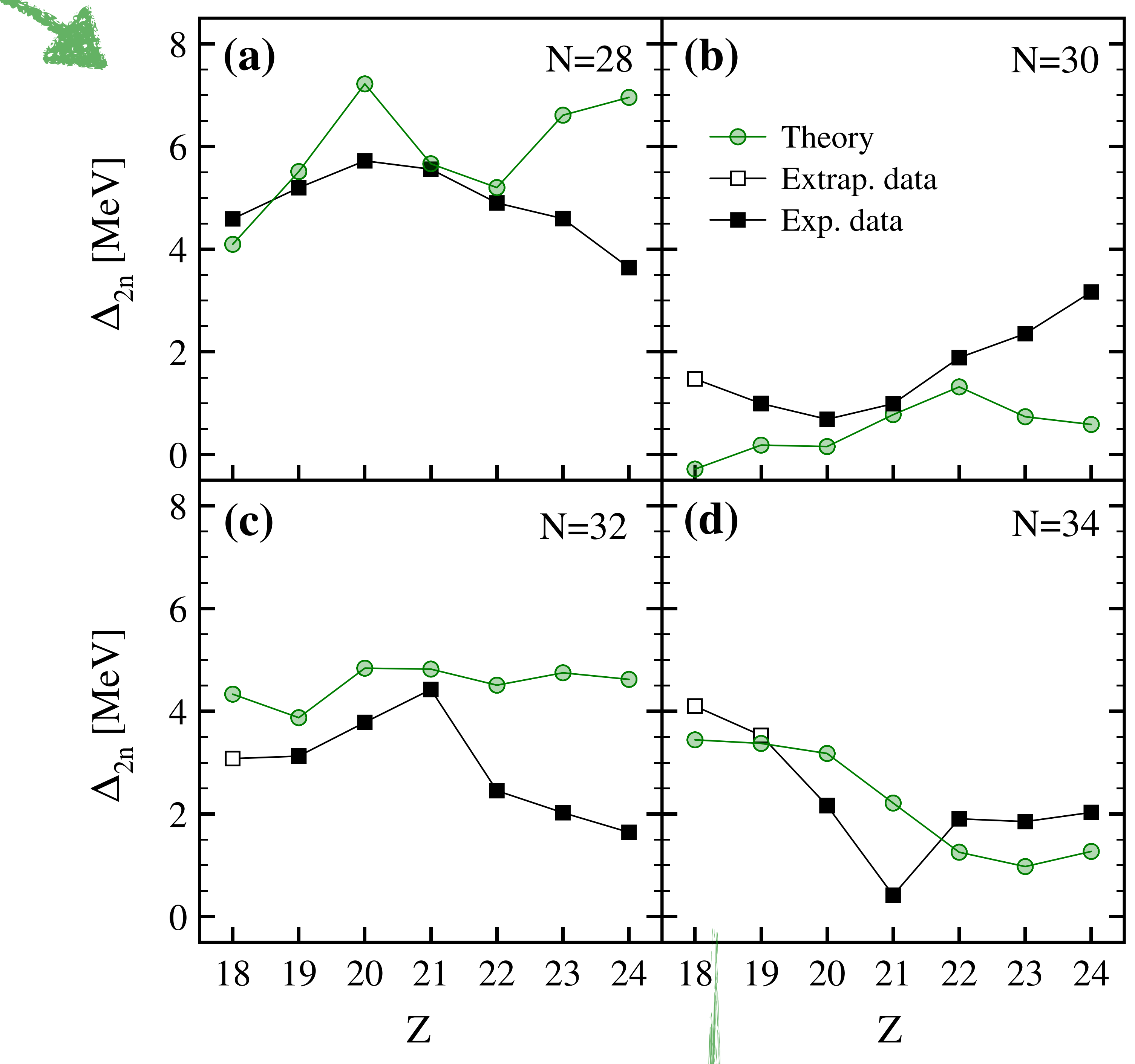
When energies are fine…

⦿ Differential quantities (“mass filters”) reveal the **emergence of magic numbers**

[Somà *et al.*, 2021]







- ○ **Quantitative** reproduction of some (but not all) magic peaks
- ○ **Description deteriorates** away from semi-magic calcium

- ○ Evolution with Z roughly captured

Diagnostic summary

- Rms deviation from experimental data of **ADC(2)** calculations

	Ar	Ca	Ti	Cr
***NN*+3*N*(lnl)**				
E [MeV]	14.1	10.3	14.2	19.2
E/A [MeV]	0.34	0.21	0.29	0.35
S_{2n} [MeV]	2.90	1.56	2.05	2.22
Δ_{2n} [MeV]	3.84	1.96	2.98	2.48
$\langle r^2_{ch} \rangle^{1/2}$ [fm]	0.211	0.219	0.241	0.242
$\delta \langle r^2_{ch} \rangle^{1/2}$ [fm]	0.012	0.023	0.020	0.016
NNLO$_{\text{sat}}$				
$\langle r^2_{ch} \rangle^{1/2}$ [fm]	0.008	0.022	0.019	0.010
$\delta \langle r^2_{ch} \rangle^{1/2}$ [fm]	0.008	0.024	0.023	0.013

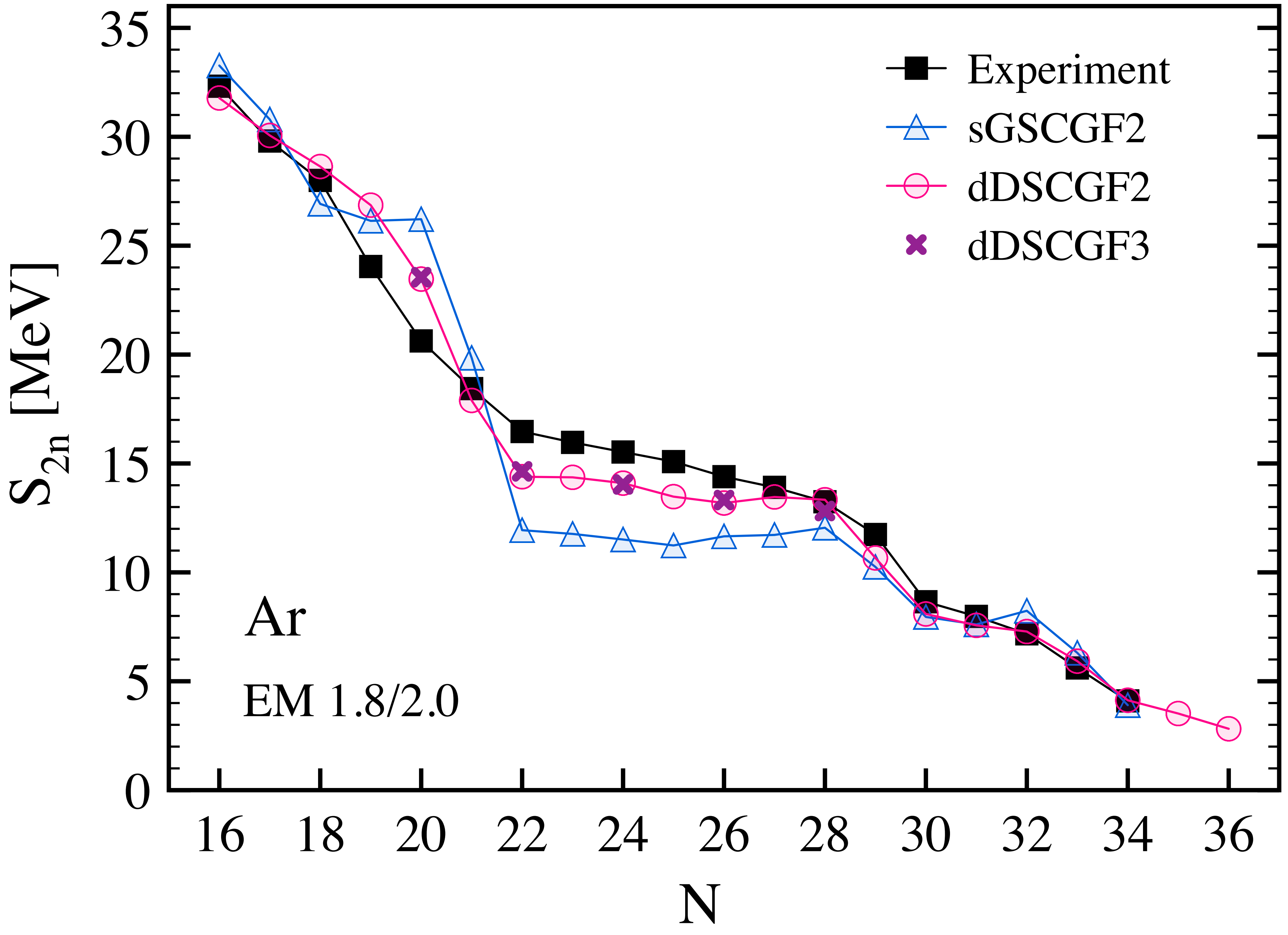
ADC(3)
(sub-shell closures only)

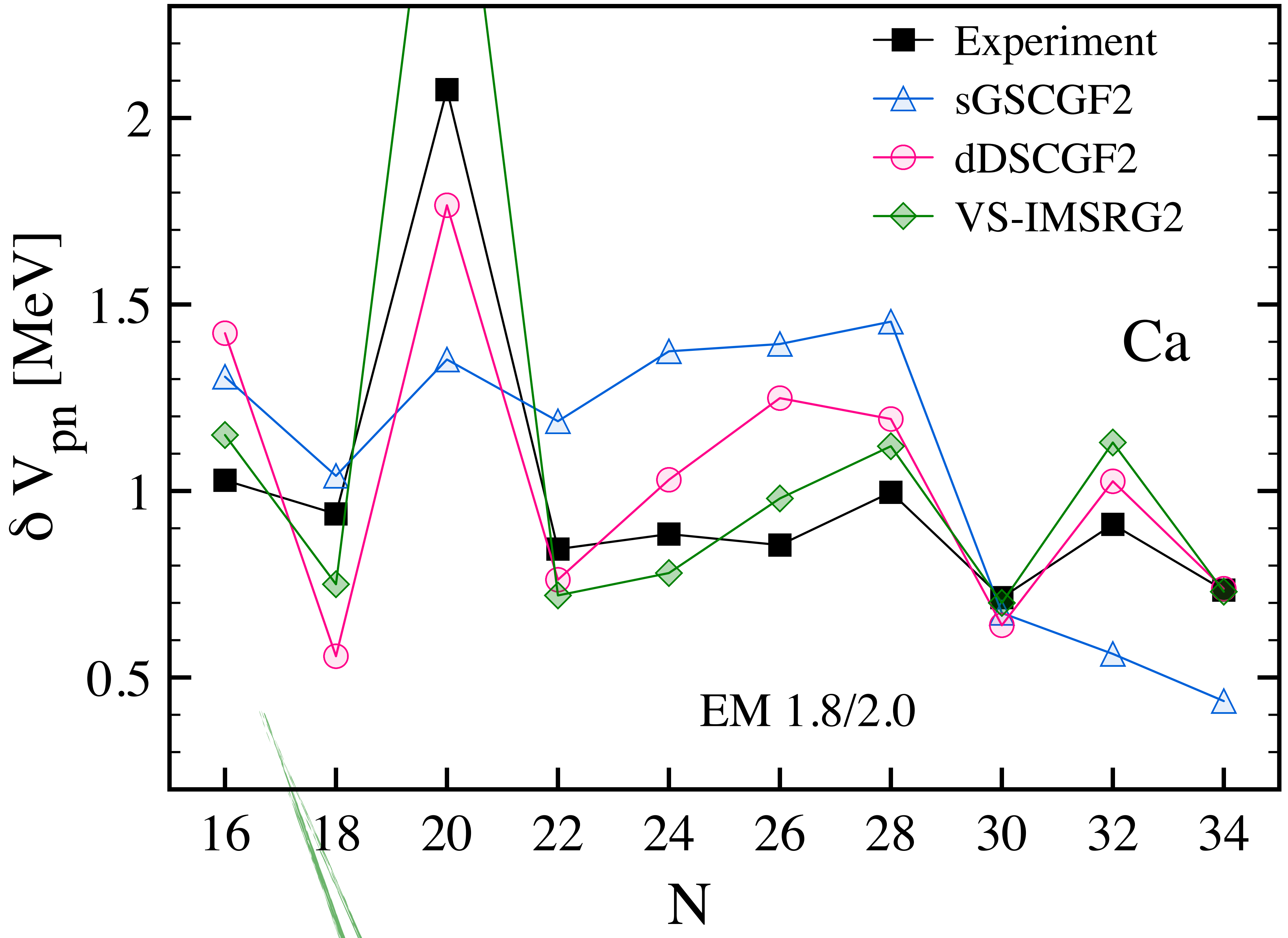
→ 2.5
→ 0.06

Going doubly open-shell — energies

- ⦿ First application of deformed SCGF
  - ○ Flexibility in controlling the breaking of rotational symmetry (**axial**, triaxial, …)
  - ○ Direct access to **odd-even** and **odd-odd** systems (full implementation in progress)

[Scalesi *et al.*, unpublished]





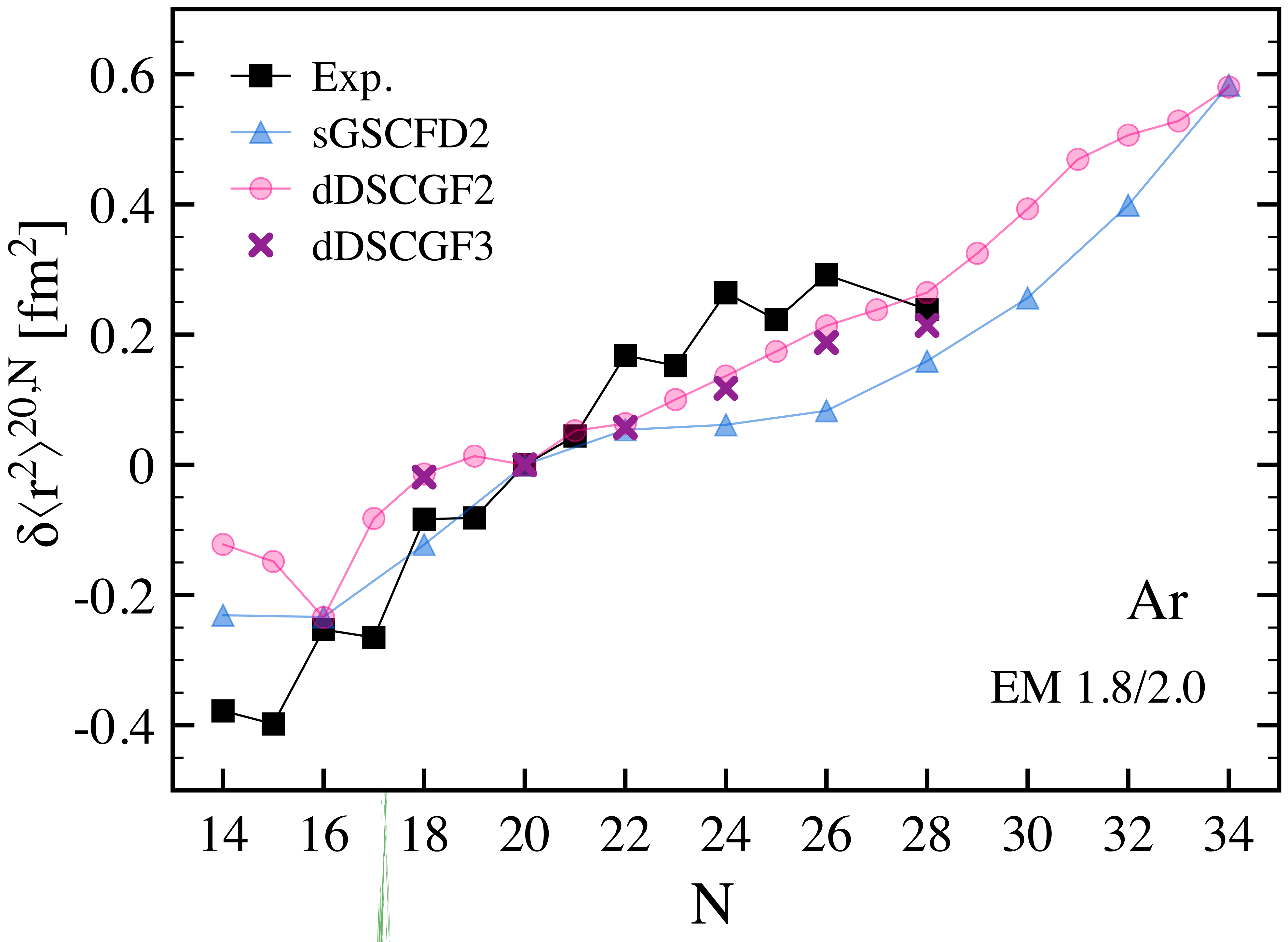
$$\delta V_{\mathrm{pn}}(N,Z) \equiv \frac{1}{4}[S_{2\mathrm{n}}(N,Z) - S_{2\mathrm{n}}(N,Z-2)]$$

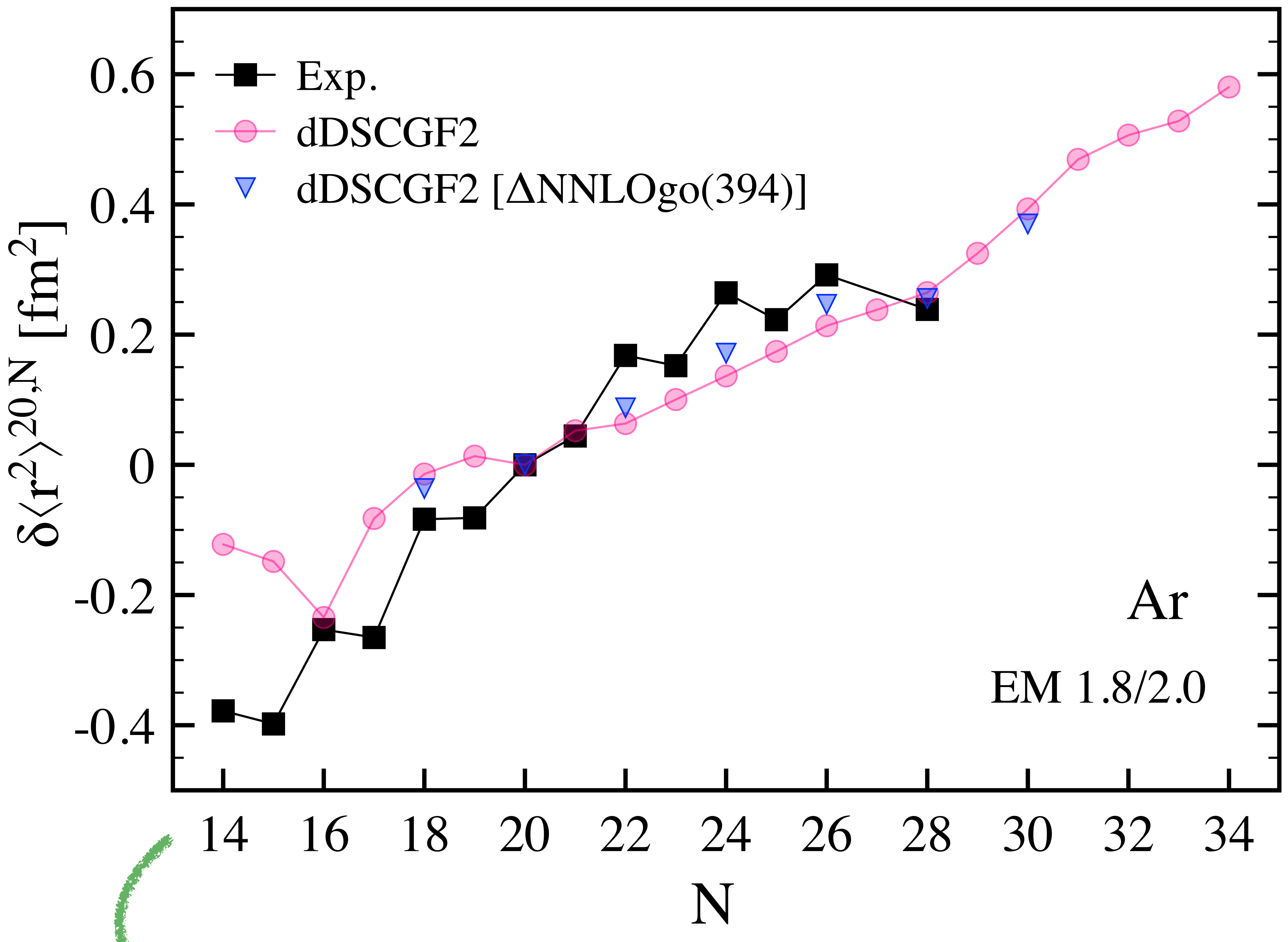
- ○ Clear impact of the explicit account of deformation
- ○ **ADC(3) now available** → differential energies only slightly affected

Going doubly open-shell — radii

- Charge radii along Ar chain

[Scalesi *et al.*, unpublished]



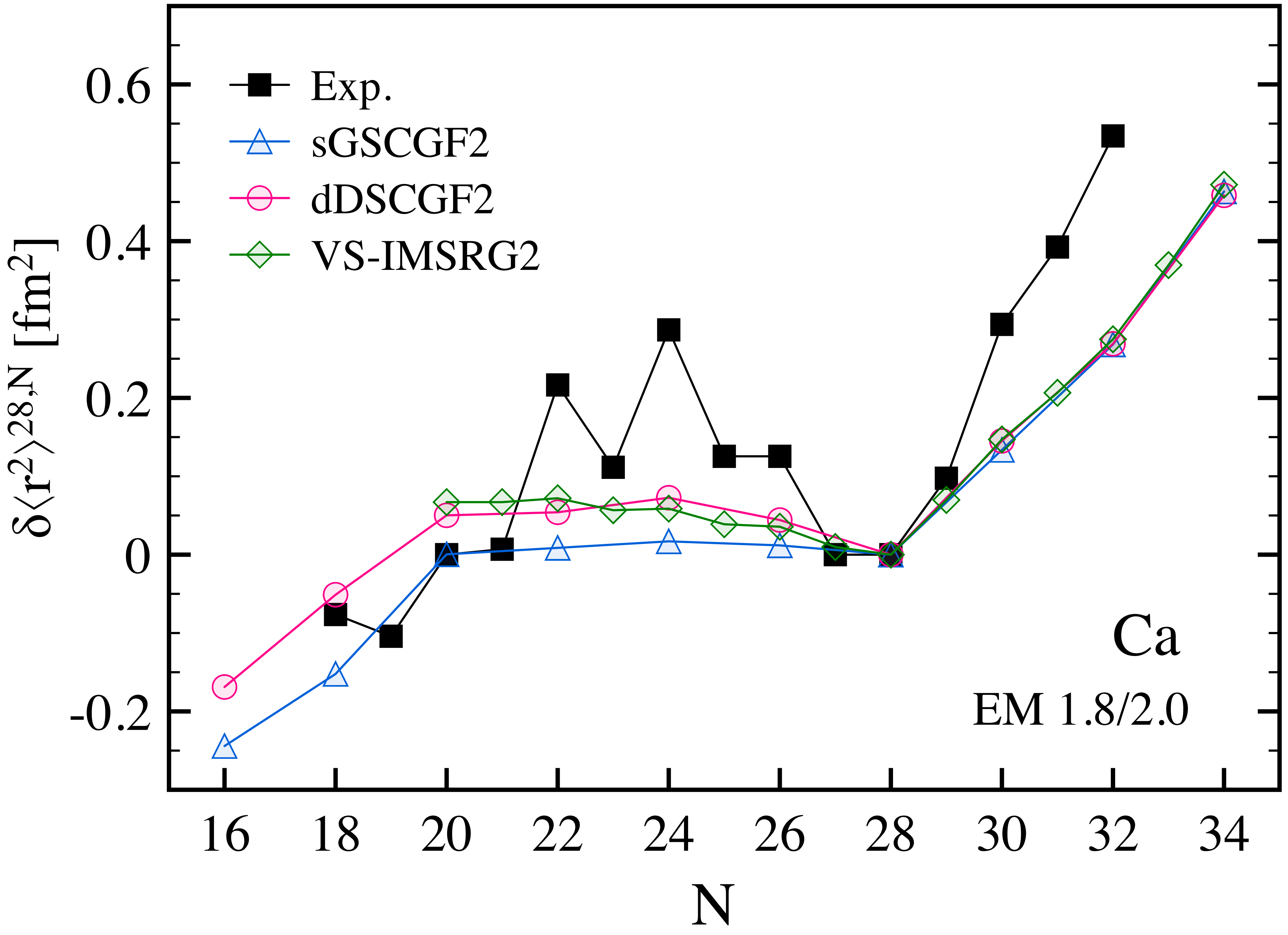


- Deformed calculations improve trend
- However, parabolic behaviour not reproduced
- ADC(3) does not change the picture

Some dependence on the input Hamiltonian observed

Problem #1 — Ca charge radii

⦿ Similar results for Ca isotopes show even more dramatic failure

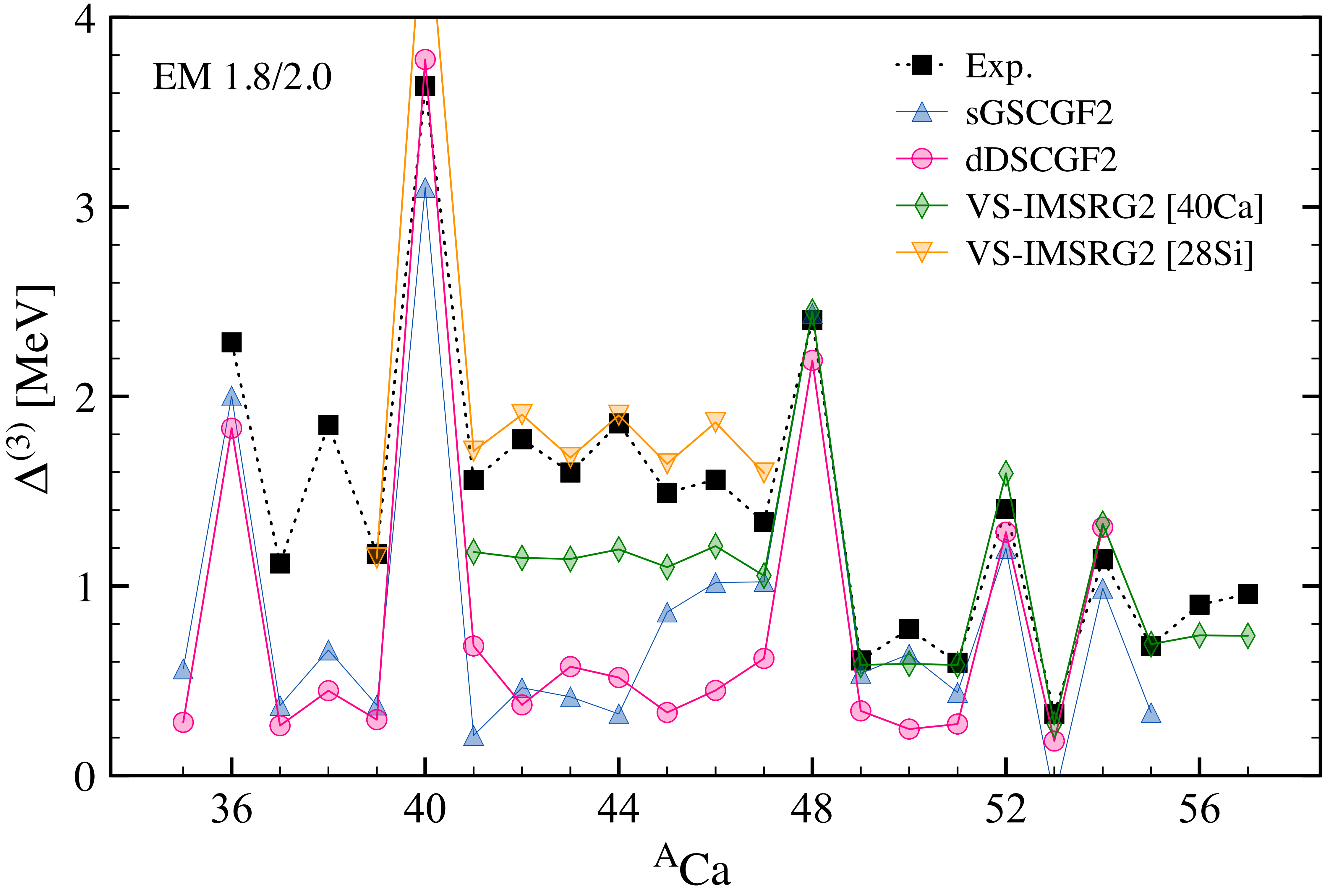


[Scalesi *et al.*, unpublished]

- ○ **Parabolic trend** between N=20 and N=28 completely missed by SCGF calculations
- ○ VS-IMSRG does not improve the situation → Odd-even staggering also barely visible
- ○ Other Hamiltonians [ΔNNLOgo(394) and EM 1.8/2.0(7.5)] lead to similar results

Problem # 2 — Pairing

⦿ Pairing typically estimated via **three-point mass differences** $\Delta^{(3)}(N) \equiv \frac{(-1)^N}{2}\left[E(N-1) - 2E(N) + E(N+1)\right]$



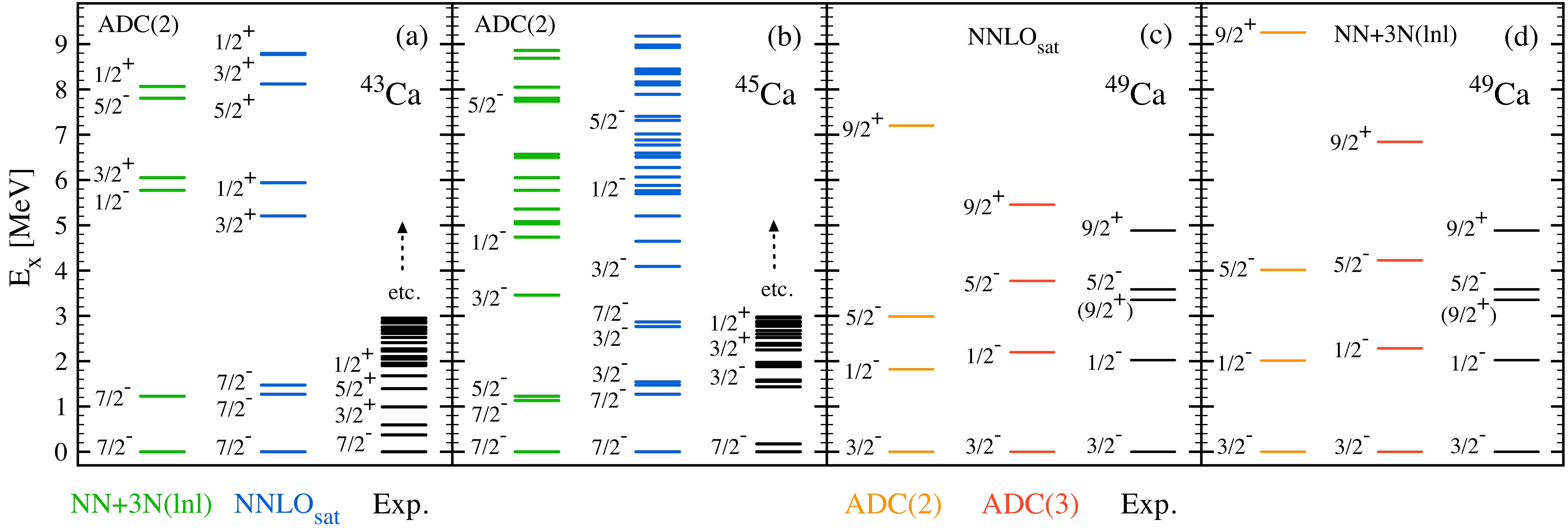
[Scalesi *et al.*, unpublished]

- ○ **Explicit accounting for pairing** (at second order) does not lead to reproducing experimental data
- ○ Deformation alone does not help (neither it does in combination with pairing, see BMBPT)
- ○ VS-IMSRG seems to solve the problem, but **convergence VS-IMSRG2 → VS-IMSRG3 unclear** [Miyagi *et al.*]

Problem # 2 — Pairing

- Same problem can be diagnosed by looking at low-lying spectra

[Somà *et al.*, 2020]

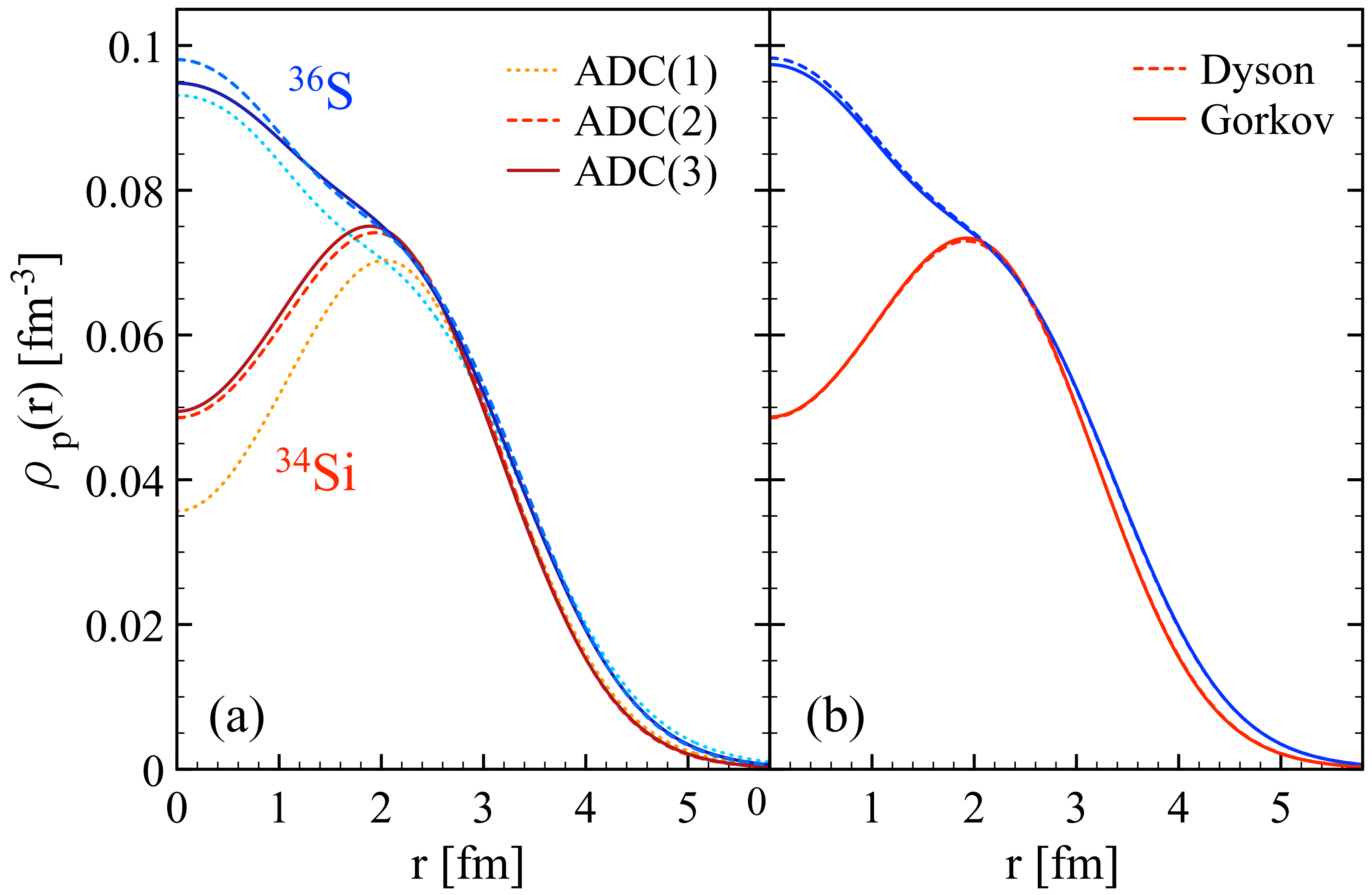


- One-neutron addition from closed-shell ^{48}Ca shows good agreement with data
- Spectra from open-shell ^{48}Ca display much lower density of states → Another signature of **too low effective mass**

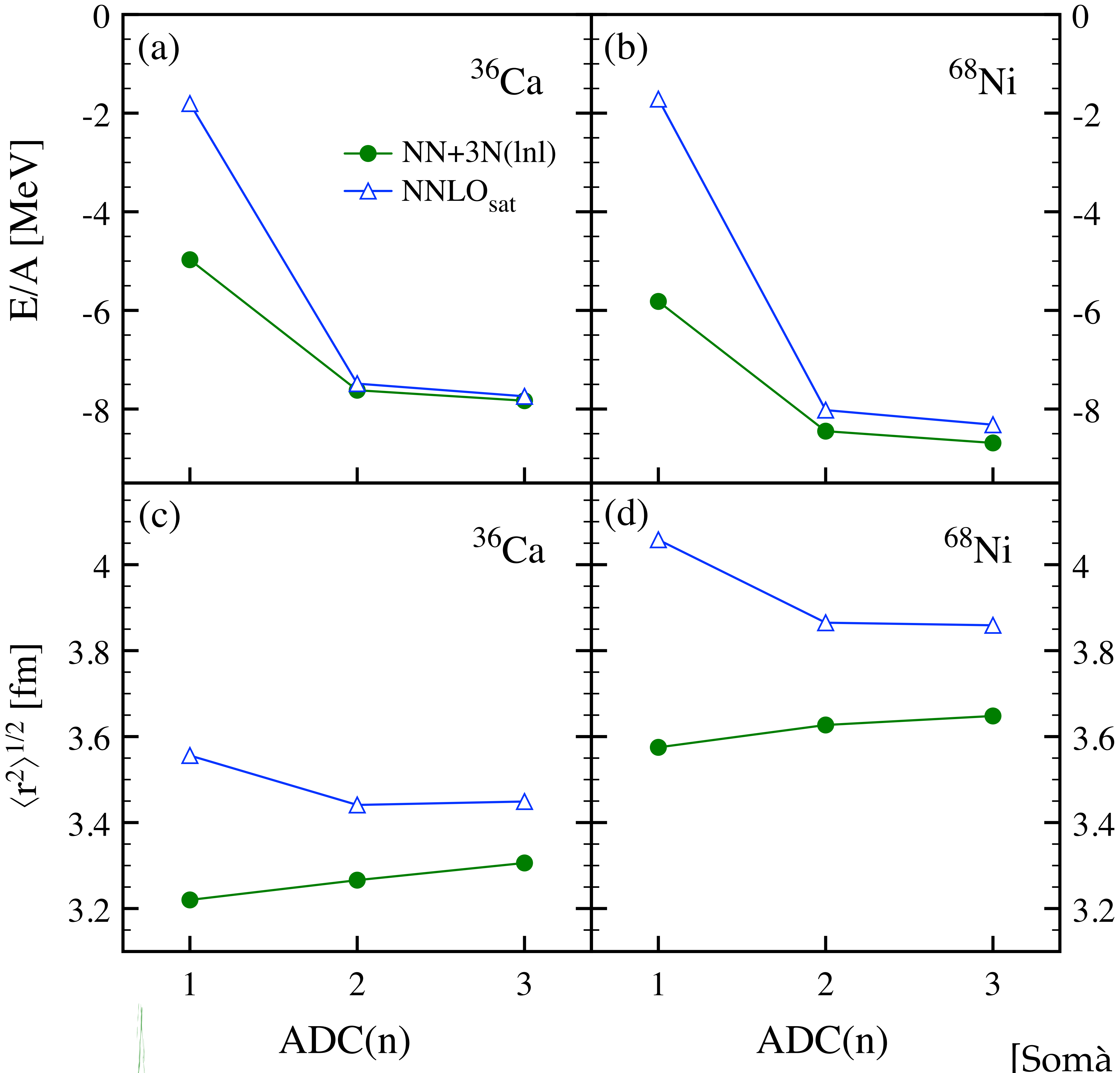
Many-body convergence & other uncertainties

[Somà *et al.*, 2021]

	NN+$3N$(lnl)		NNLO$_{\text{sat}}$
	E	r_{ch}	r_{ch}
Model space (e_{max})	0.5%	$< 0.1\%$	0.5%
Model space ($e_{3\text{max}}$)	0.2%	0.2%	0.3%
ADC truncation	2%	0.5%	$< 0.1\%$
U(1) breaking	0.2%	$< 0.1\%$	$< 0.1\%$
Neglected induced op.	2%	1%	–
Total	2.9%	1.1%	0.6%



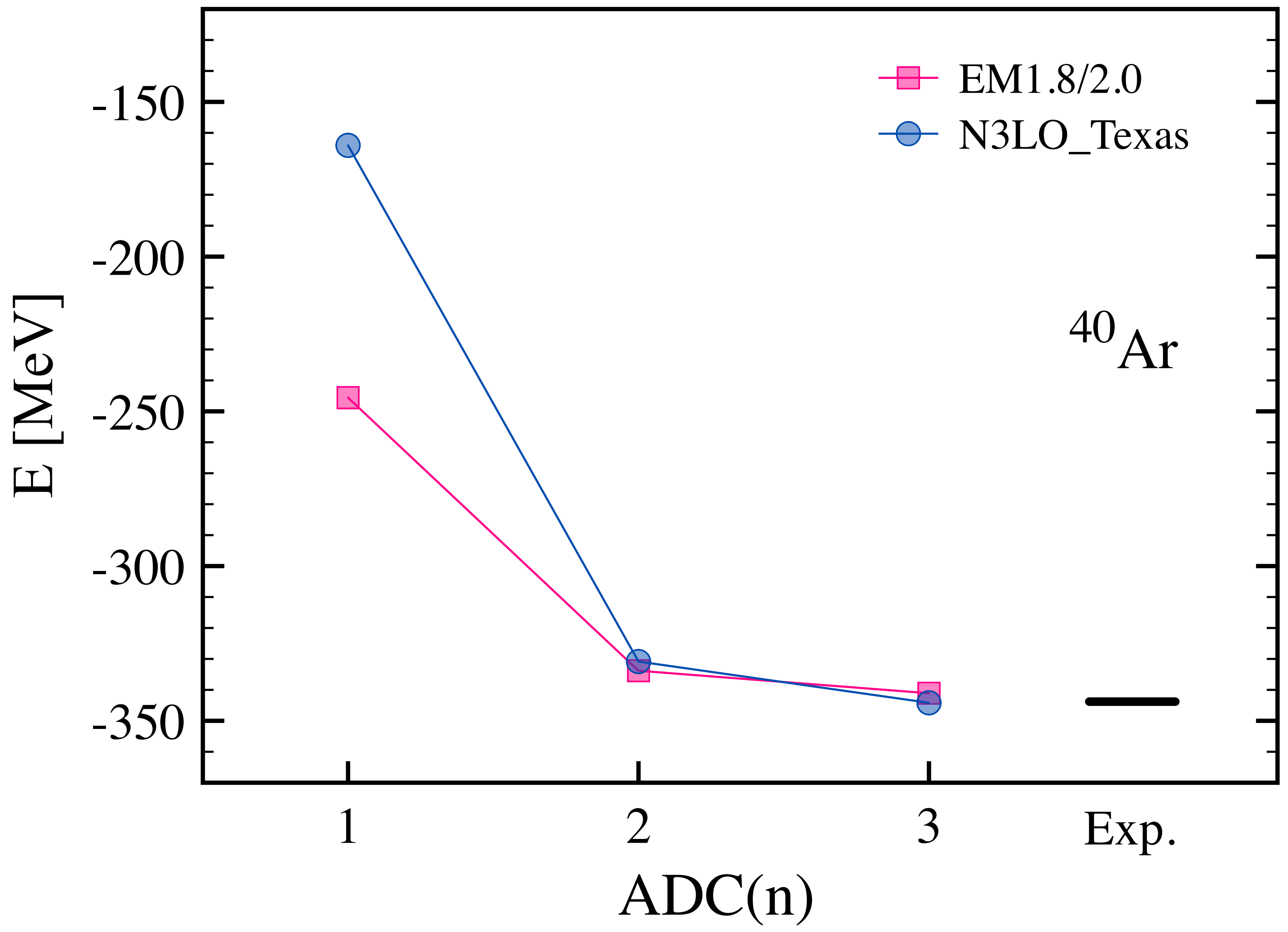
[Duguet *et al.*, 2017]

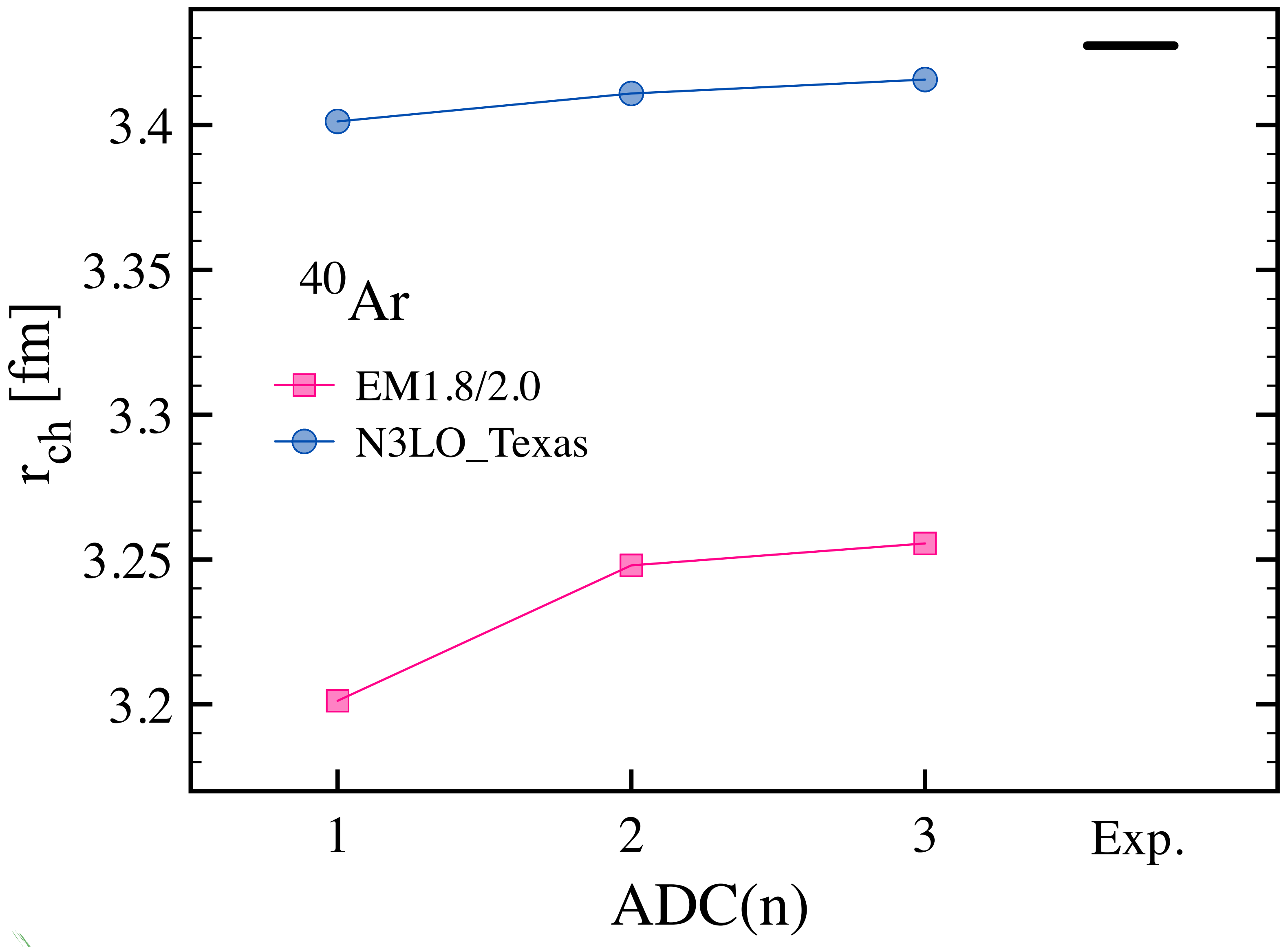


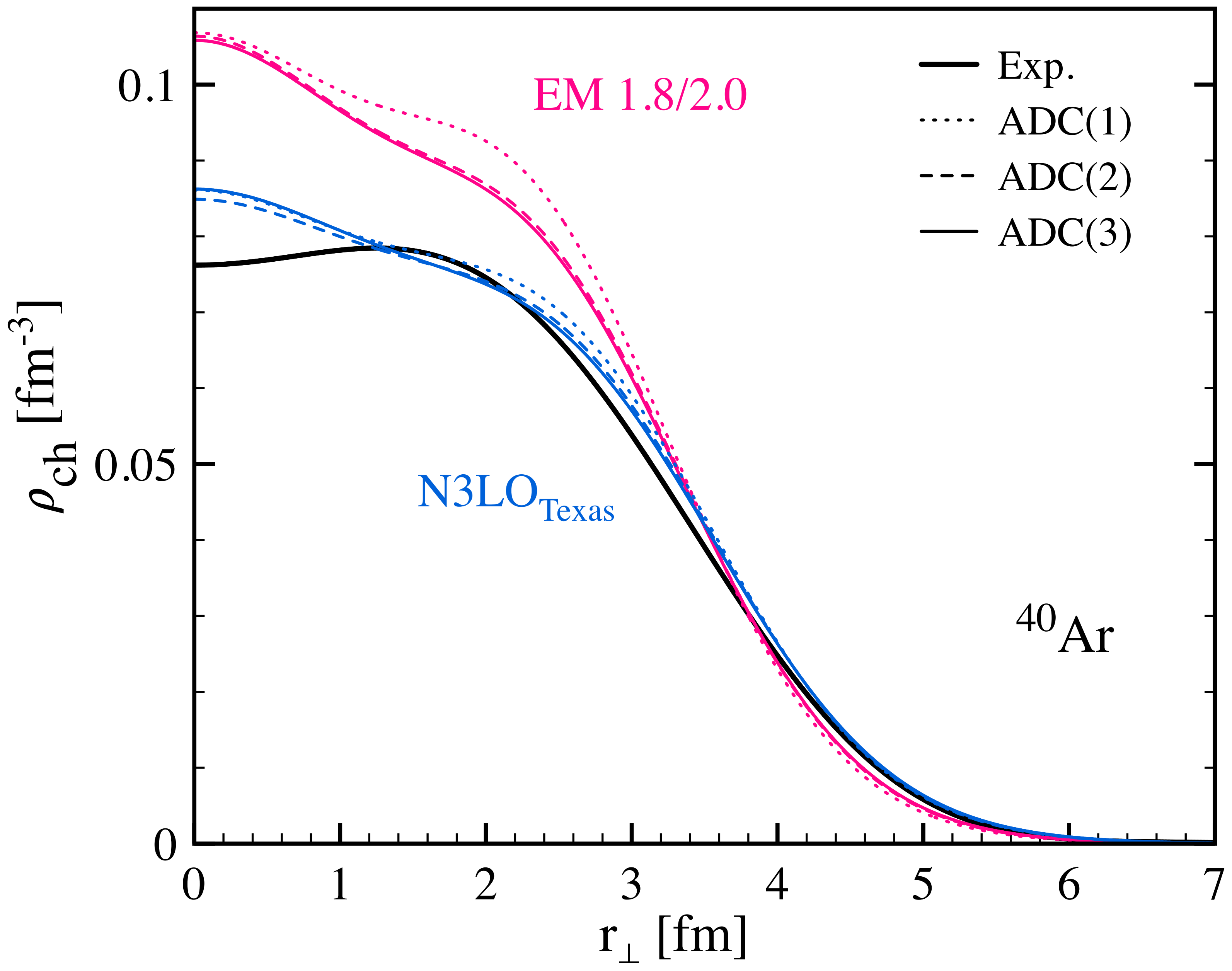
[Somà *et al.*, 2020]

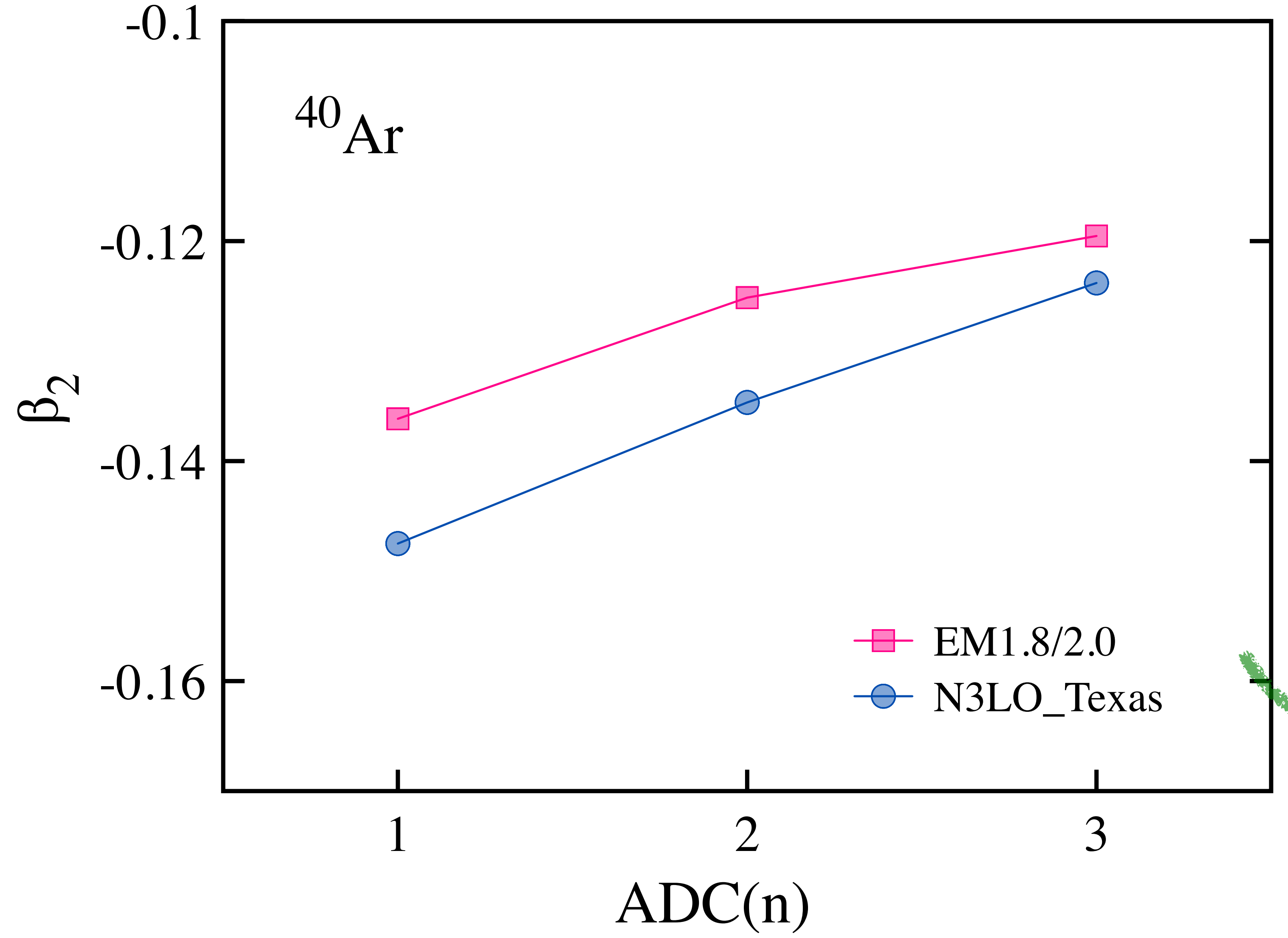
- ○ Clear convergence patterns → similar to e.g. CC
- ○ Specific convergence depend on Hamiltonian & observable

Many-body convergence in deformed SCGF









- ○ No qualitative difference w.r.t. spherical case
- ○ Only partial account of MB convergence → **More general ref. state?**

Deformation decreases, as expected, but slowly

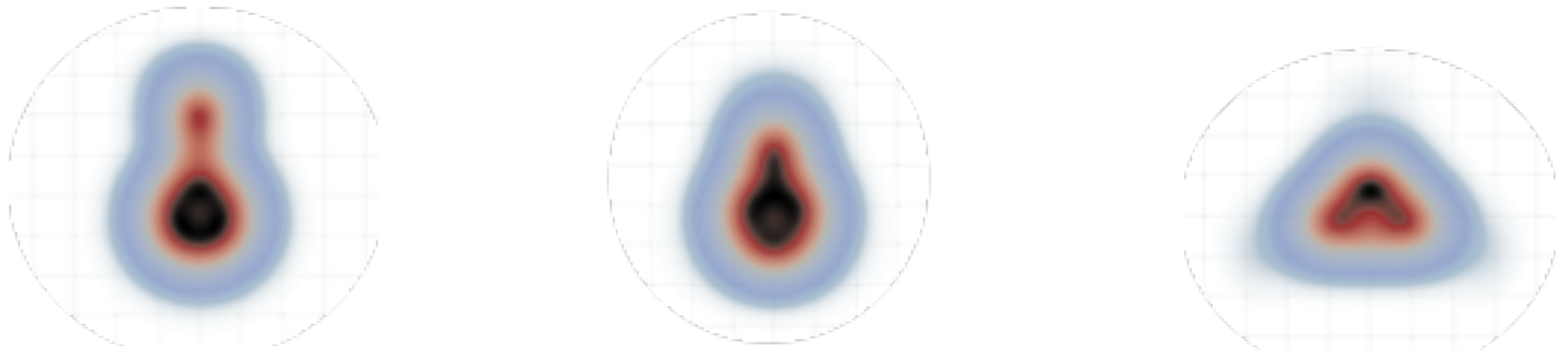
[Scalesi *et al.*, unpublished]

3. PGCM-PT

Projected generator coordinate method

- **Alternative strategy: break symmetries, project, then expand**
  - Construction of the unperturbed state via **projected generator coordinate method** (PGCM)
  - Low-dimensional linear combination of *non-orthogonal* projected Bogolyubov product states (← EDF)

Def. vacua



$|\Phi(q_1)\rangle$ $|\Phi(q_2)\rangle$ $|\Phi(q_3)\rangle$

Projection

$\tilde{\sigma} \equiv (J^{\Pi}, N, Z)$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_2)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_3)\rangle$ → *Rotational modes*

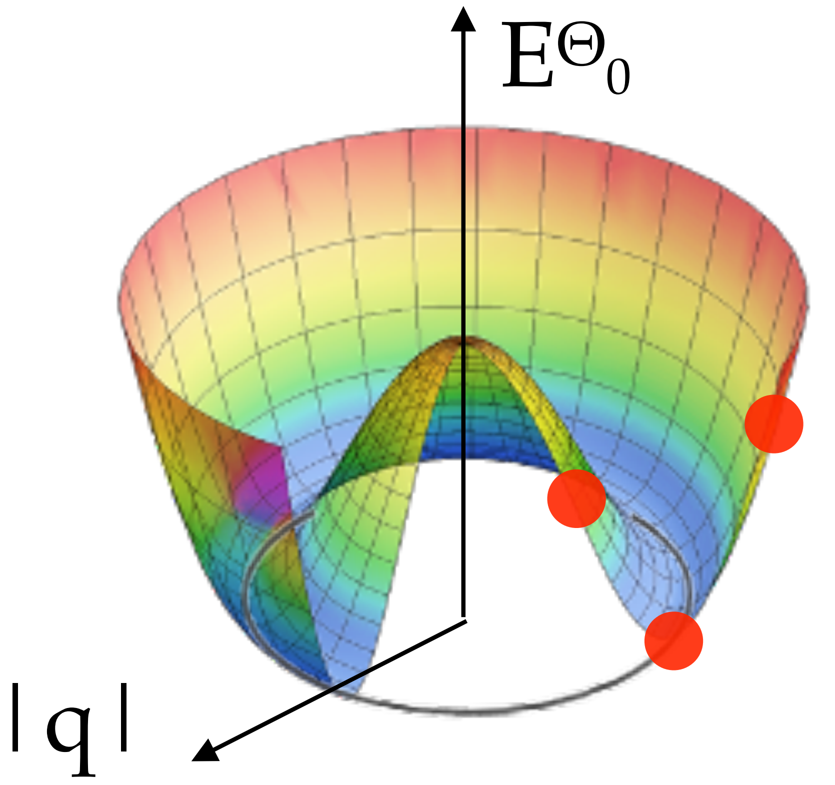
Shape mixing

$$|\Theta^{\tilde{\sigma}}_{\mu}\rangle = \sum_q f^{\tilde{\sigma}}_{\mu}(q)\, P^{\tilde{\sigma}}\, |\Phi(q)\rangle$$

→ *Vibrational modes*

Variational principle → **Hill-Wheeler-Griffin equation**

$$\sum_q H^{\tilde{\sigma}}_{qp} f^{\tilde{\sigma}}_{\mu}(q) = \epsilon^{\tilde{\sigma}}_{\mu} \sum_q N^{\tilde{\sigma}}_{qp} f^{\tilde{\sigma}}_{\mu}(q)$$

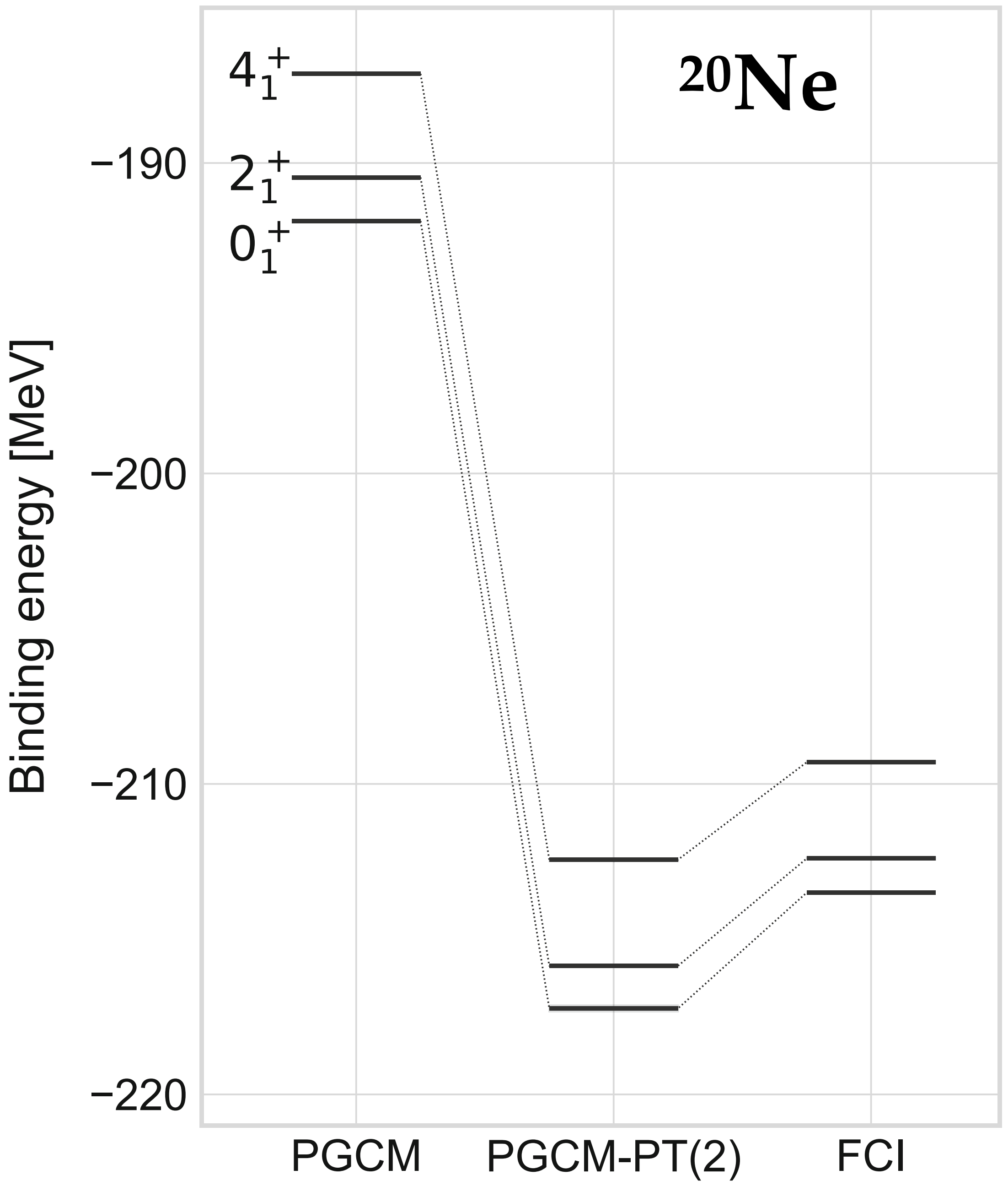


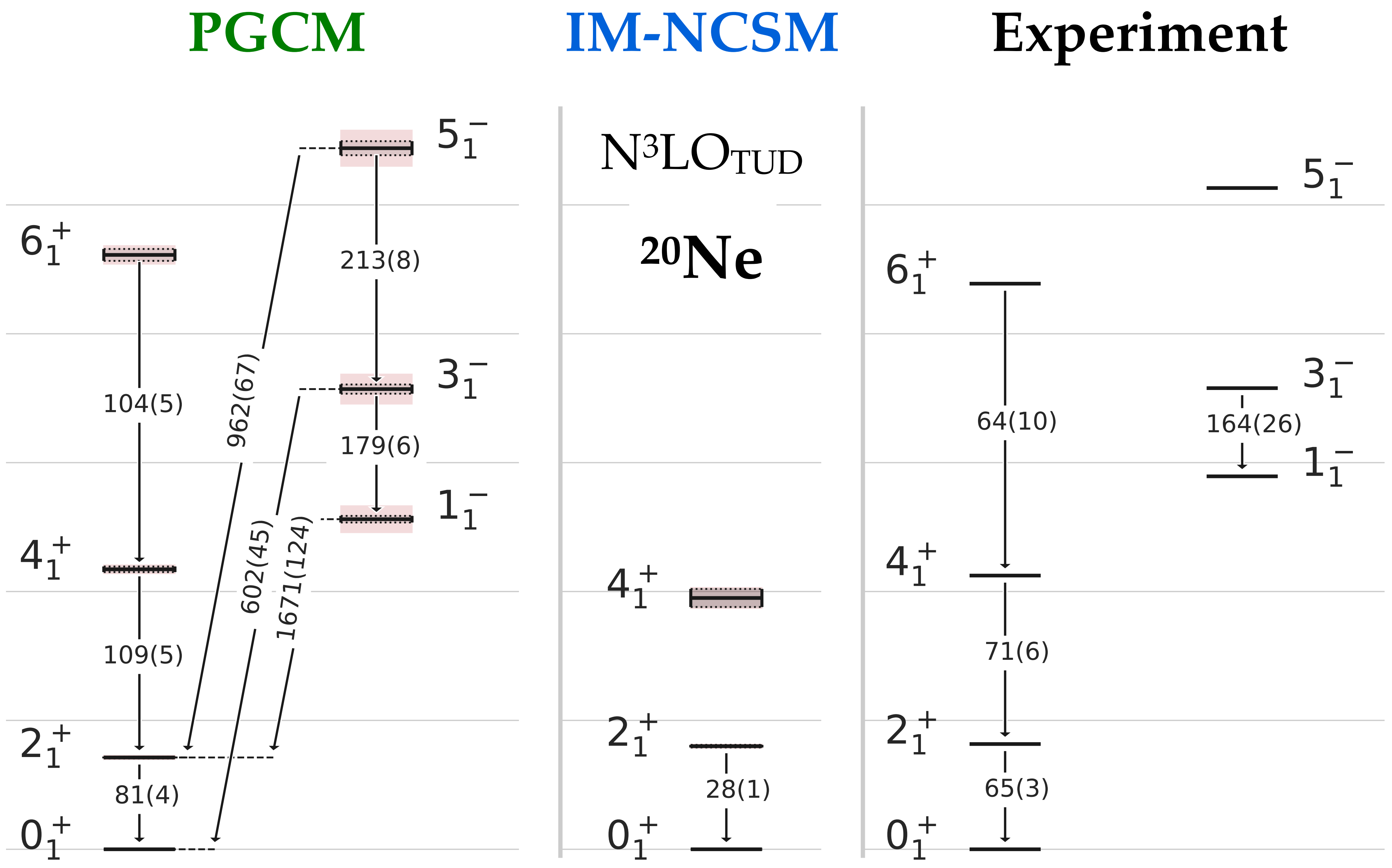
Perturbation theory on top of PGCM states

PGCM-PT

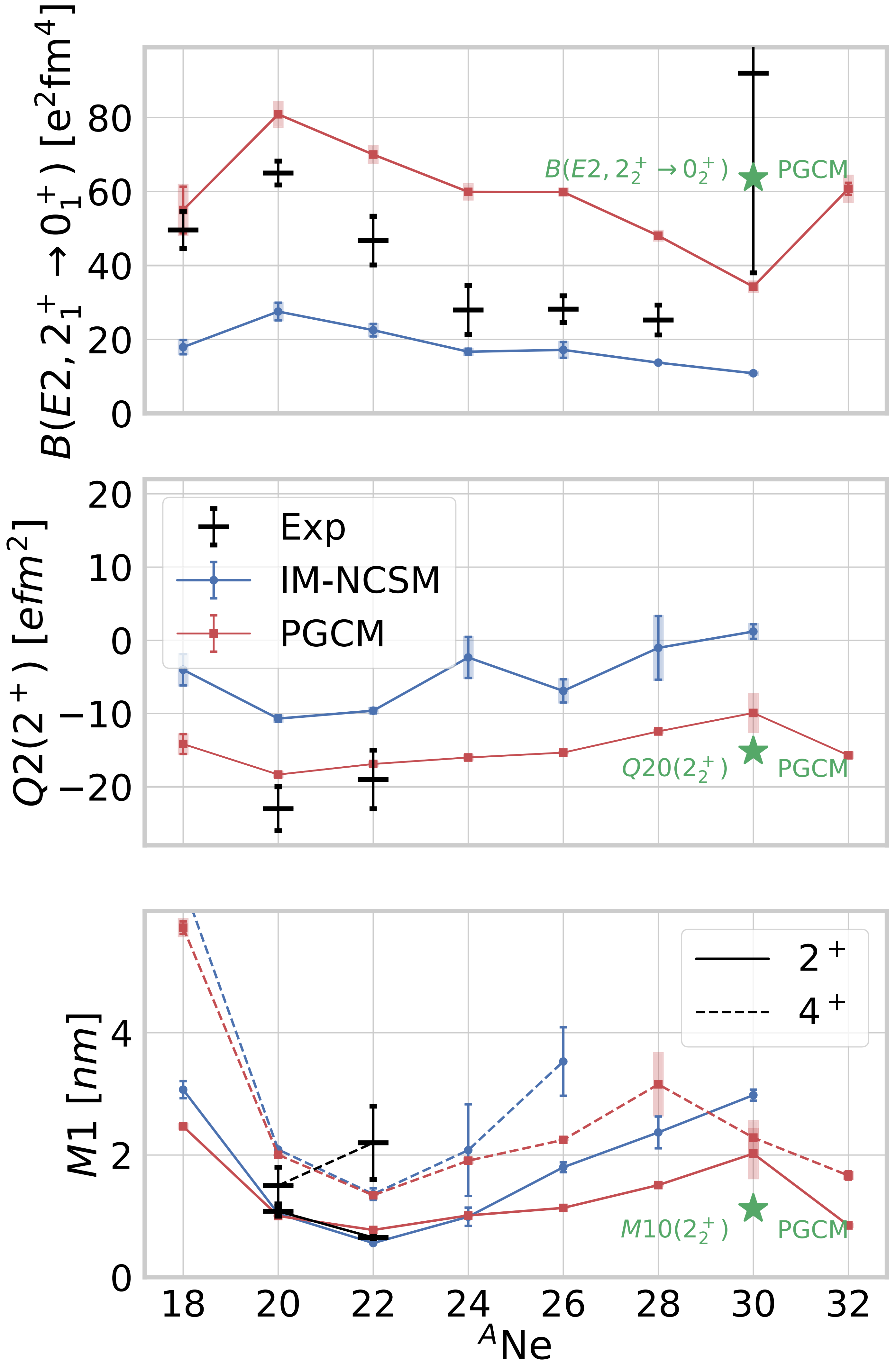
[Frosini *et al.*, 2022]

PGCM — low-lying spectroscopy & EM moments





[Frosini *et al.*, 2022]

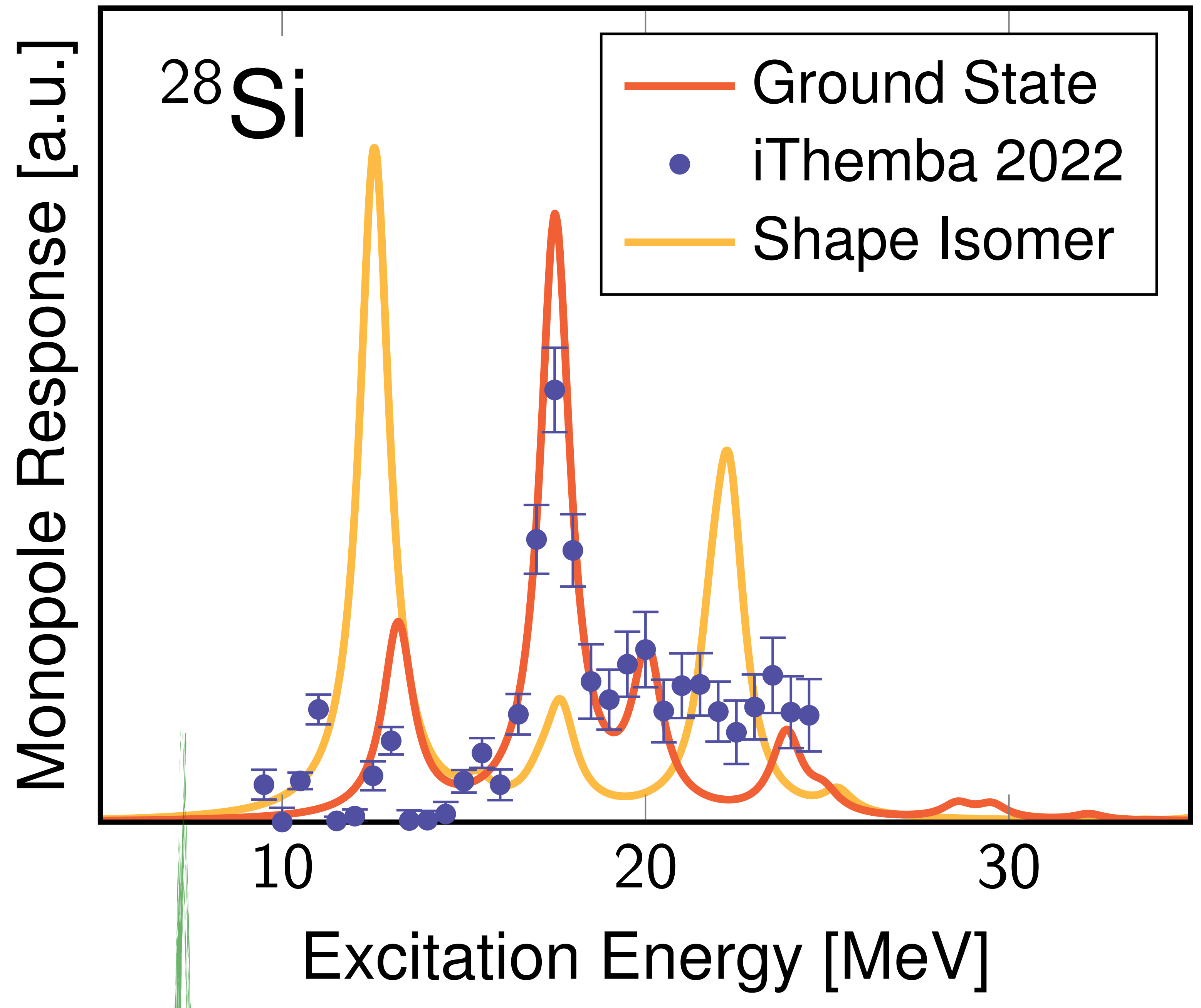


- ○ Dynamical correlations similar in different states → **cancel out in excitation spectra**
- ○ Spectra compare well with NCSM and experiment
- ○ EM observables at hand along isotopic chains → trends OK with exceptions

PGCM — giant resonances

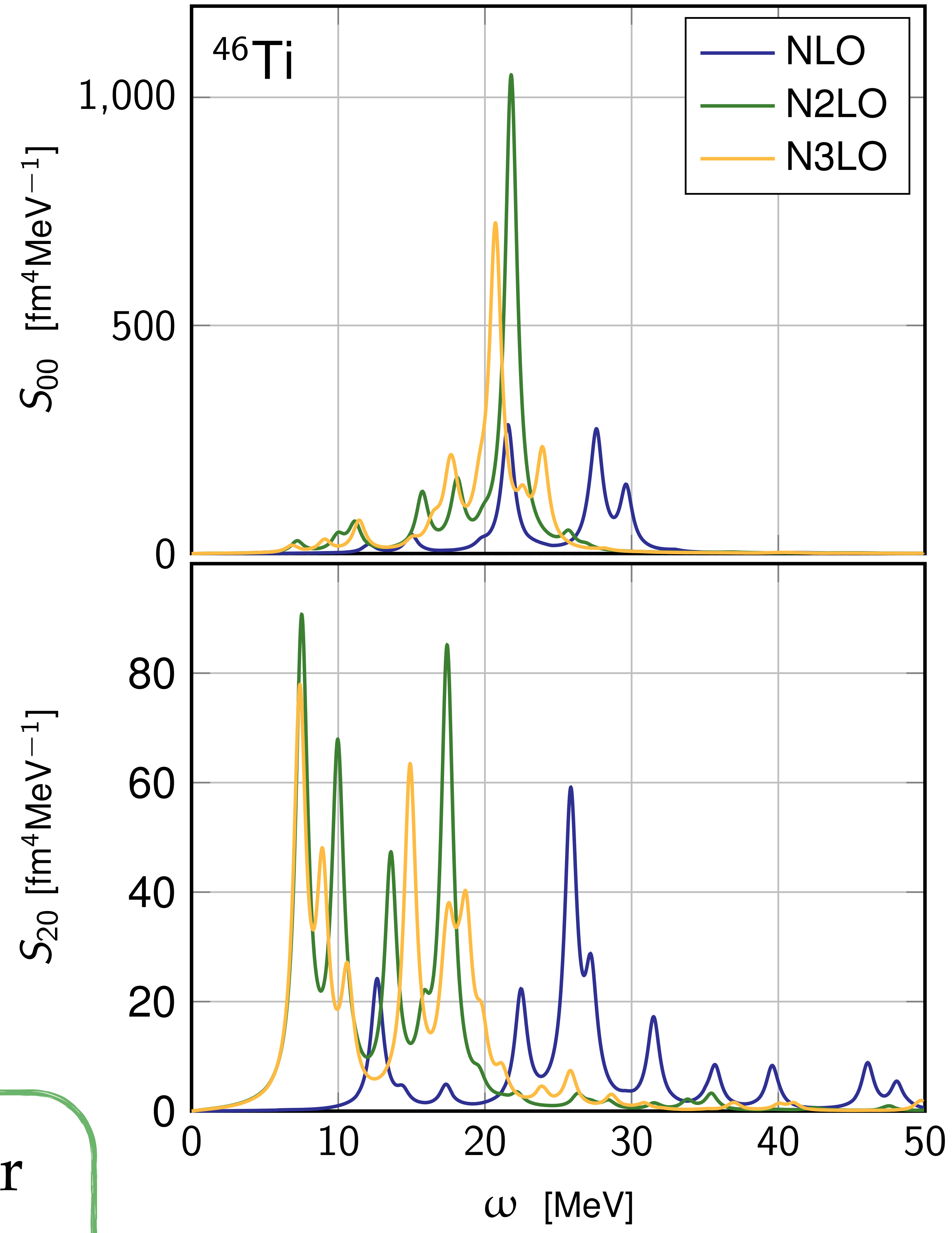
- PGCM can access also collective excitations at larger energies → **giant resonances** [Porro *et al.*, 2024]

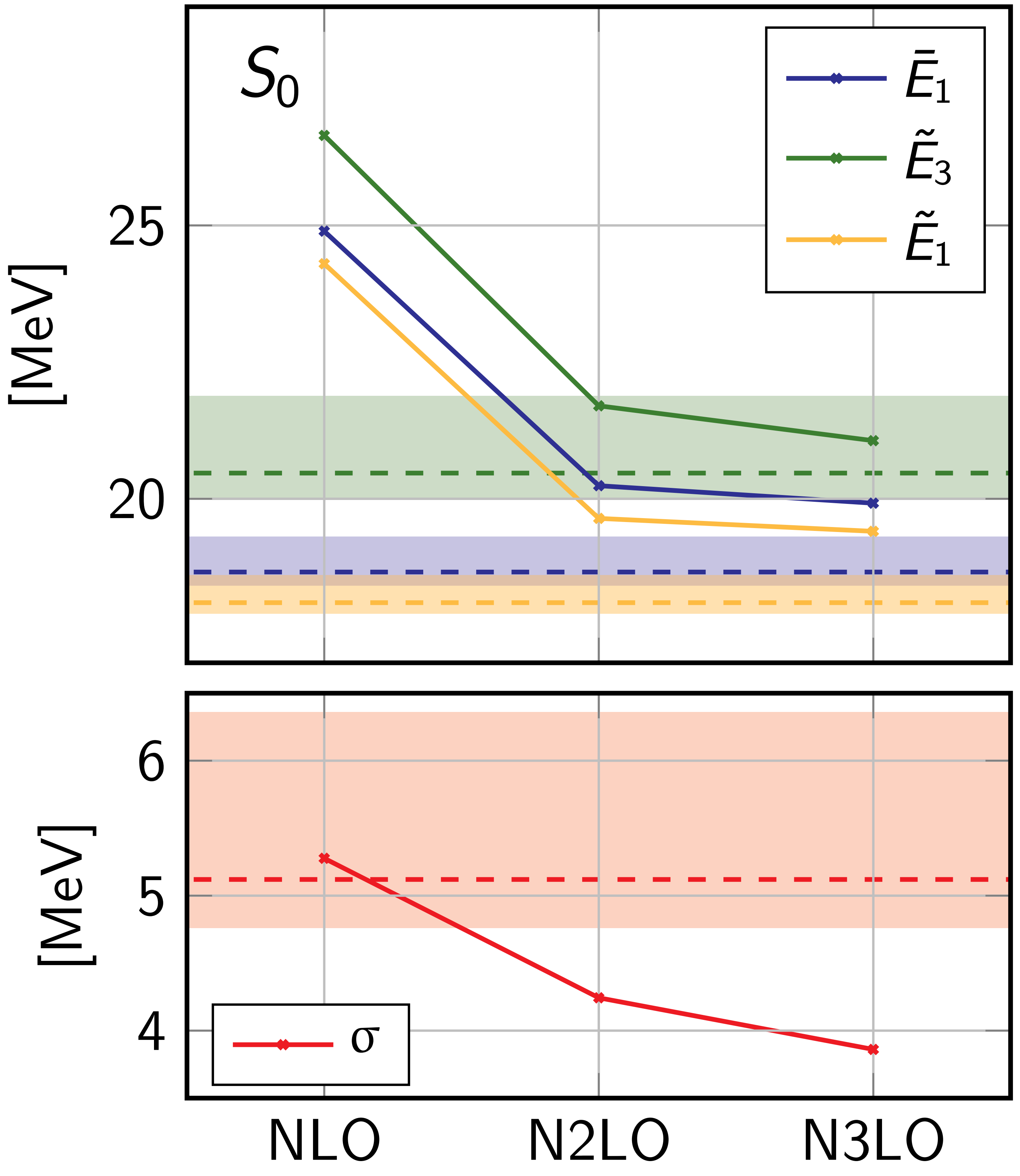
$$S_F(\omega) \equiv \sum_{\nu\sigma} |\langle \Psi_\nu^\sigma | F | \Psi_0^{\sigma_0} \rangle|^2 \, \delta(E_\nu^\sigma - E_0^{\sigma_0} - \omega)$$



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

Order-by-order convergence





Response → Mean energy & dispersion

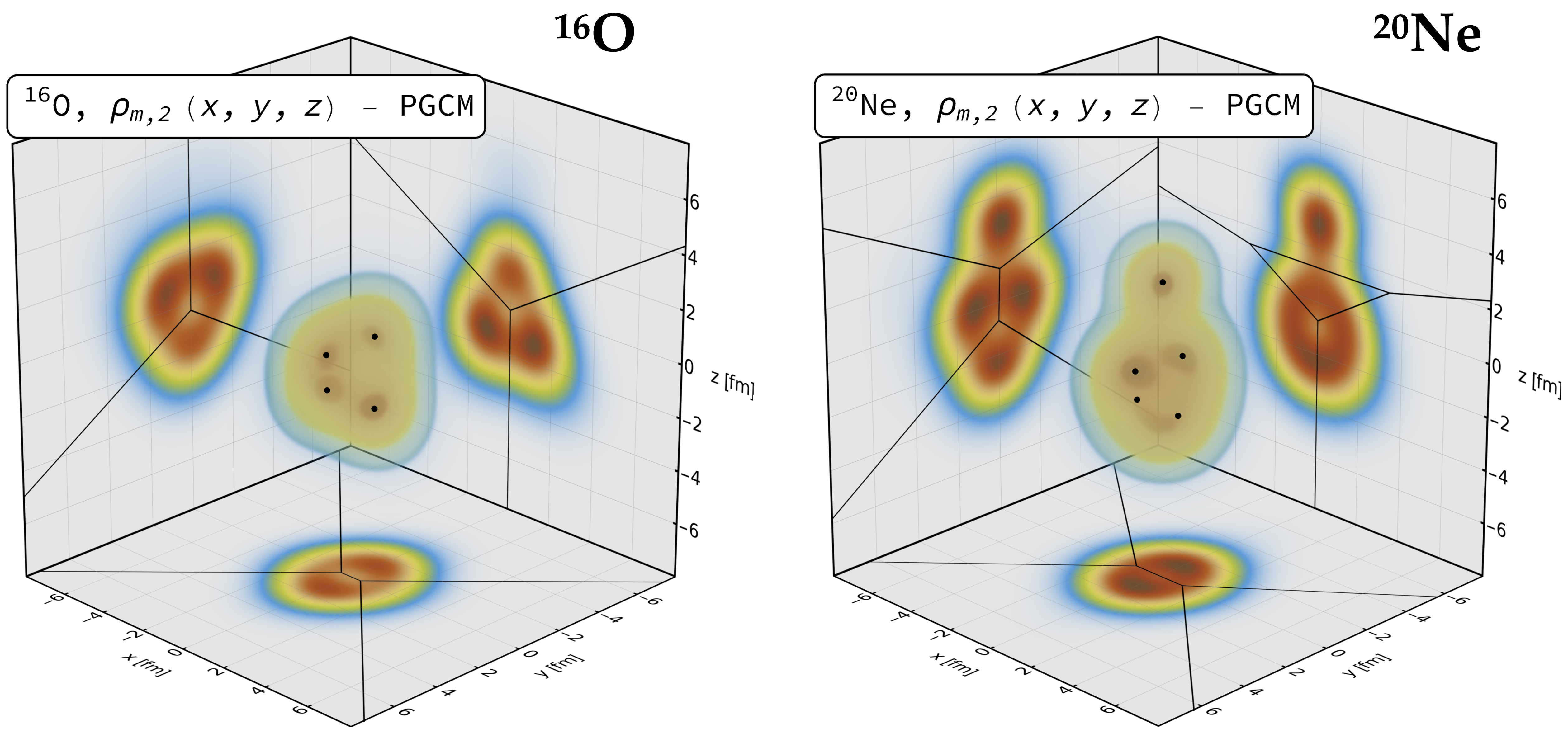
Nuclear structure & relativistic ion collisions

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

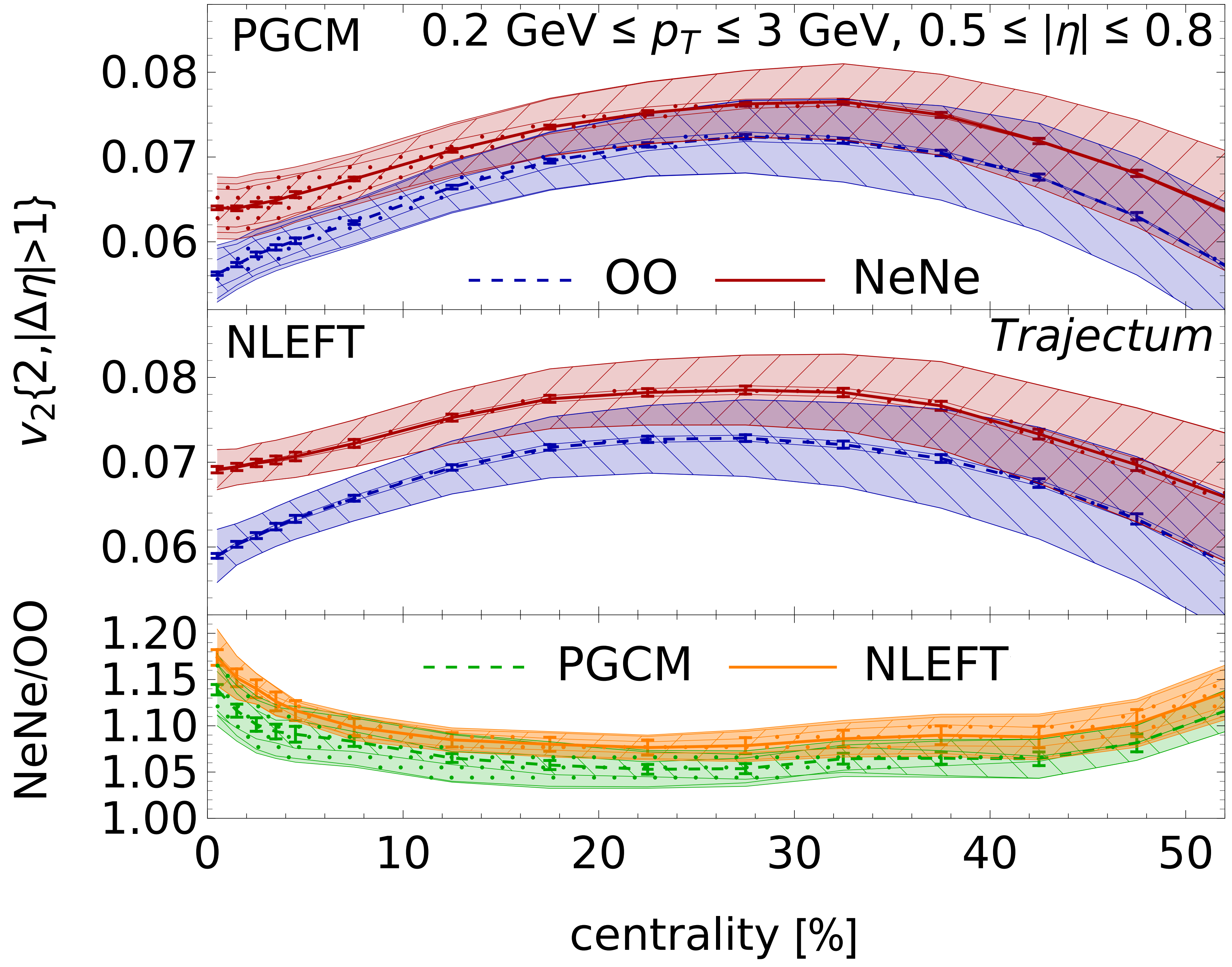
→ Test of the hydrodynamic QGP paradigm for small systems

→ New observables to test nuclear structure models

Elliptic flow



[Calculations by B. Bally]



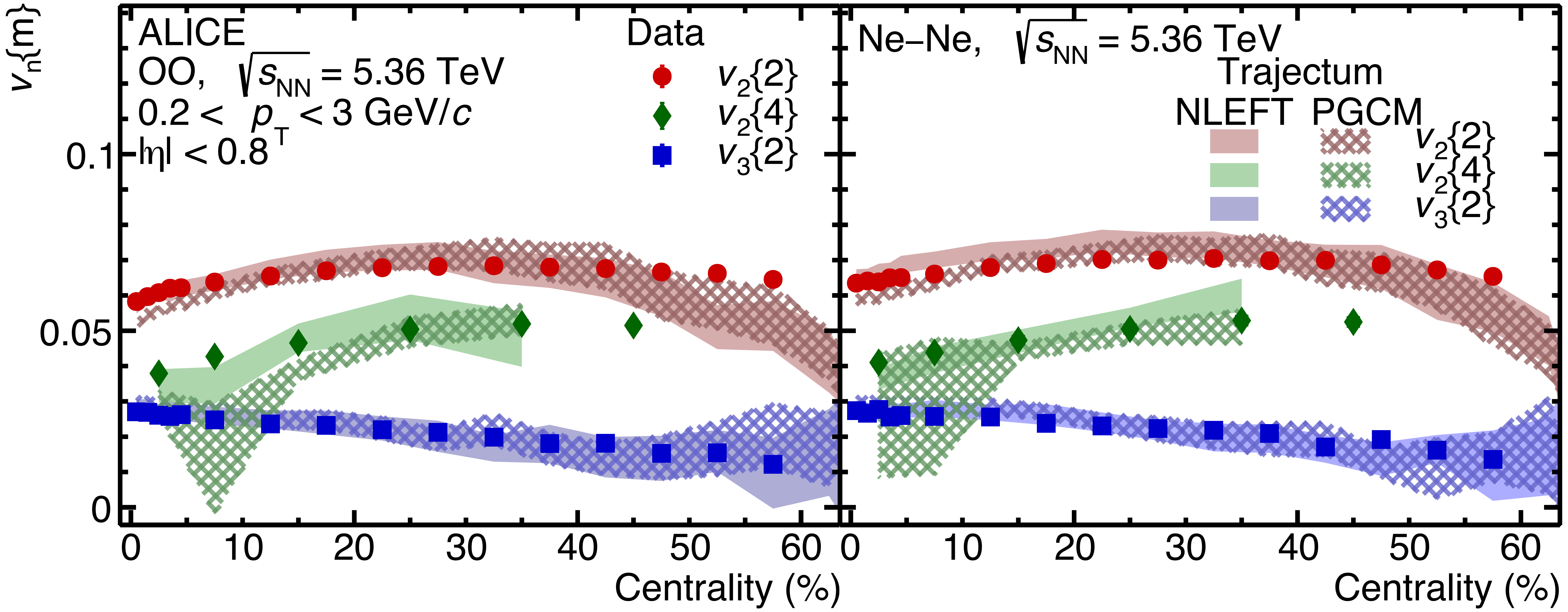
[Giacalone *et al.*, 2025]

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

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

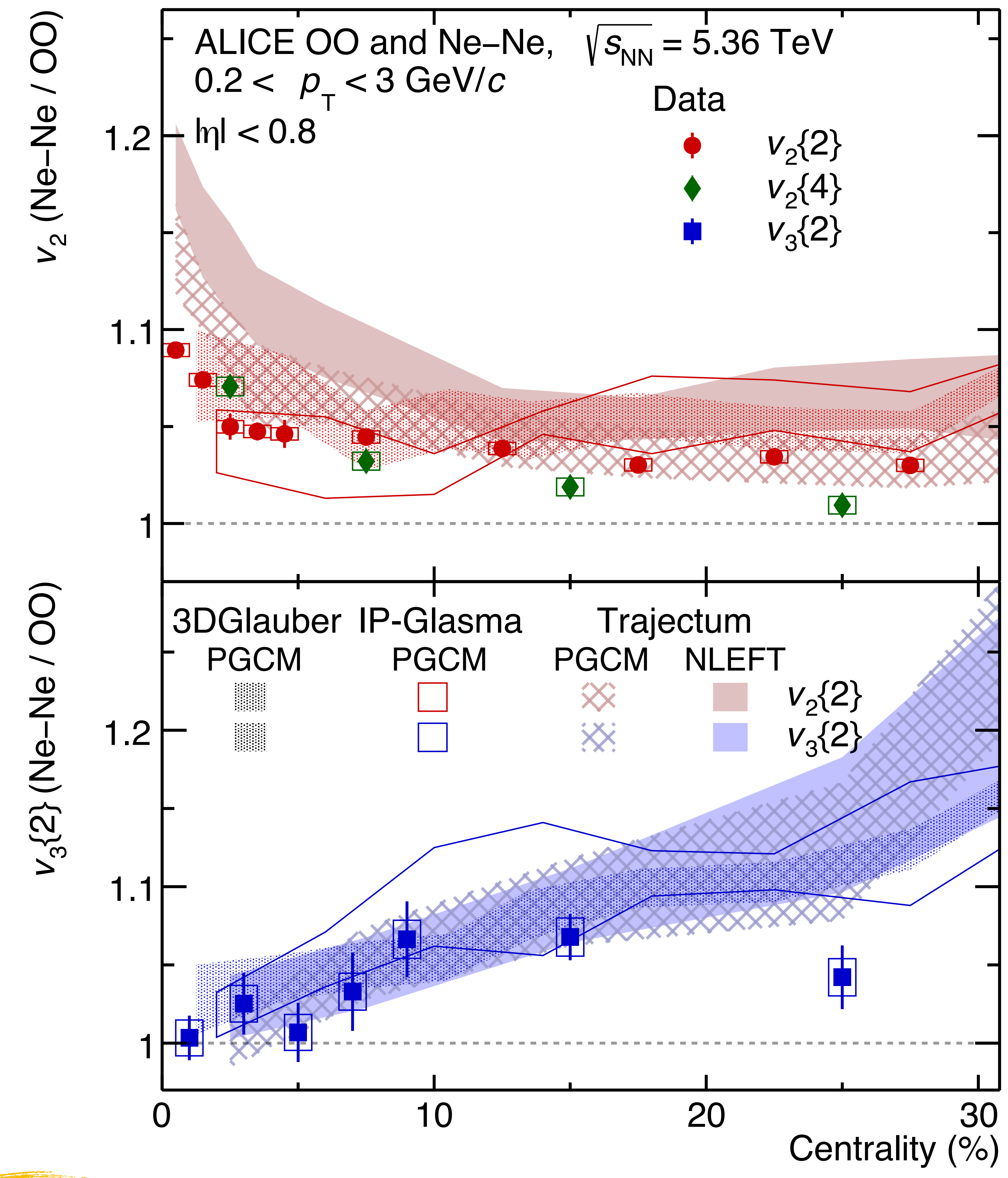
Nuclear structure & relativistic ion collisions

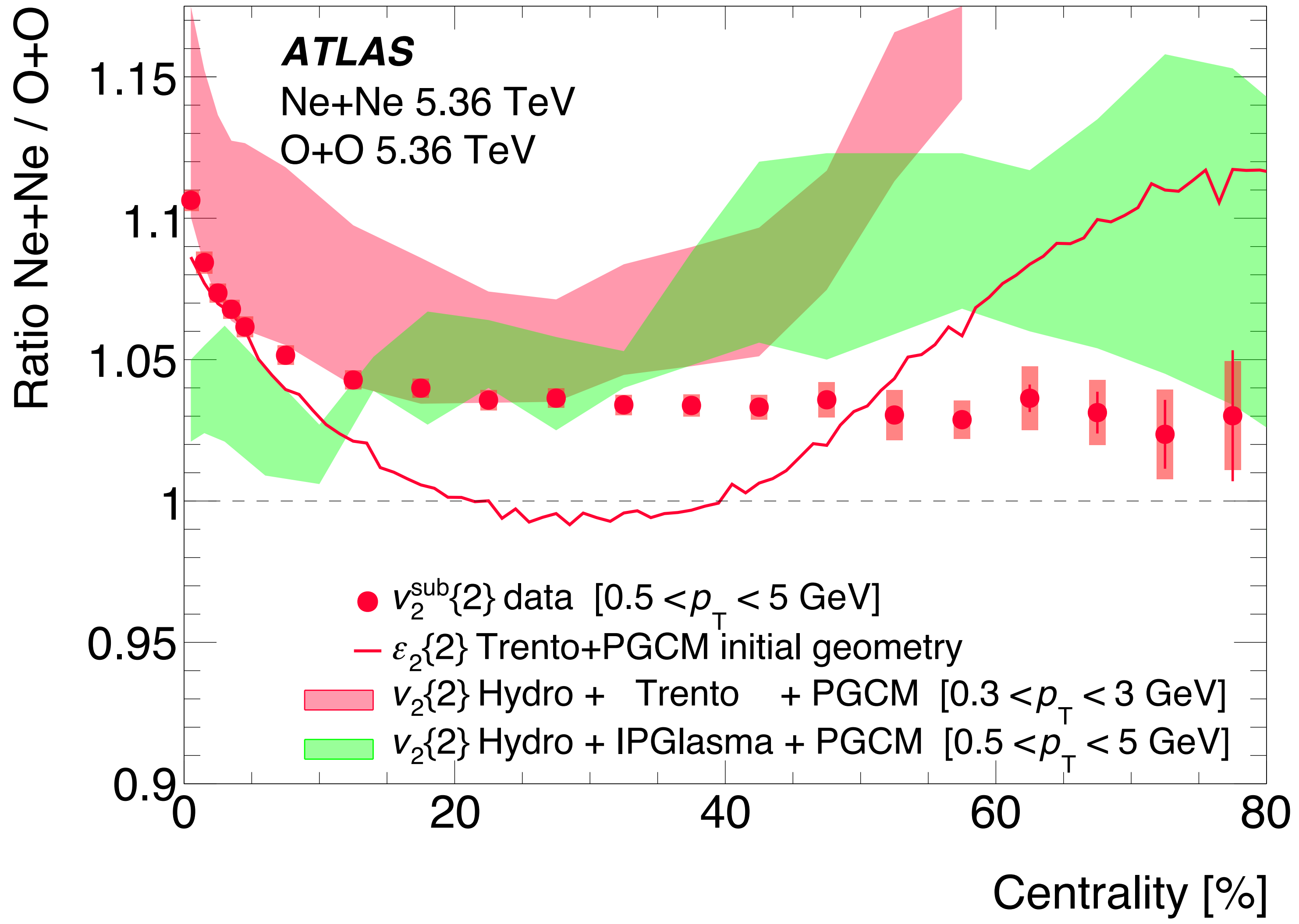
○ **First analyses of experimental measurements confirm PGCM predictions!**

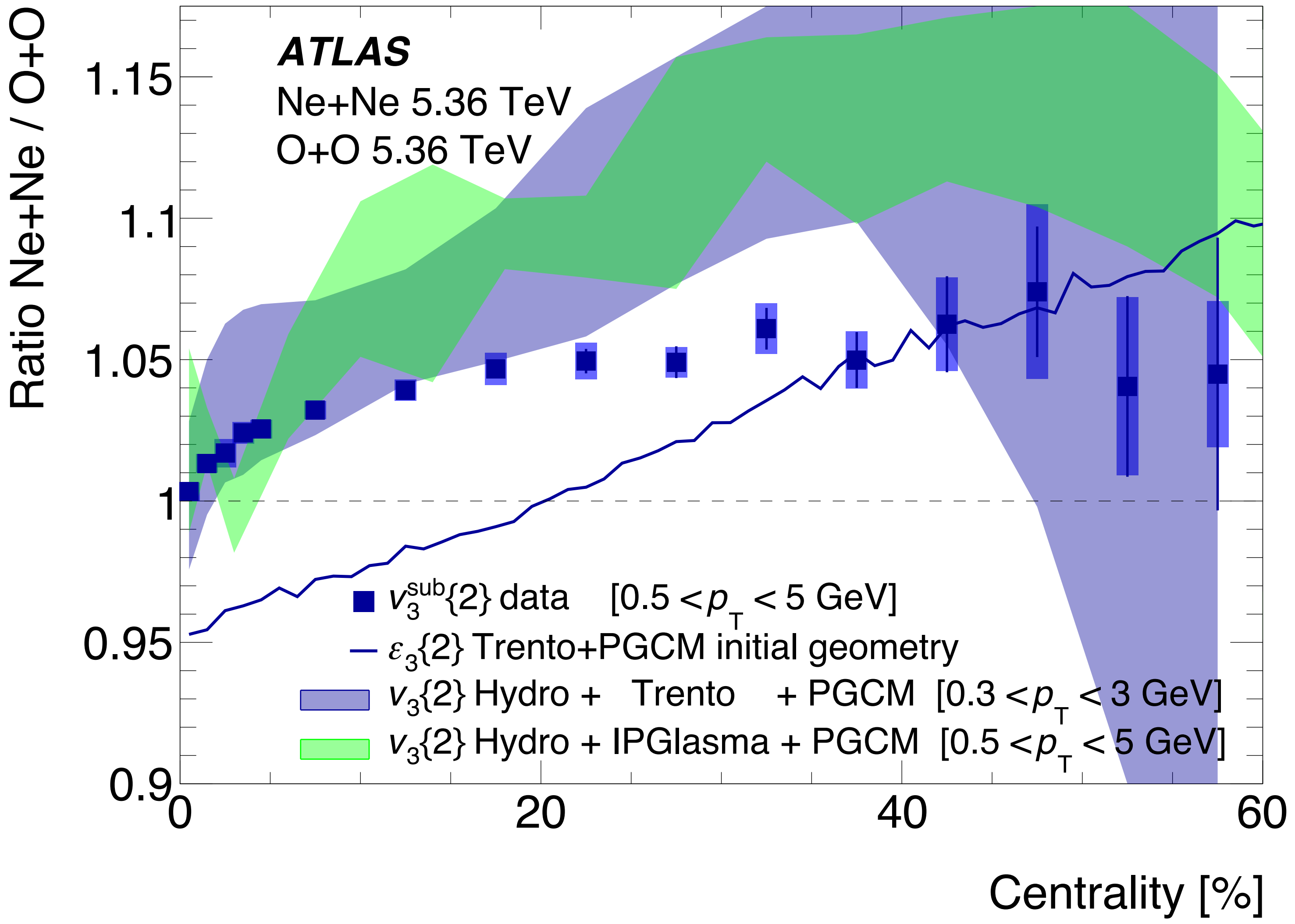


ALICE

[ALICE collaboration, 2509.06428]







ATLAS

[ATLAS collaboration, 2509.05171]

Perspectives and challenges

⦿ **Progress** in ab initio calculations of (medium/heavy) open-shell nuclei

- Many **complementary methods** → BMBPT, SCGF, PGCM(-PT) + CC, (VS-)IMSRG, …
- **Symmetry breaking & restoration** proves effective in capturing strong static correlations

⦿ **Challenges**

- Thorough assessment of **many-body uncertainties**
- Current bottleneck on the way to heavy nuclei → rank-reduction of **three-nucleon forces**
- High computational costs
  - → Development of **dimensionality-reduction techniques** (importance truncation, natural orbitals, tensor factorisation, …)
  - → Development of **emulators**

⦿ **INT 26-1 challenges**

- **Failures**: is it the many-body method or the Hamiltonian? Or both? → Less evident than in light or closed-shell nuclei
- Open-shell observables in **fitting** procedure? In **importance resampling**?
- How to develop **reliable emulators** for open-shell, possibly heavy systems?