Recent progress and open questions in ab initio simulations of nuclei
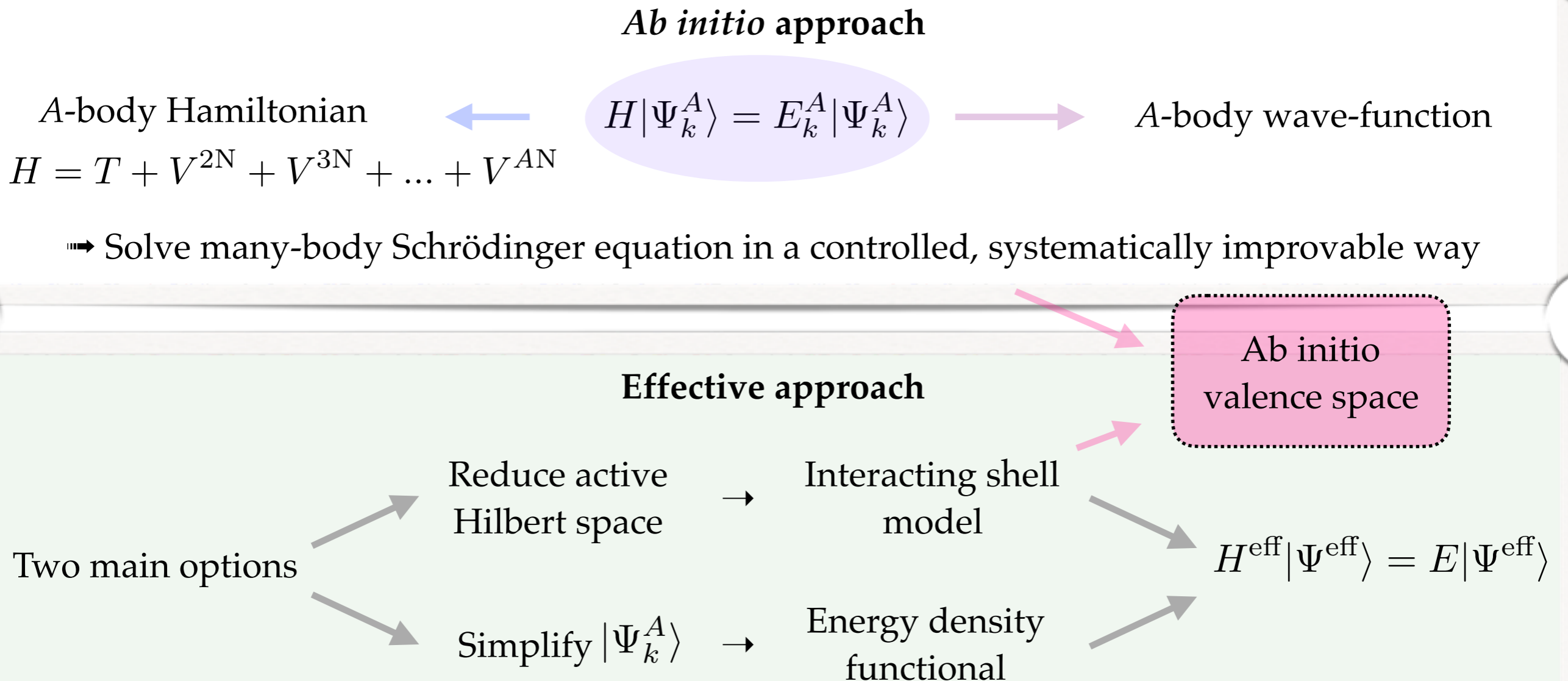
Vittorio Somà
IRFU, CEA Saclay, France

GDR RESANET - Working group 3 meeting
12-13 November 2018

Ab initio vs. effective approach

Ab initio approach

A-body Hamiltonian $\longleftarrow$ $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ $\longrightarrow$ A-body wave-function

$$H = T + V^{2\mathrm{N}} + V^{3\mathrm{N}} + ... + V^{A\mathrm{N}}$$

⇒ Solve many-body Schrödinger equation in a controlled, systematically improvable way

Effective approach

Ab initio valence space

Two main options

Reduce active Hilbert space $\rightarrow$ Interacting shell model

Simplify $|\Psi_k^A\rangle$ $\rightarrow$ Energy density functional

$$H^{\mathrm{eff}}|\Psi^{\mathrm{eff}}\rangle = E|\Psi^{\mathrm{eff}}\rangle$$

	Ab initio	Shell model	EDF
Accuracy	🌤️	☀️	🌤️
Reach across the mass table	🌧️	🌧️	☀️
Predictive power/error estimate	🌤️	🌧️	🌦️

Evolution of ab initio nuclear chart

⊙ "Exact" approaches
- ○ Since 1980's
- ○ Monte Carlo, CI, …
- ○ Factorial / exponential scaling

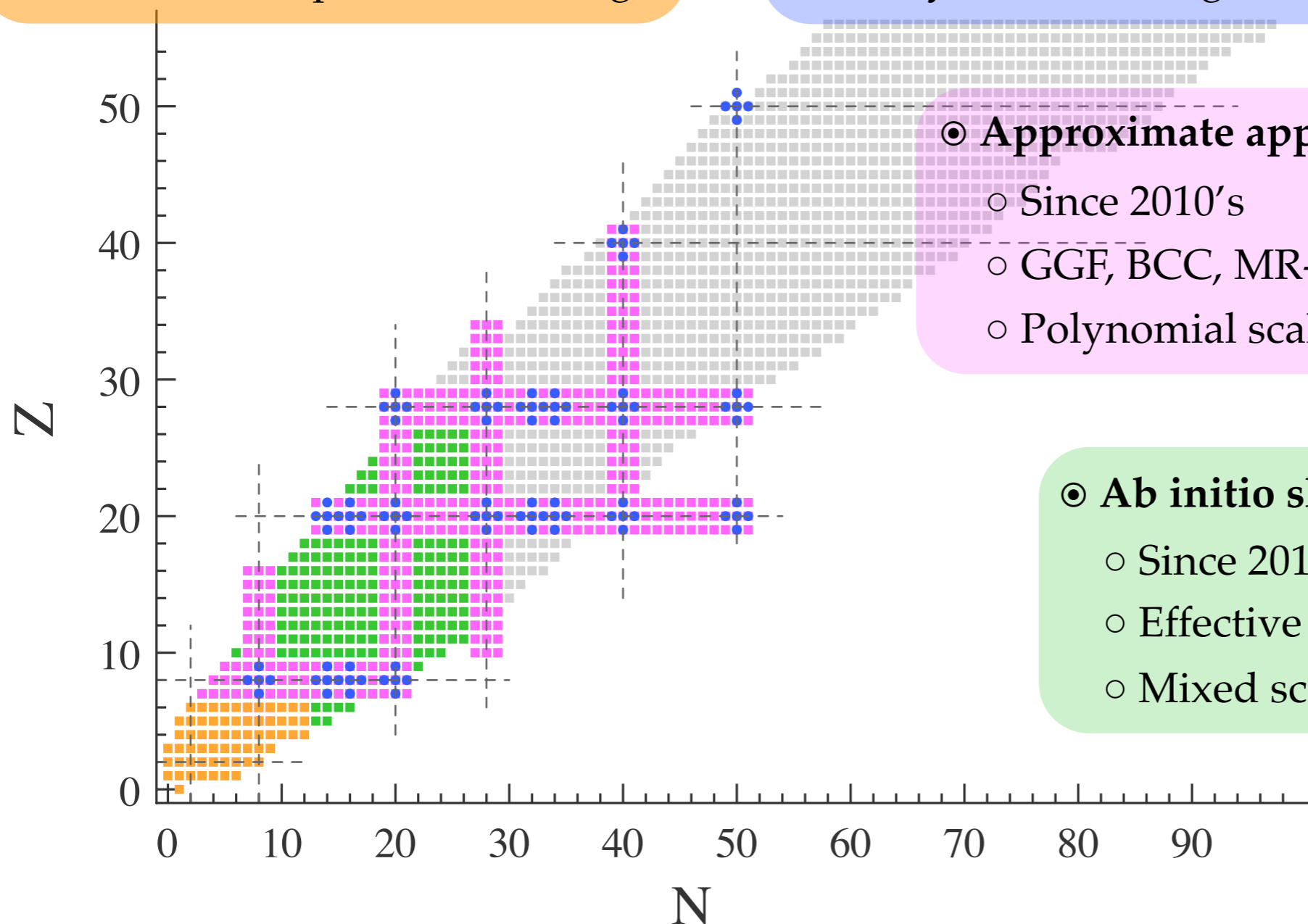**⊙ Approximate approaches for closed-shell nuclei**
- ○ Since 2000's
- ○ SCGF, CC, IMSRG
- ○ Polynomial scaling

⊙ Approximate approaches for open-shells
- ○ Since 2010's
- ○ GGF, BCC, MR-IMSRG
- ○ Polynomial scaling

⊙ Ab initio shell model
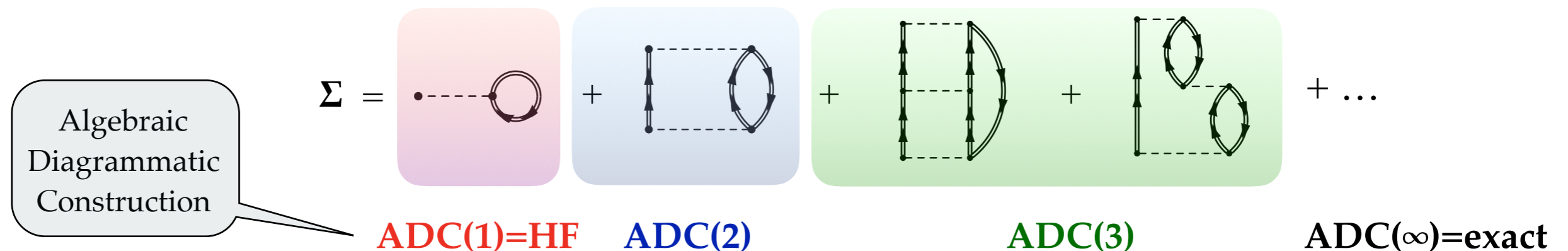- ○ Since 2014
- ○ Effective interaction via CC / IMSRG
- ○ Mixed scaling

Self-consistent Green's function approach

⊙ **Solution of the *A*-body Schrödinger equation** $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ **achieved by**

1) Rewriting it in terms of **1-, 2-, …. *A*-body objects** $G_1 = G$, $G_{2, \dots}$ G_A (**Green's functions**)

2) Expanding these objects in perturbation (in practise **G ⇒ one-body observables**, etc..)

○ **Self-consistent** schemes resum (infinite) subsets of perturbation-theory contributions

⊙ **Self-energy expansion**

Algebraic Diagrammatic Construction

$$\Sigma = \quad + \quad + \quad + \quad + \dots$$

ADC(1)=HF   **ADC(2)**   **ADC(3)**   **ADC(∞)=exact**

⊙ **Access a variety of quantities**

○ One-body GF → Ground-state properties of even-even *A* + spectra of odd-even neighbours

○ Two-body GF → Excited spectrum of even-even *A*

○ Self-energy → Optical potential for nucleon-nucleus scattering

Chiral effective field theory & nuclear interactions

⊙ Chiral EFT aims to provide a **systematic** framework to construct AN interactions (A=2, 3, …)

⊙ Main features:

   ○ High-energy physics unresolved → **soft potentials** → improved many-body convergence

   ○ Many-body forces and currents consistently derived

   ○ A **theoretical error** can be, in principle, assigned to each order in the expansion
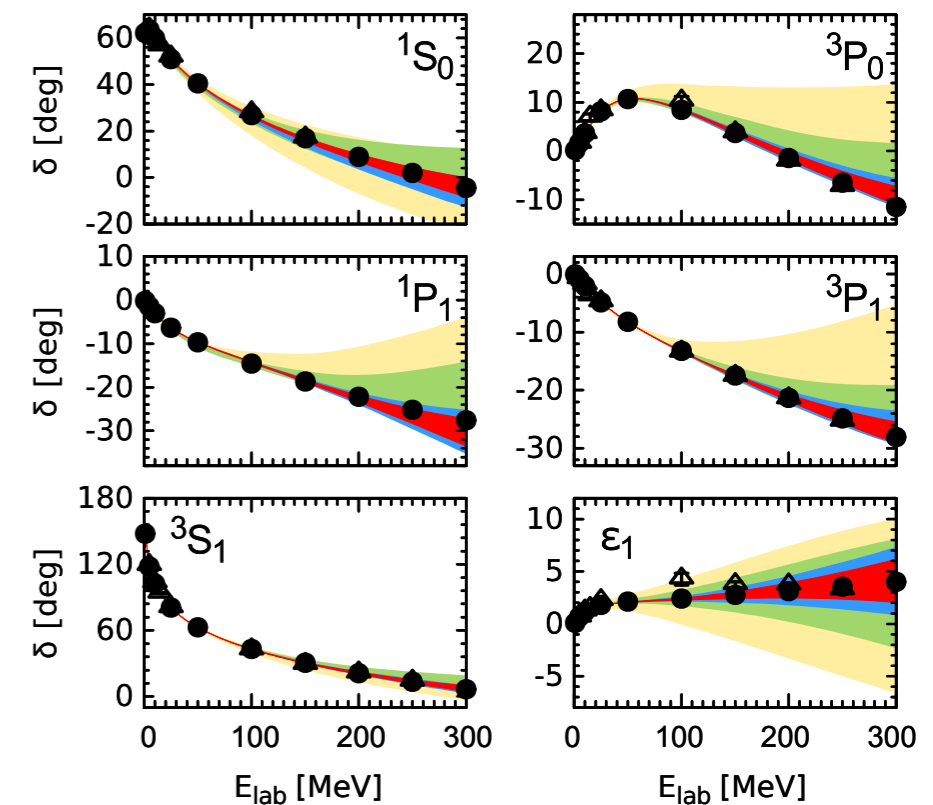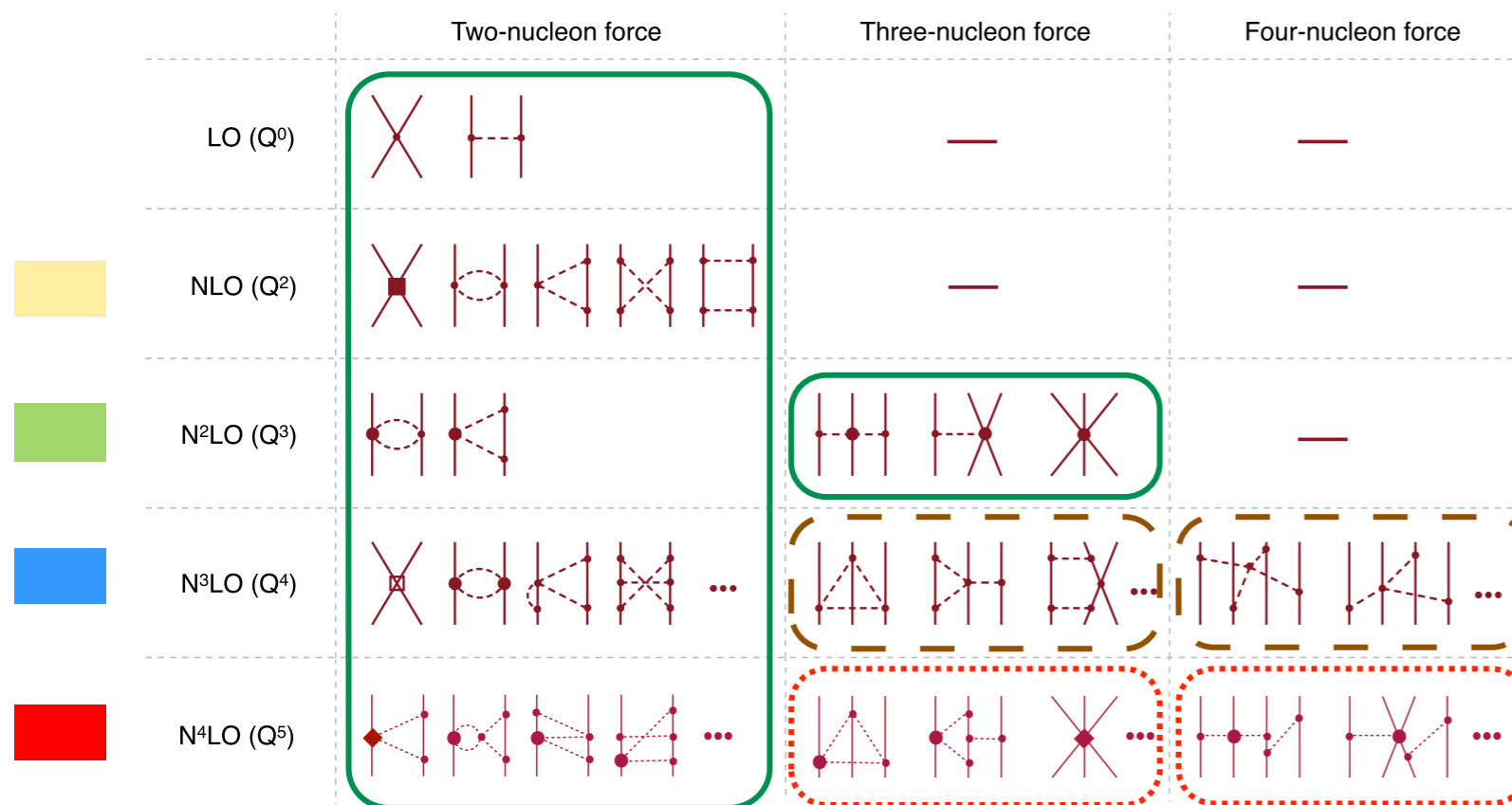
[Meißner 2016]

⇨ **Ideally: apply to the many-nucleon system (and propagate the theoretical error)**

Chiral effective field theory & nuclear interactions

⊙ Renormalisability ⟷ independence of UV physics

⊙ Most commonly used power counting scheme (Weinberg PC) not renormalisable

⊙ Two alternatives:

Fix-cutoff approach

○ Phenomenological success

○ *A posteriori* error estimate   [e.g. Epelbaum *et al.* 2015]

Renormalisable approach

○ Work in progress   [van Kolck, Pavon Valderrama, Long, ...]

○ Non-trivial impact on/from many-body approximations used   [Drissi *et al.* in preparation]

First "standard" interaction [(EM) N3LO]

obtained in large many-body spaces

Energy (MeV)

- MR-IM-SRG
- IT-NCSM
- SCGF
- Lattice EFT
- CC
- AME 2012

Mass Number A
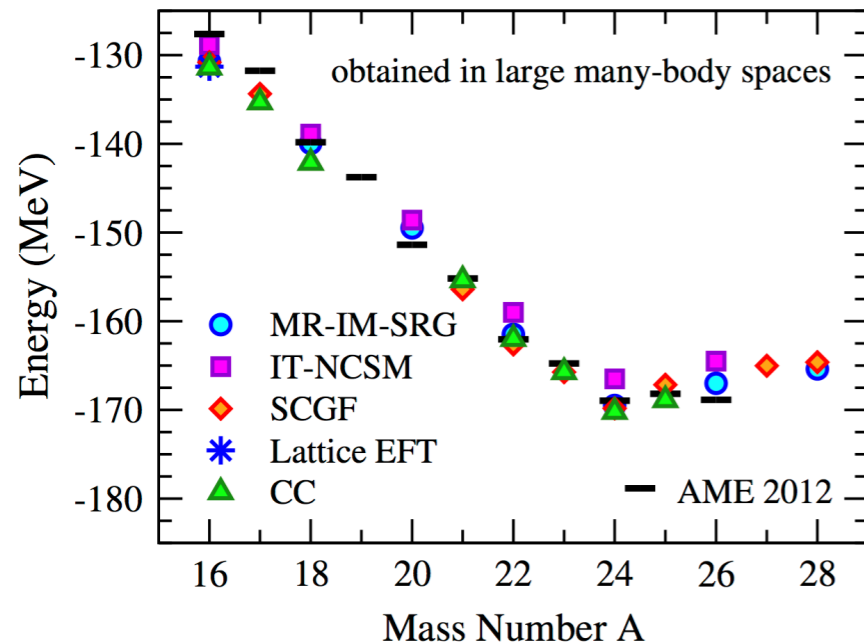
[Hebeler *et al.* 2015]

✔ **Successful benchmarks**

- Experiment
- NN + 3N (full)
- NN + 3N (ind.)
- SM (NN + 3N)
- CC

S_{2n} [MeV]

^{A}Ca
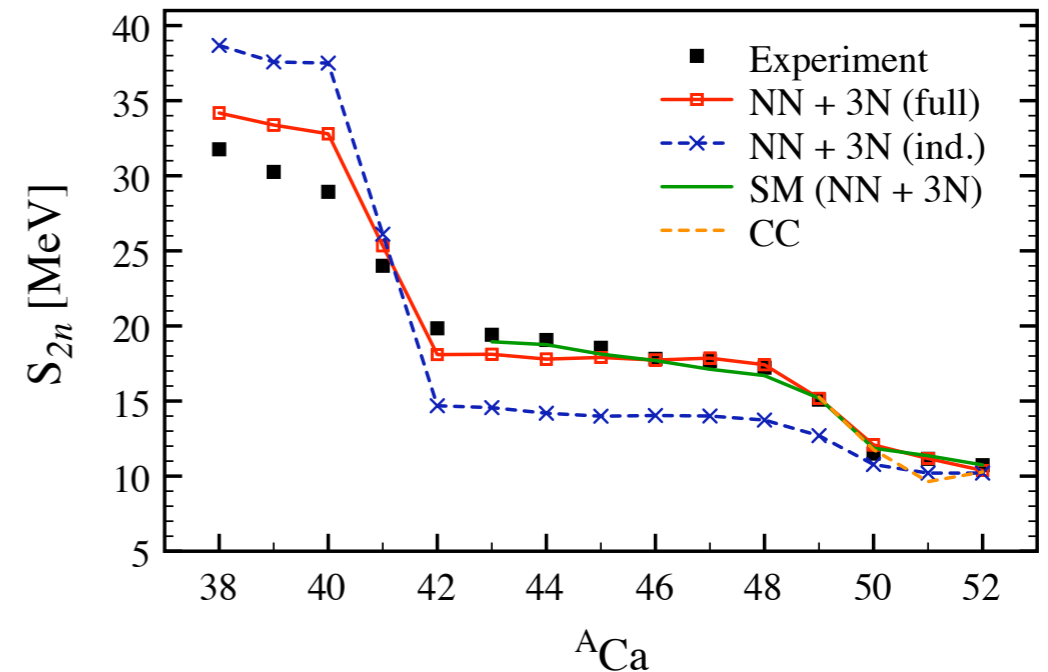
[Somà, *et al.* 2014]

✔ *N=28 gap reproduced*

- GGF [NN + 3N (ind.)]
- GGF [NN + 3N (full)]
- ADC(3) "corrected"
- IM-SRG [NN + 3N (full)]

$N_{max} = 9$

$N_{max} = 13$

E_0^A [MeV]

$N_{max} = 13$

^{A}Ca
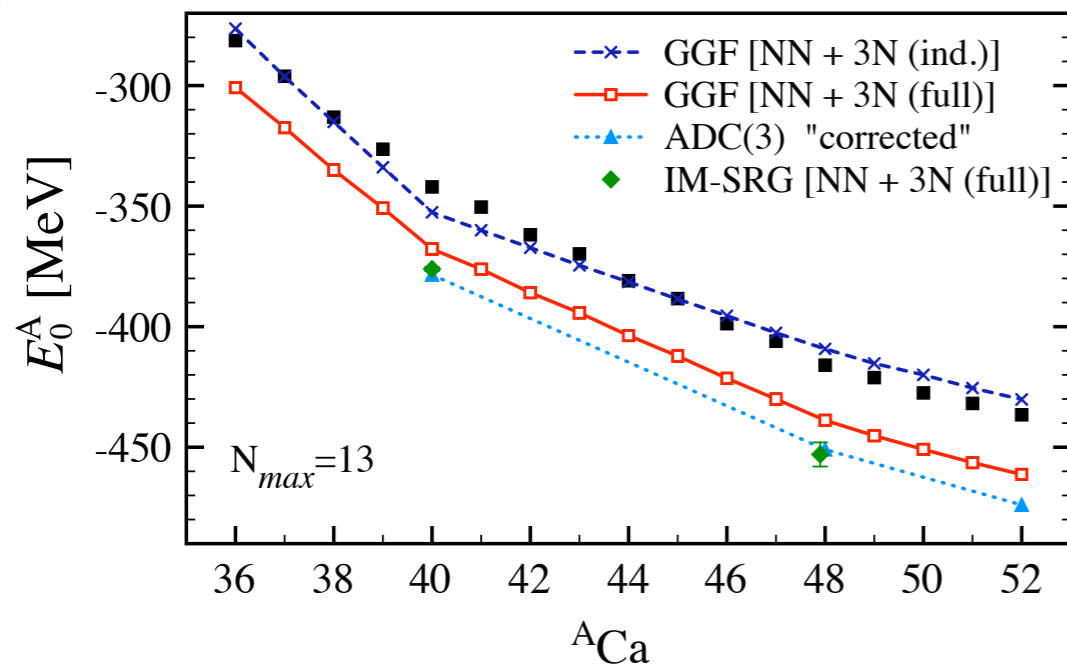
[Somà, *et al.* 2014]

✗ **Overbinding**

- Exp.
- EM

r_{ch} [fm]

^{16}O ^{40}Ca ^{50}Ca ^{58}Ni ^{64}Ni

^{18}O ^{48}Ca ^{52}Ca ^{60}Ni
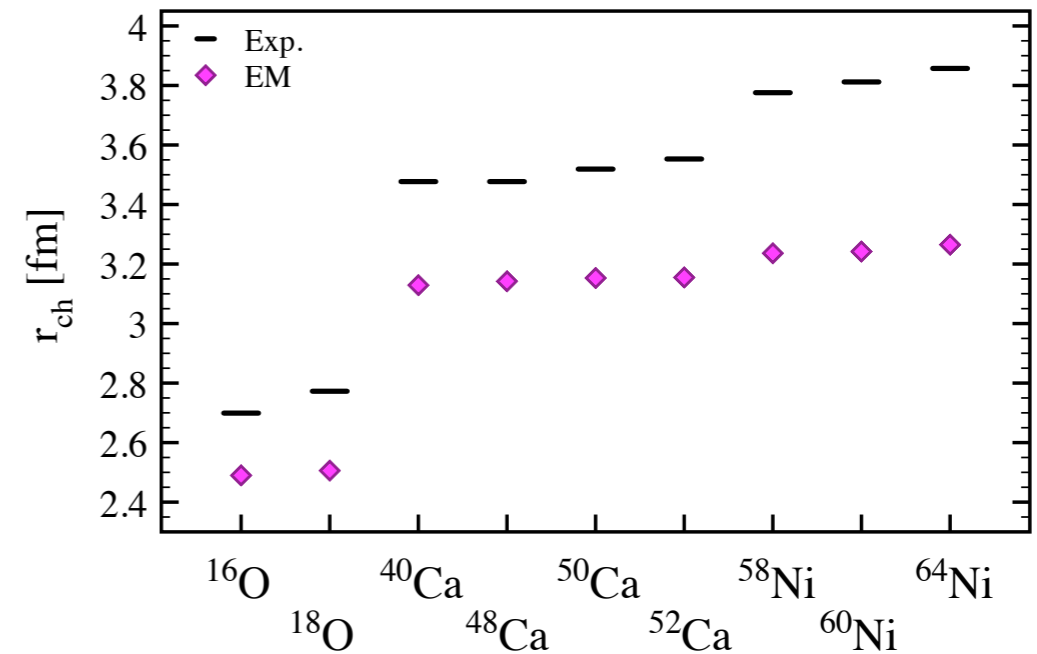
✗ **Radii underestimated**

Testing interactions, pt. 1

[Simonis et al. 2017]
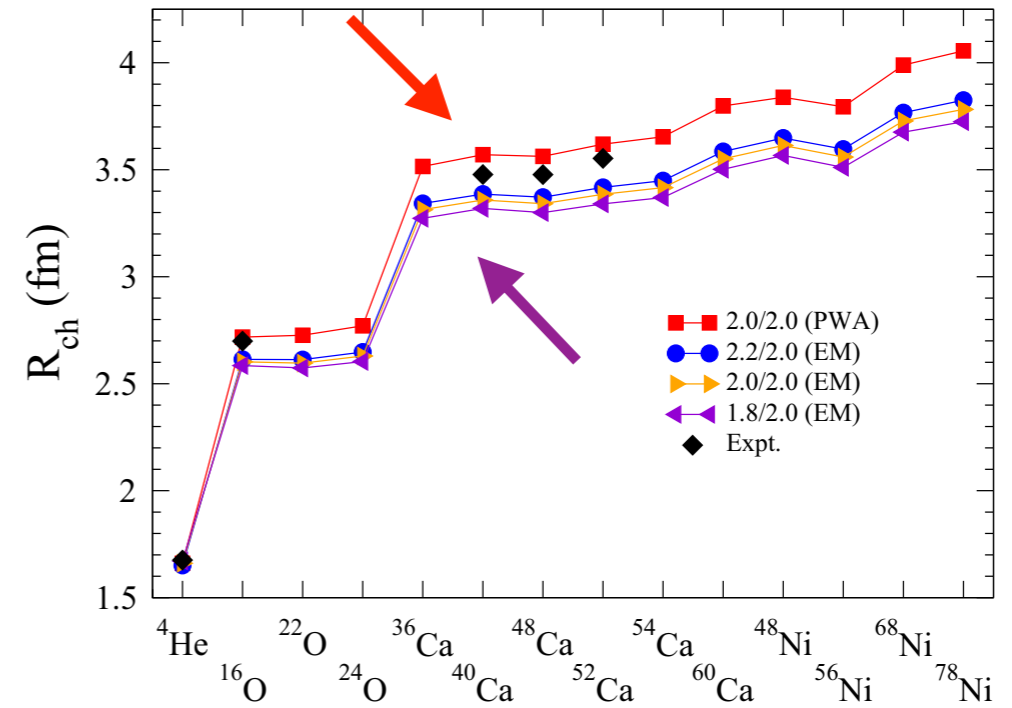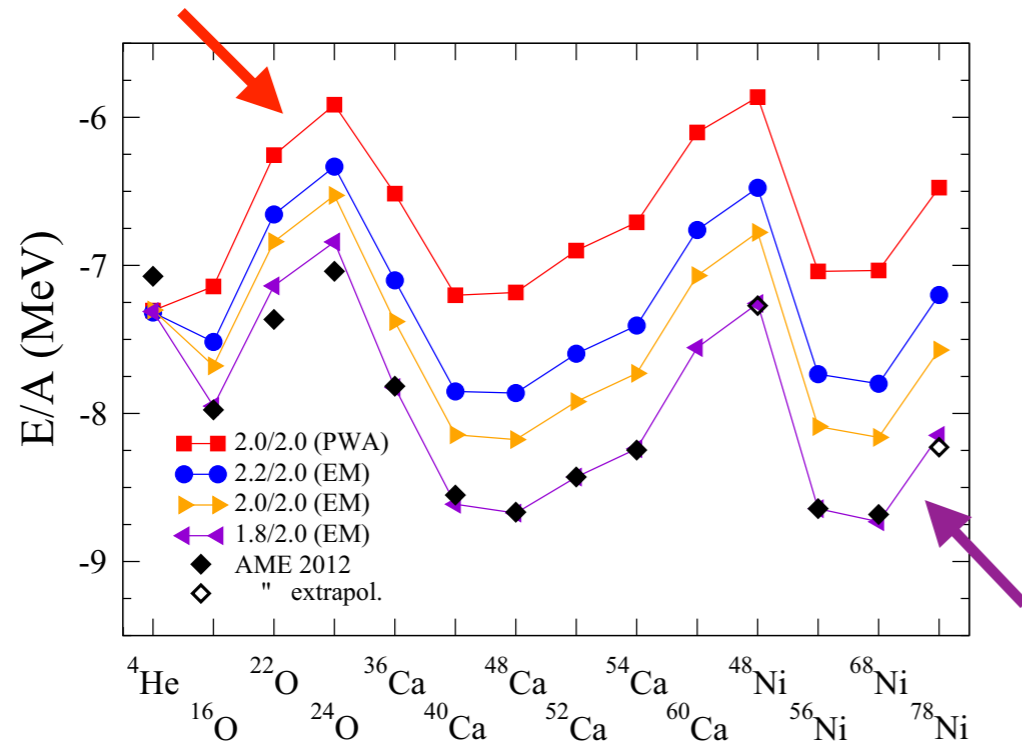
[Drischler et al. 2017]
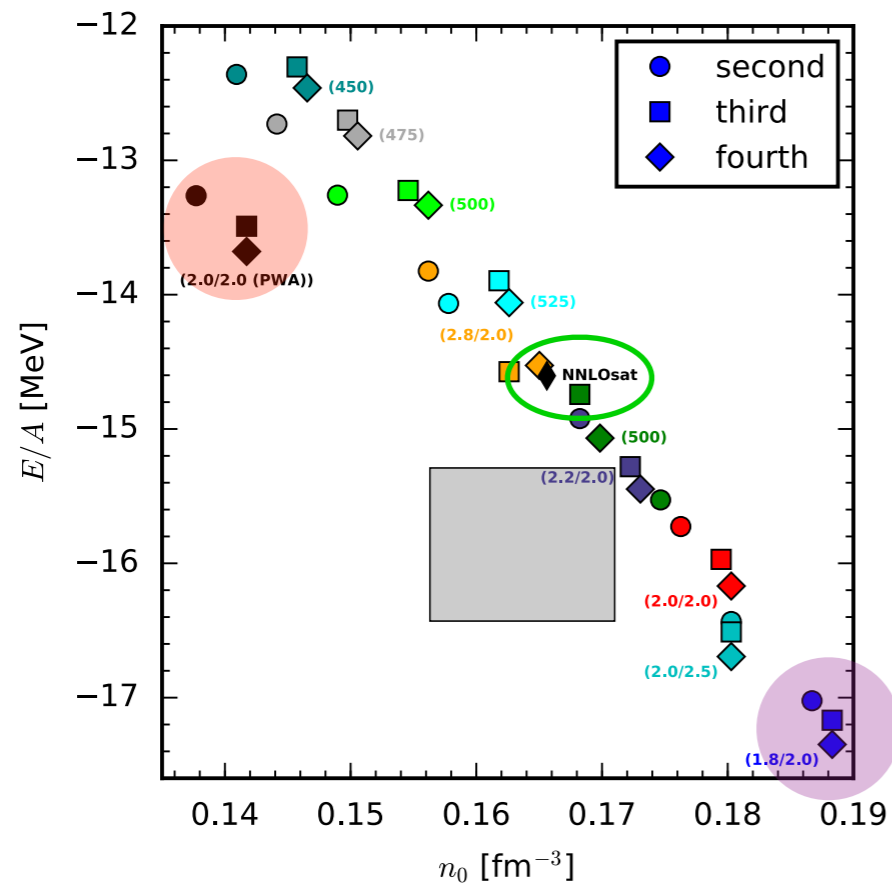
○ "Family" of SRG-evolved interactions

○ Radii ~OK only with strong underbinding

○ Correlation with saturation properties

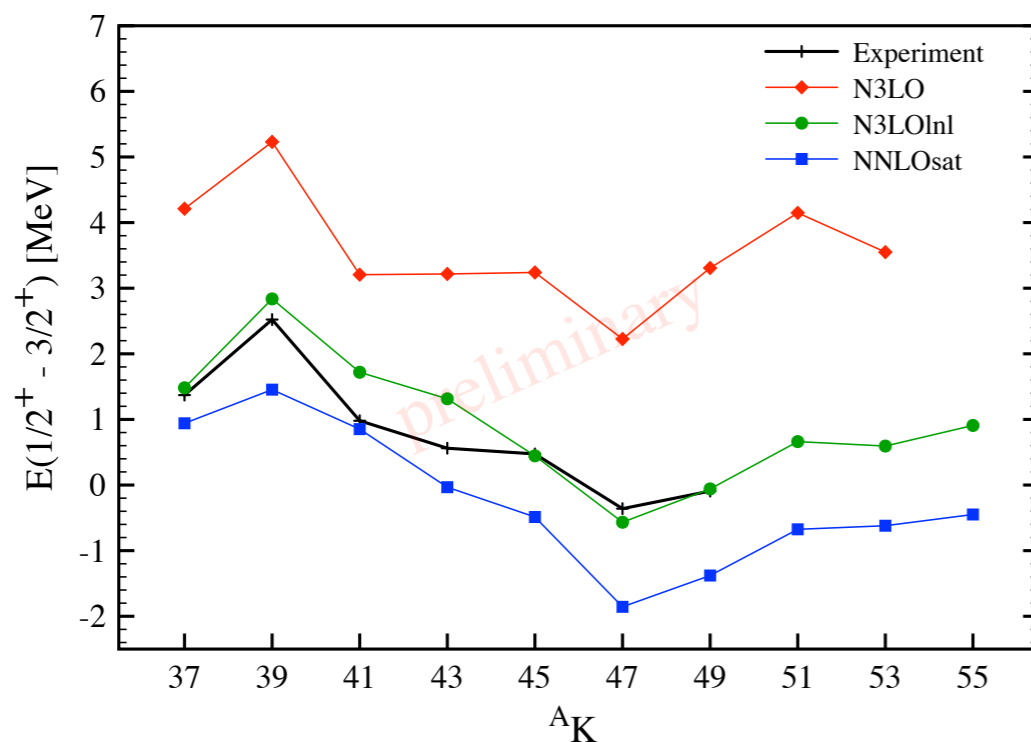○ More sophisticated studies needed!

Testing interactions, pt. 2

Total energies

Charge radii

Low-lying spectra

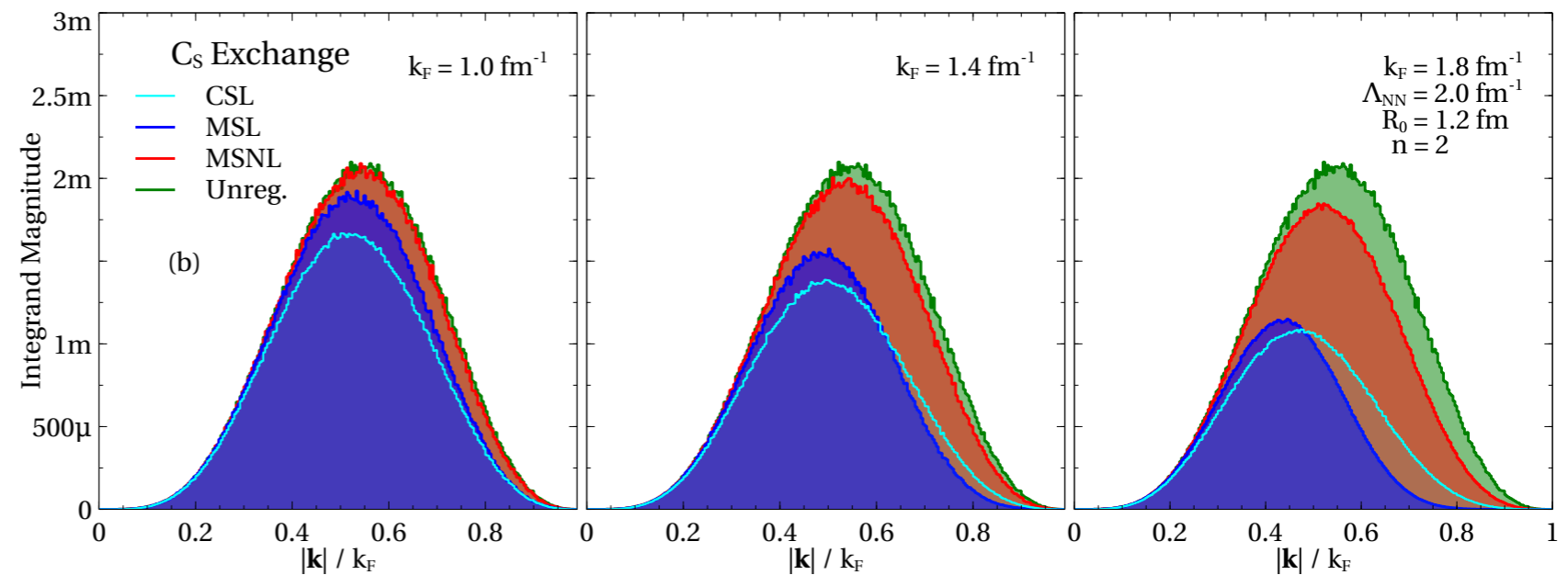[Somà *et al.* in preparation]

○ New interactions correct for overbinding

○ Radii OK when fitted!

○ NNLO$_{sat}$ not great e.g. in pf shell

○ Producing N3LO$_{sat}$ not straightforward

Re

○ **Regularisation scheme is a major source of variation** among currently employed Hamiltonians
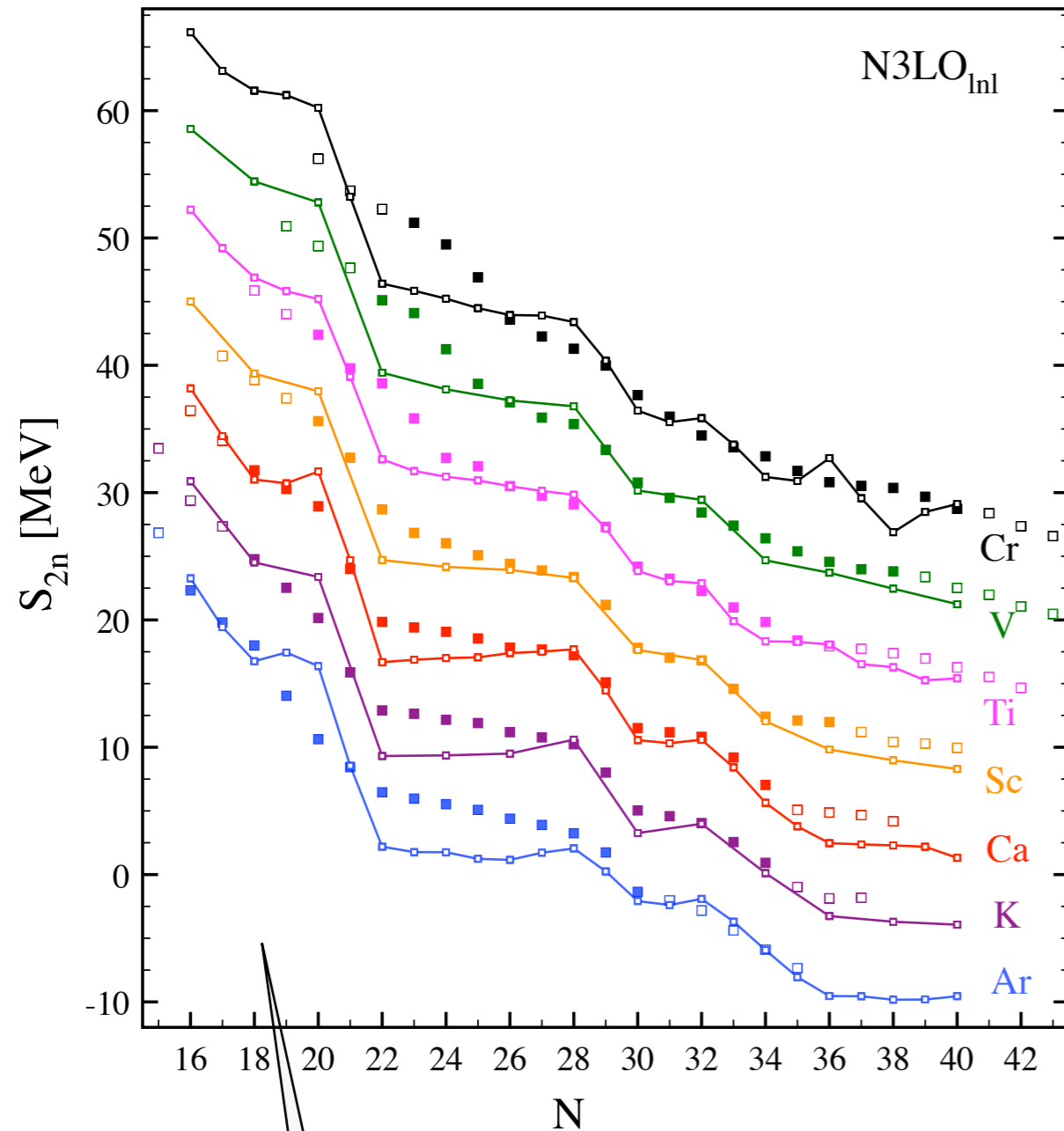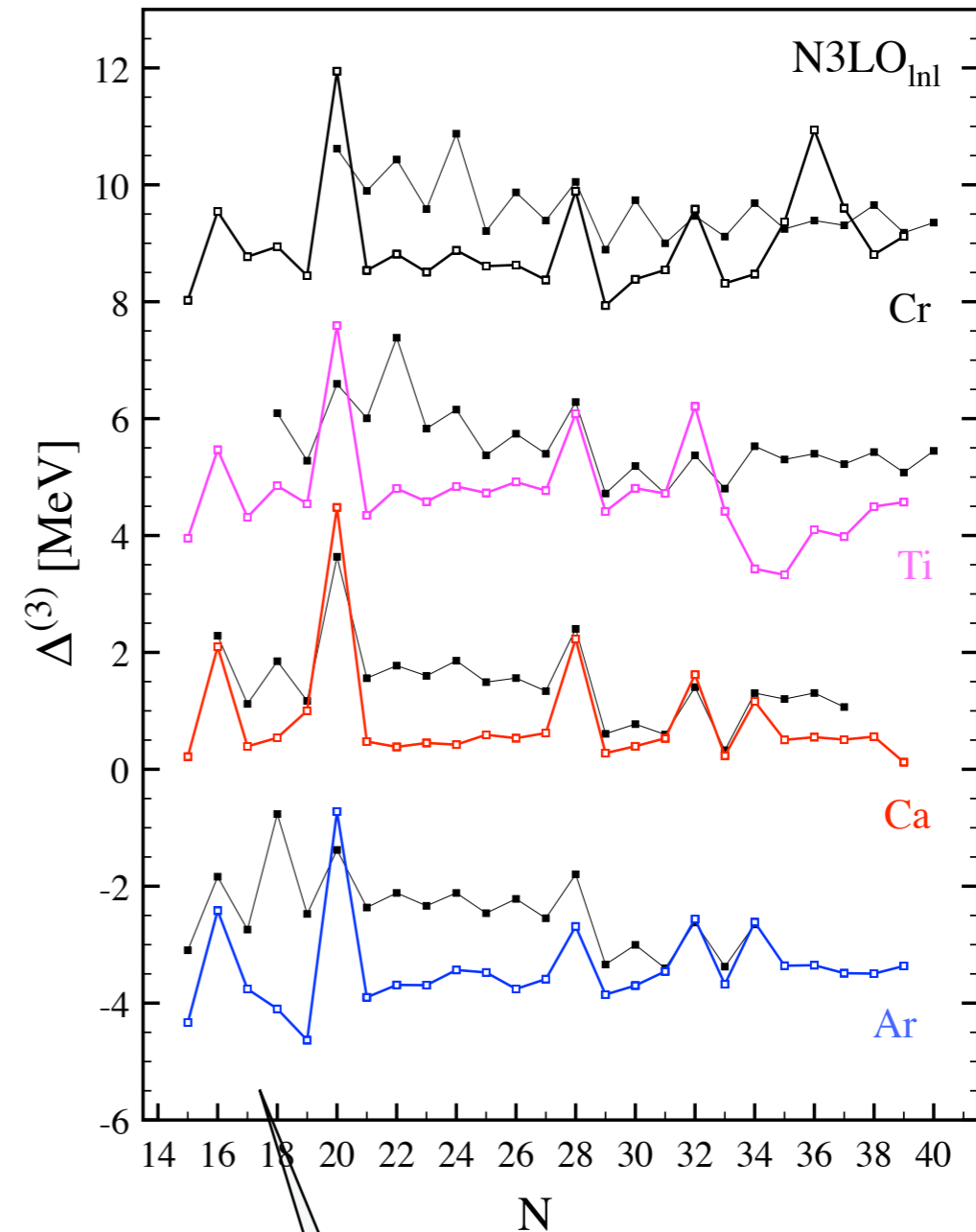
○ Effects on 2N phase space

○ Effects on 3N phase space
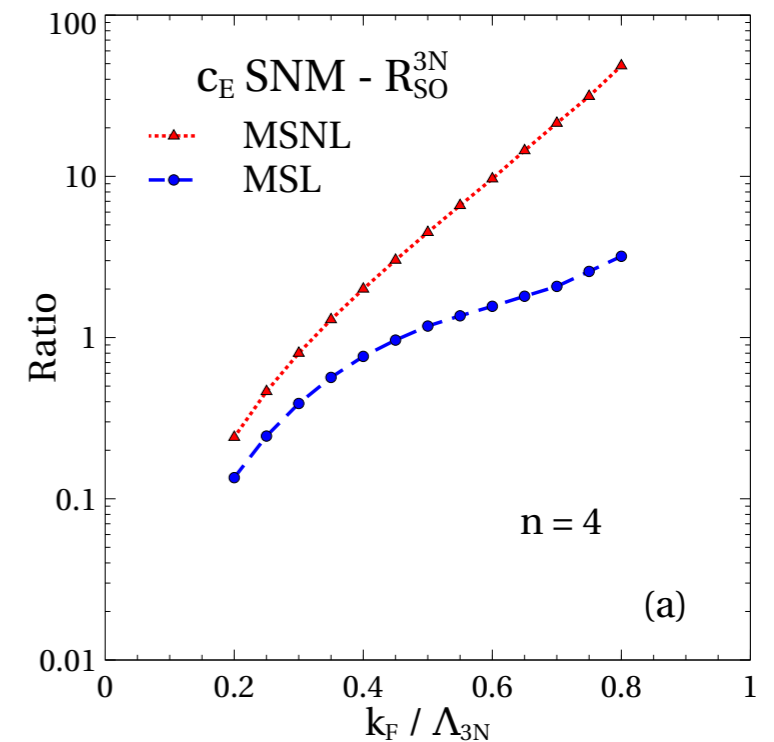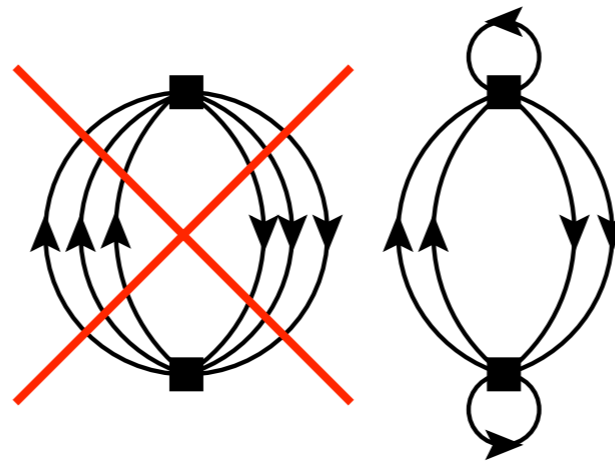
[Dyhdalo, Furnstahl, Hebeler, Tews 2016]
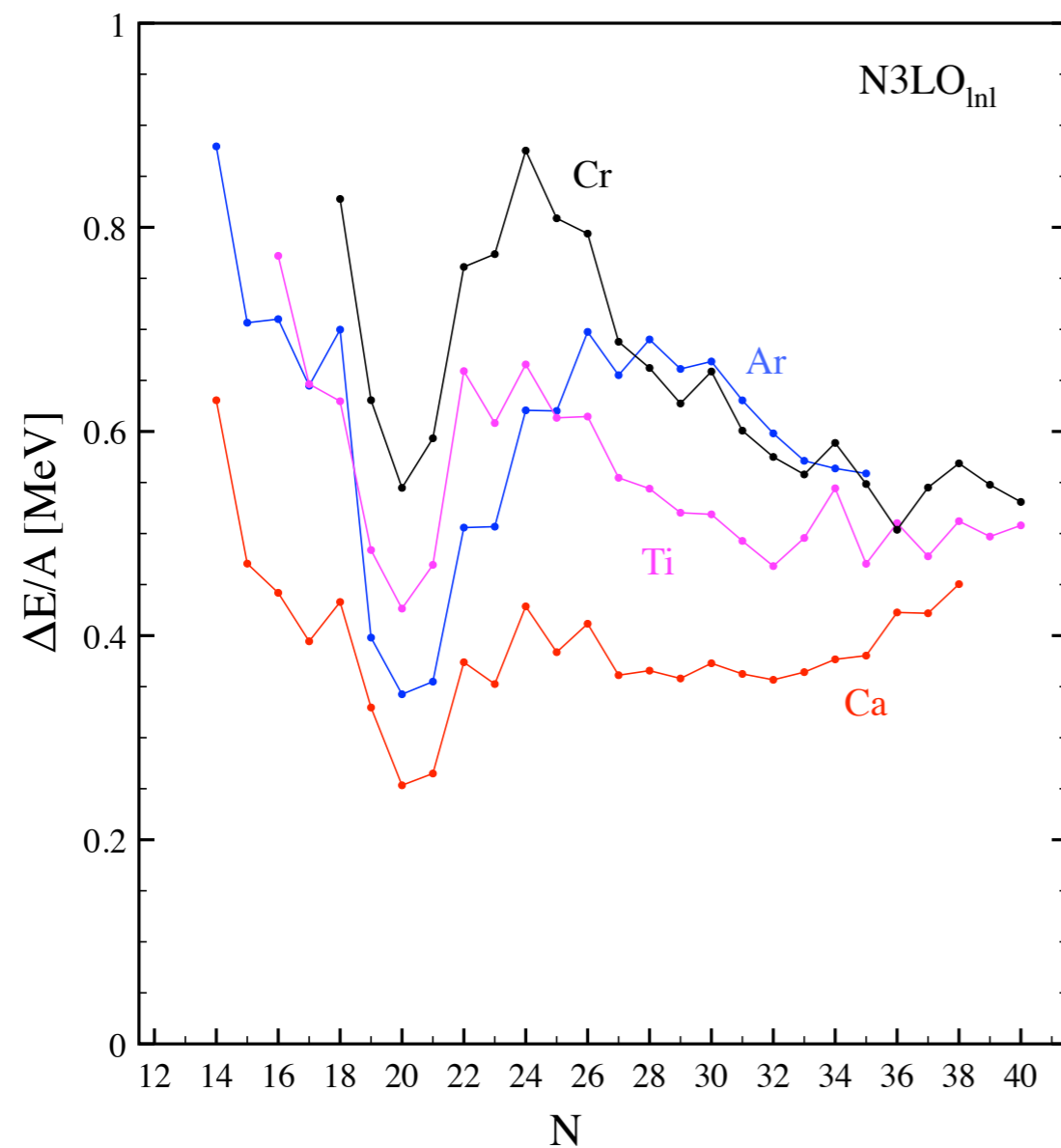
Emergence of magic numbers "ab initio"

N3LO_lnl

S_2n [MeV]

Cr
V
Ti
Sc
Ca
K
Ar

N

✗ N = 20 overestimated

✓ Good agreement for N ≥ 28

N3LO_lnl

$\Delta^{(3)}$ [MeV]

[Somà et al. in preparation]

Cr

Ti

Ca

Ar

N

✓ Main gaps nicely emerge!

✗ Pairing too weak in f_{7/2}

⊙ **Currently, description of doubly open-shell nuclei quantitatively worsens with deformation**
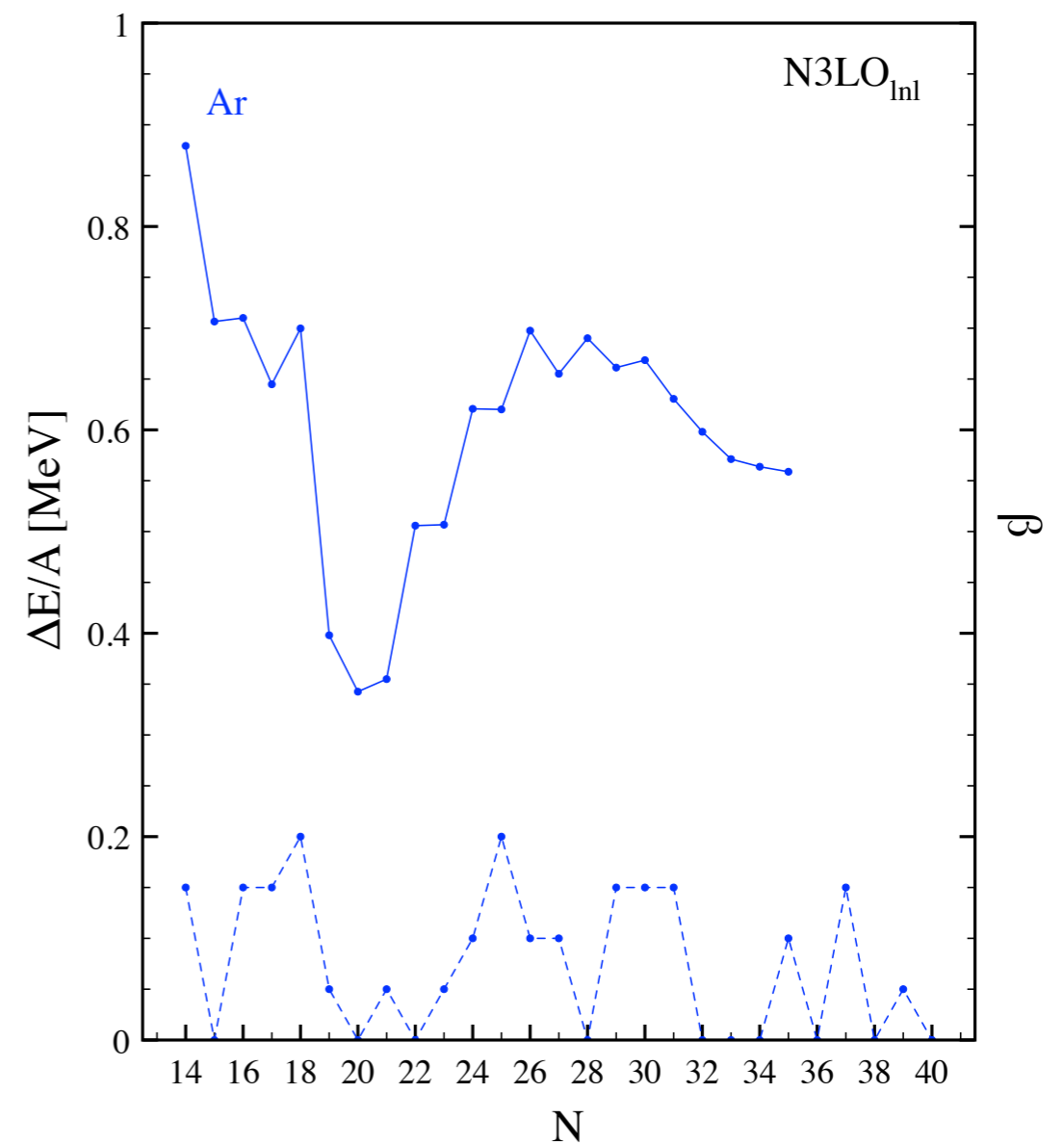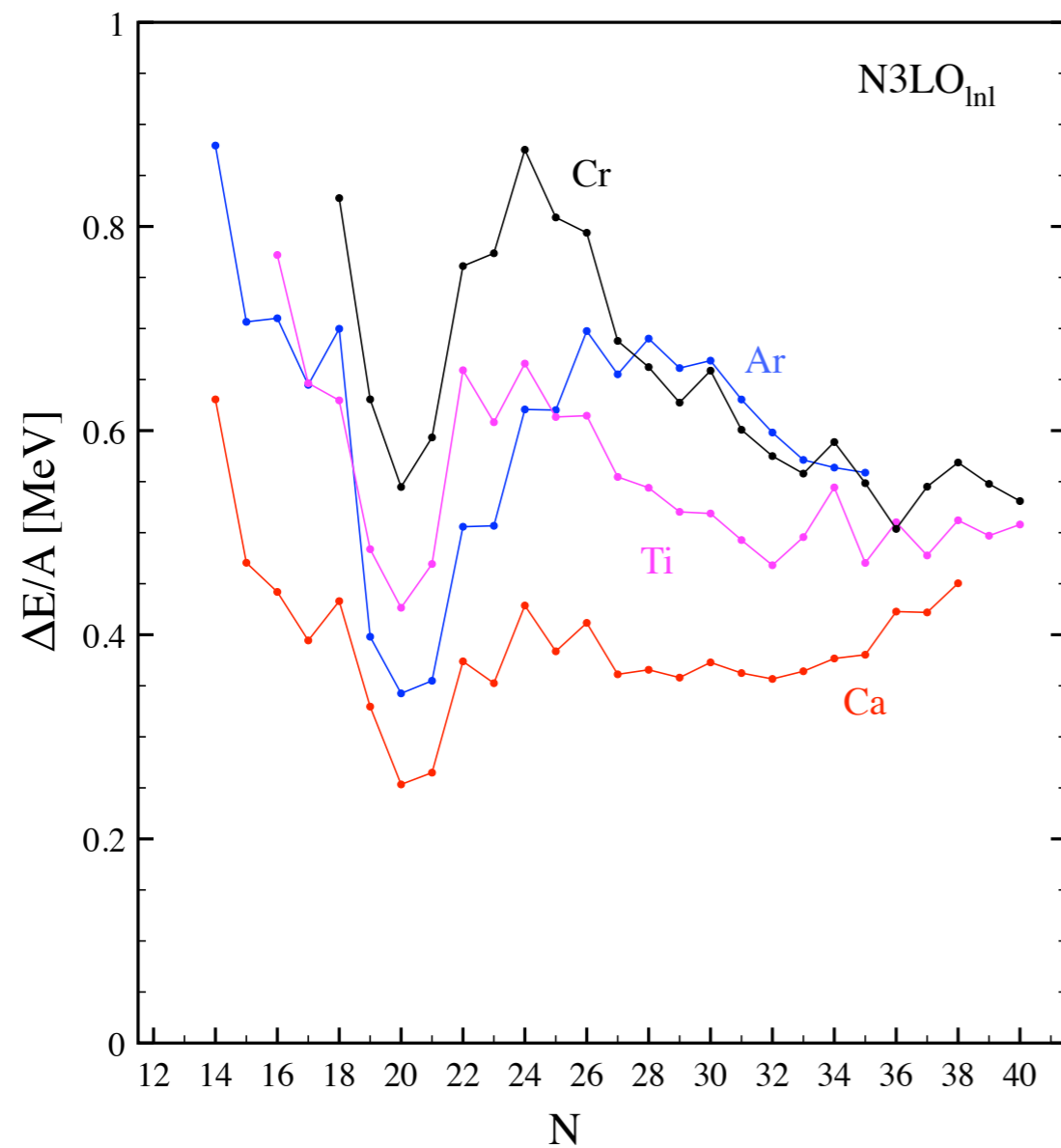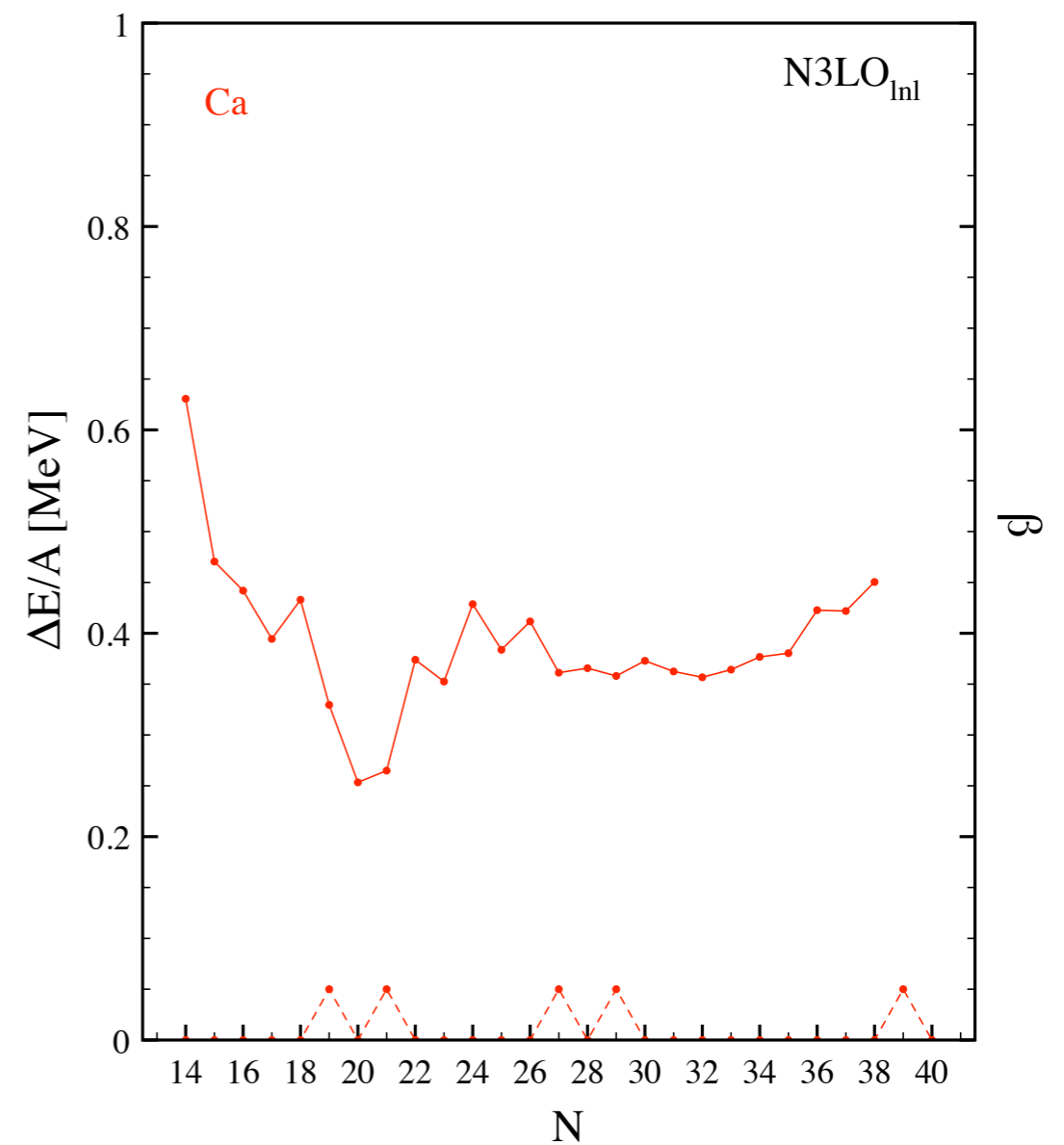

[Somà *et al.* in preparation]

Doubly open-shell nuclei

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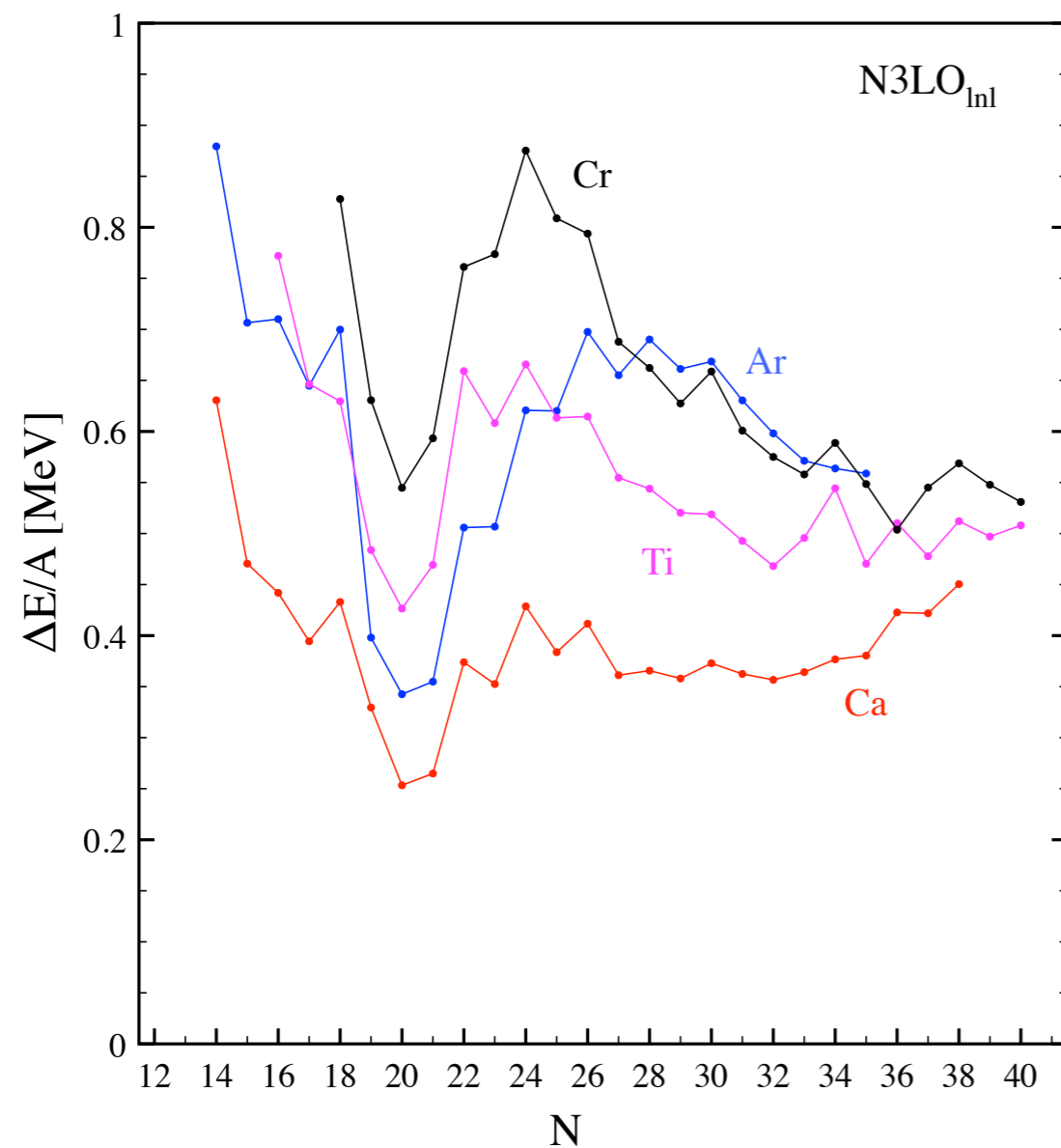⇨ Correlation with deformation parameter β   [Hilaire & Girod 2007]

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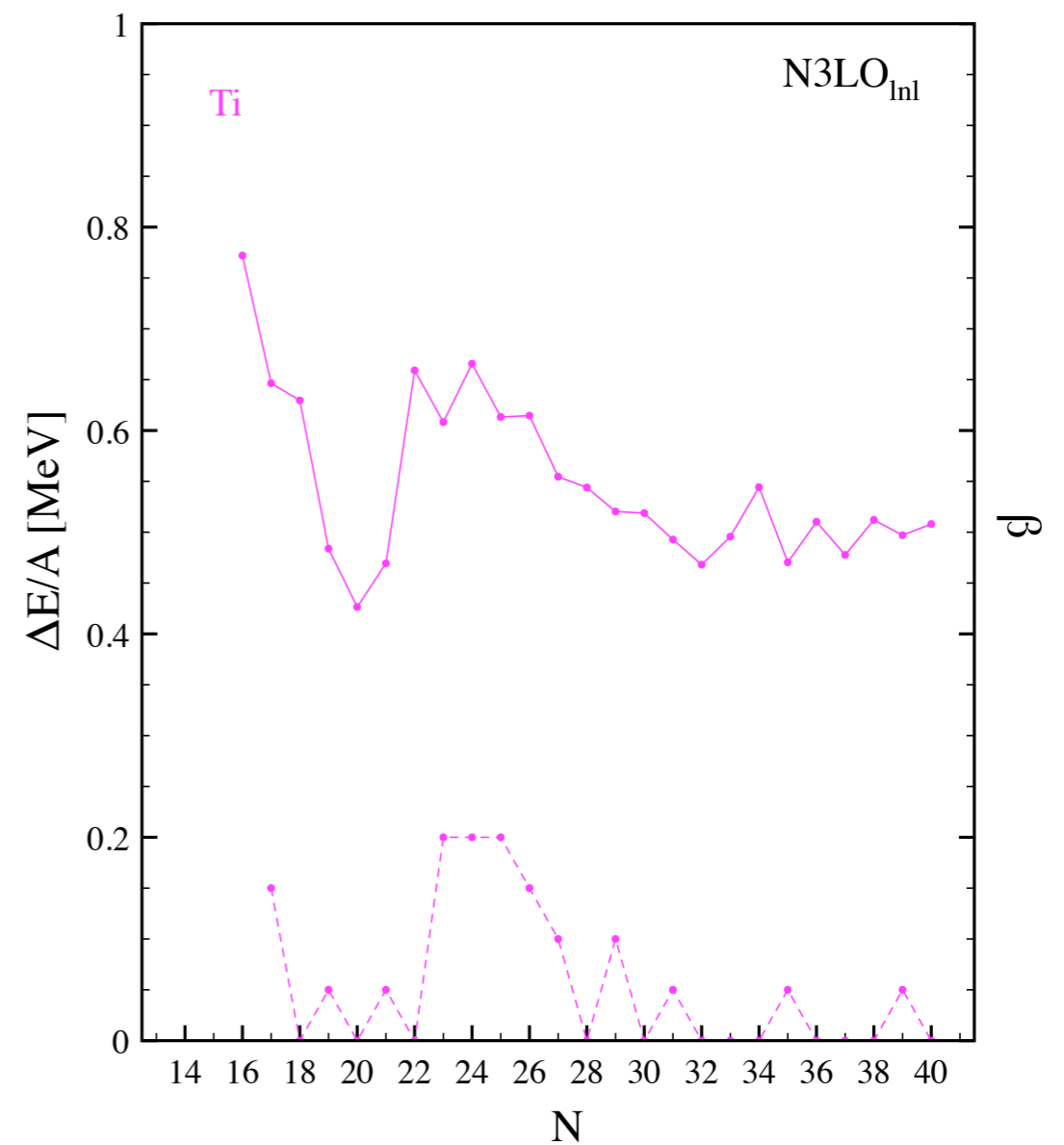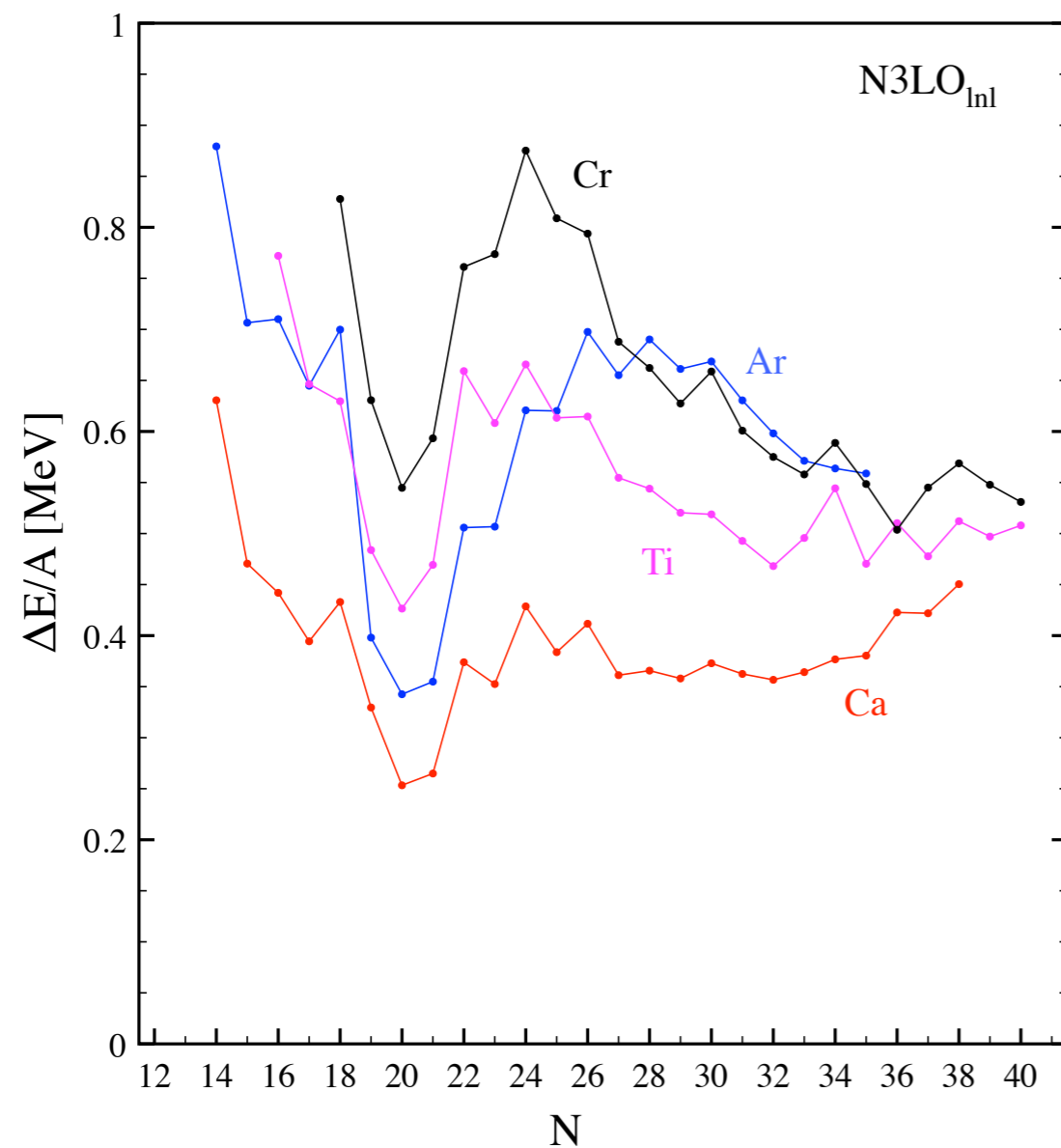⇨ Correlation with deformation parameter β   [Hilaire & Girod 2007]

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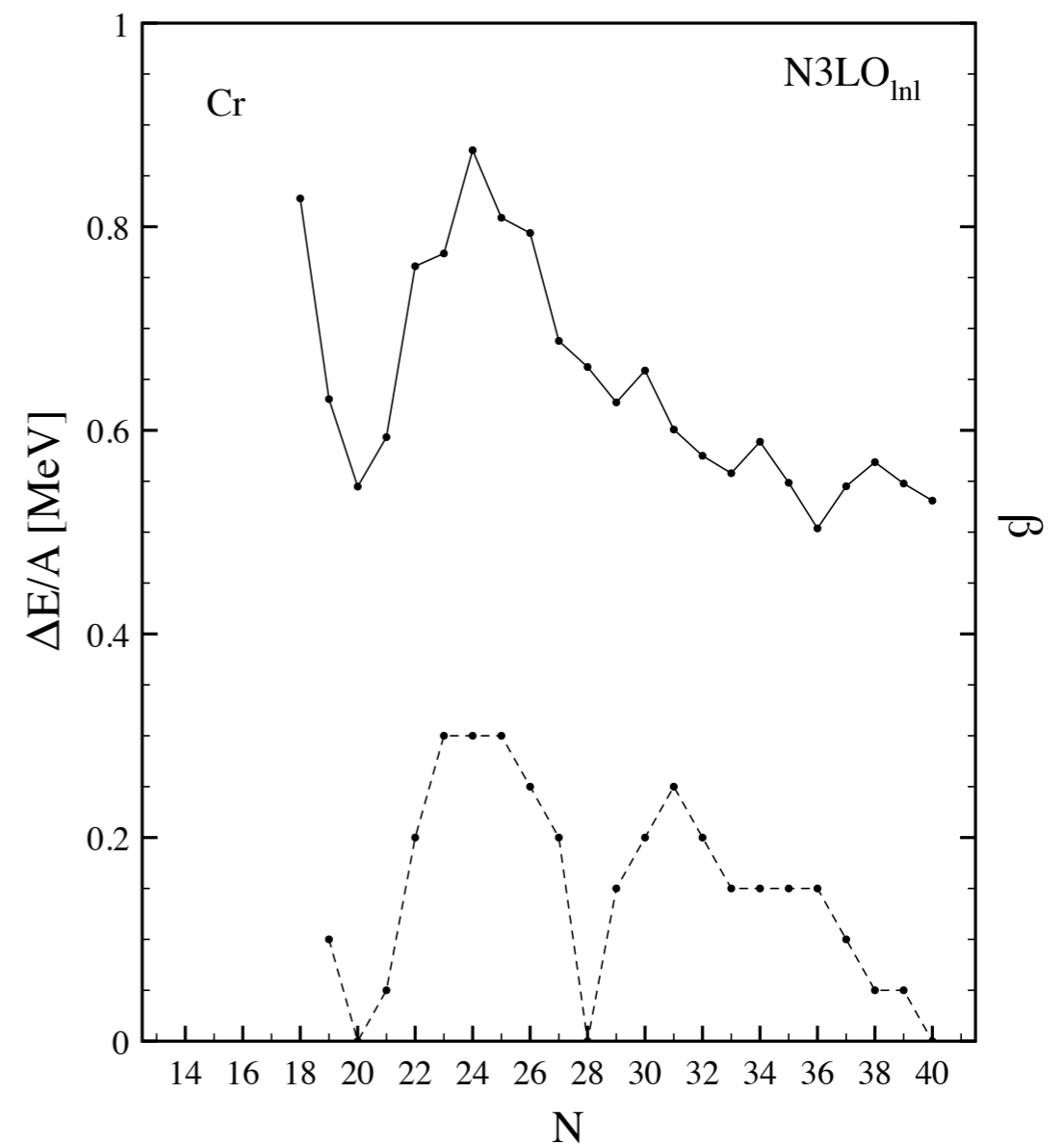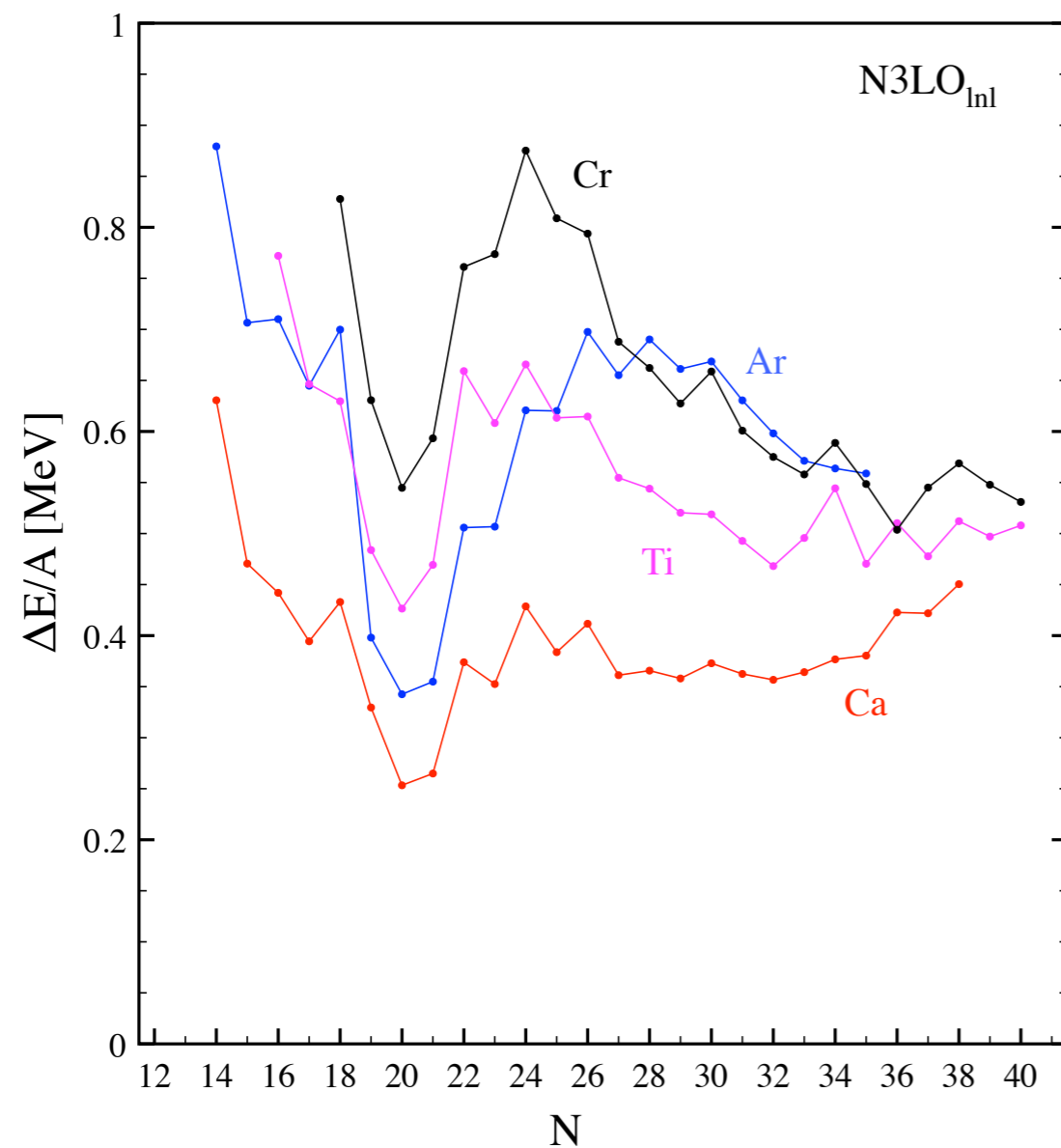

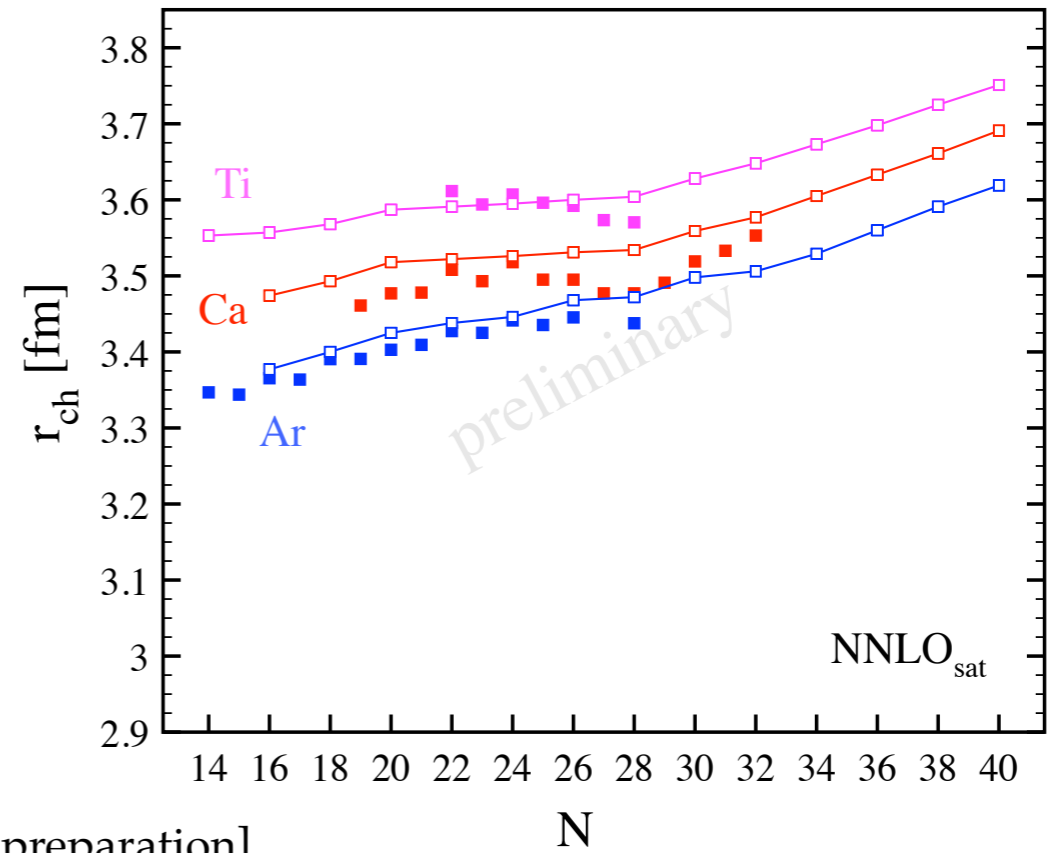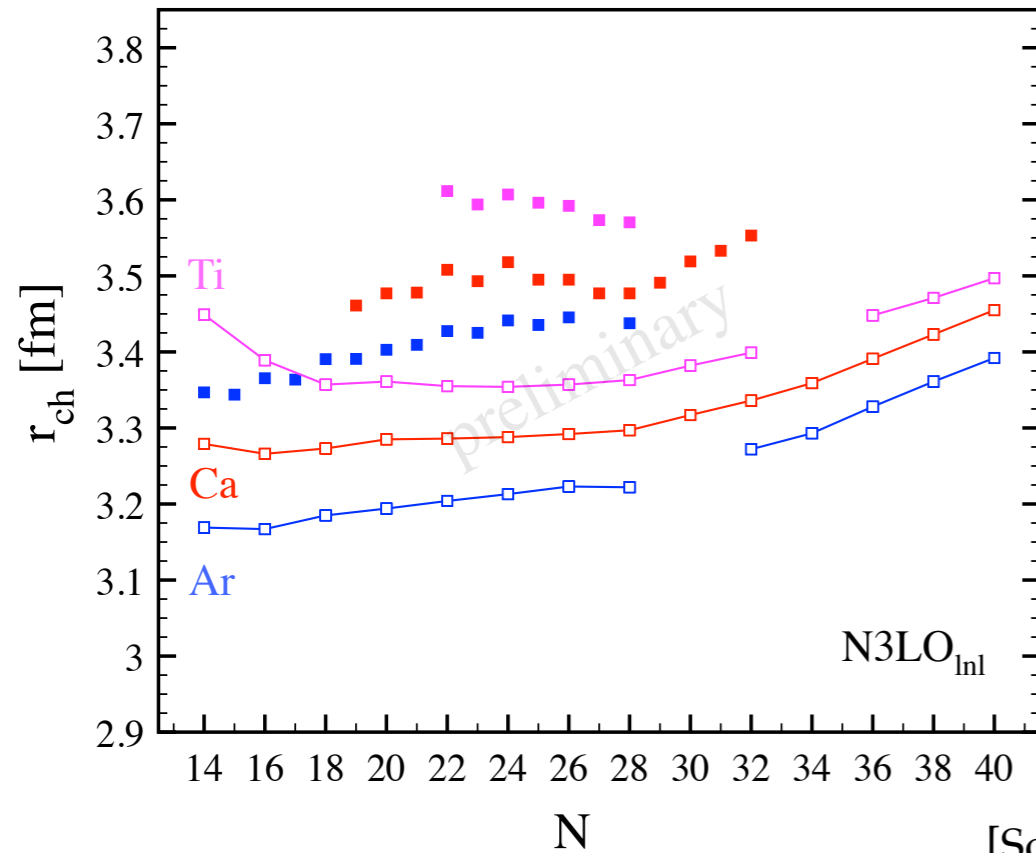[Somà *et al.* in preparation]

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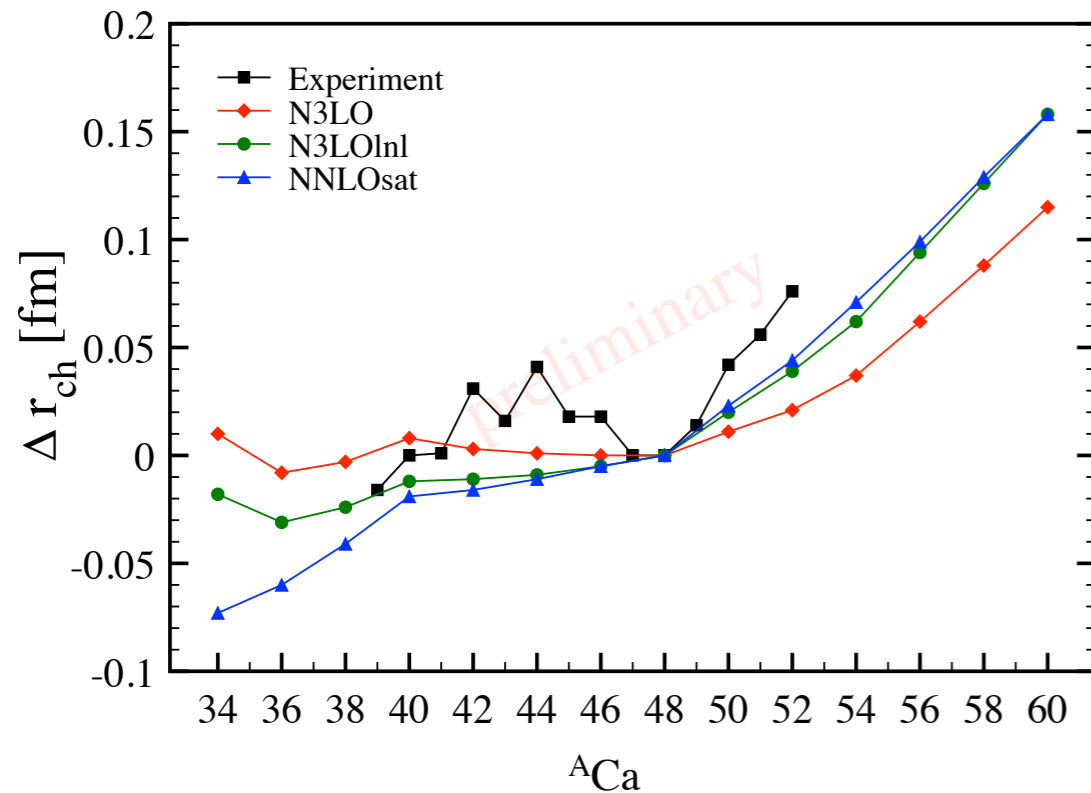

[Somà *et al.* in preparation]

Charge radii

[Somà *et al.* in preparation]

○ Qualitative difference in absolute

○ Ca chain challenge even for NNLO$_{sat}$

○ Similar isotopic trend

○ SRG evolution overlooked?

The case of ^{34}Si

⊙ **Unconventional depletion** ("bubble") in the centre of ρ_{ch} conjectured for certain nuclei

⊙ **Purely quantum mechanical effect**

   ○ $\ell = 0$ orbitals display radial distribution peaked at $r = 0$

   ○ $\ell \neq 0$ orbitals are instead suppressed at small r

   ○ Vacancy of s states ($\ell = 0$) embedded in larger-ℓ orbitals might cause central depletion

⊙ **Conjectured associated effect on spin-orbit splitting**

   ○ Non-zero derivative at the interior

   ⬇

   ○ Spin-orbit potential of "non-natural" sign

   ⬇

   ○ Reduction of (energy) splitting of low-ℓ spin-orbit partners

⊙ Bubbles predicted for hyper-heavy nuclei   [Dechargé *et al.* 2003]

⊙ In light/medium-mass nuclei the **most promising candidate is ^{34}Si**
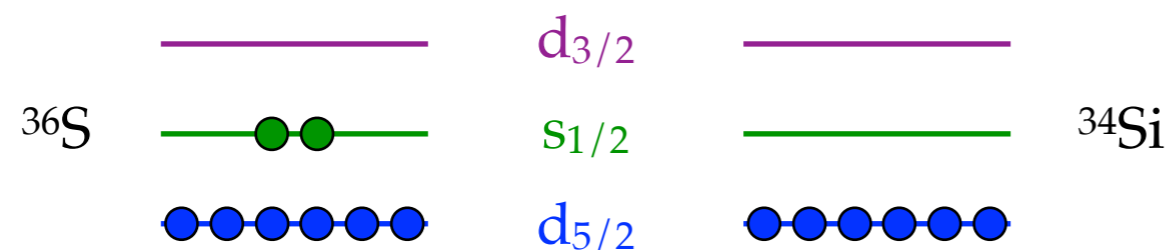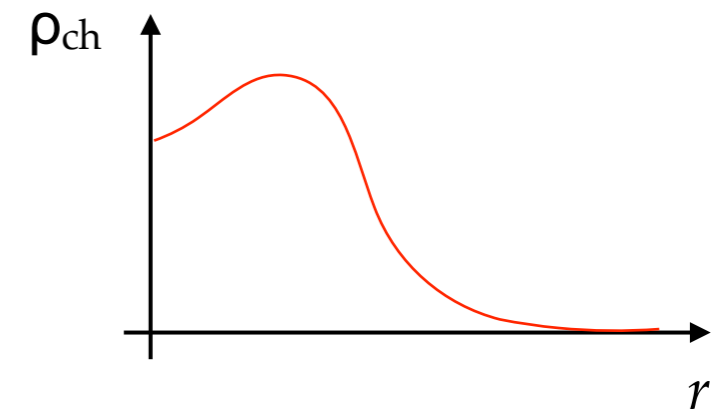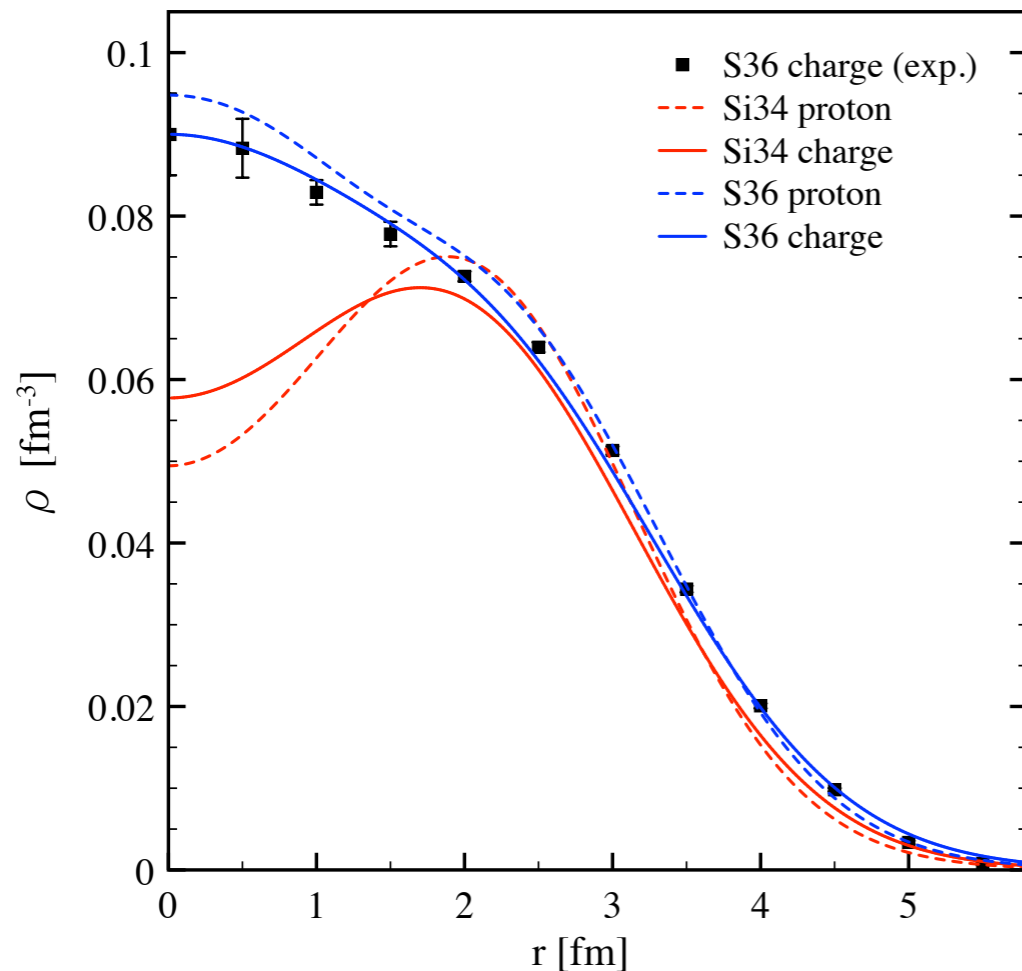
[Todd-Rutel *et al.* 2004, Khan *et al.* 2008, …]

The case of ^{34}Si

⊙ Good reproduction of g.s. properties

E [MeV]	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	-84.481	-274.626	-282.938	-283.427
^{36}S	-90.007	-296.060	-305.767	-308.714

$\langle r_{ch}^2 \rangle^{1/2}$	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	3.270	3.189	3.187	-
^{36}S	3.395	3.291	3.285	3.2985 $\pm$ 0.0024

⊙ **Mild central depletion predicted**

⇨ Charge density computed via folding with the finite charge of the proton

⇨ Folding smears out central depletion

⇨ Excellent agreement with experimental charge distribution of ^{36}S
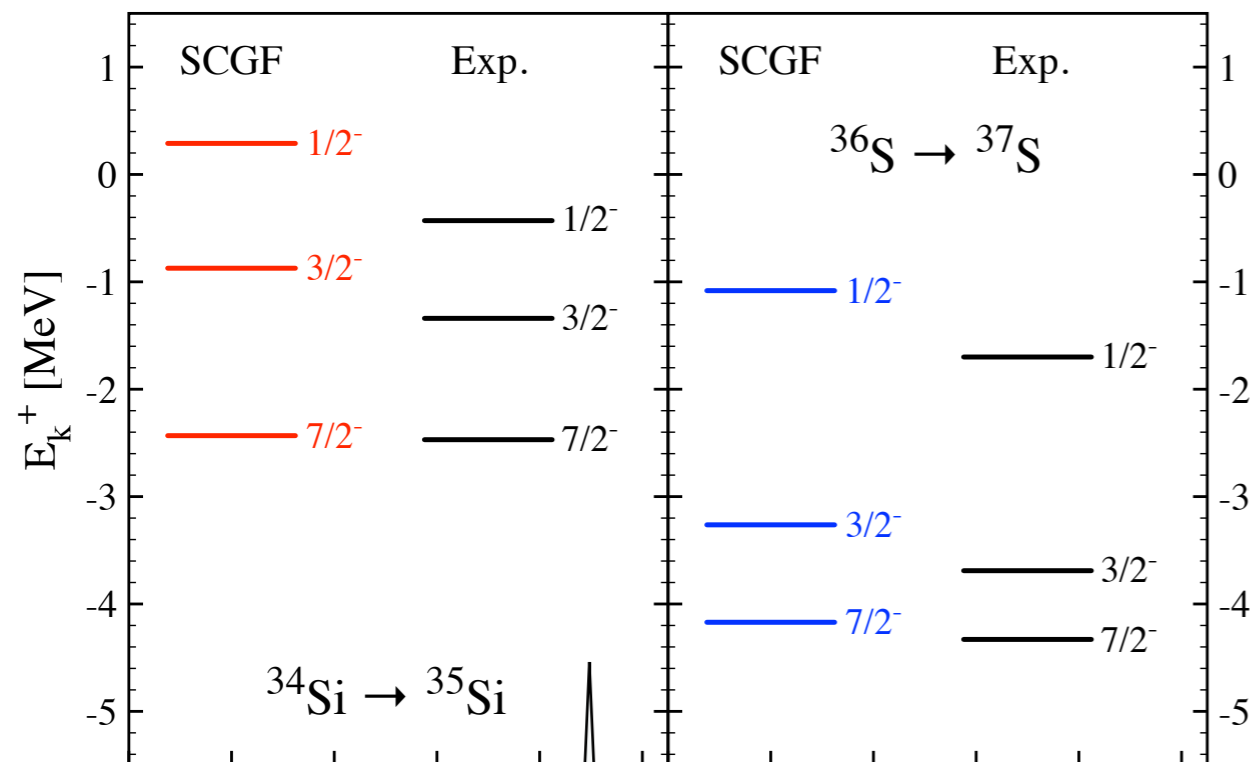
[Duguet *et al.* 2017]

The case of ^{34}Si

⊙ Addition and removal spectra compared to **transfer** and **knock-out reactions**

One-neutron addition

Exp. data:
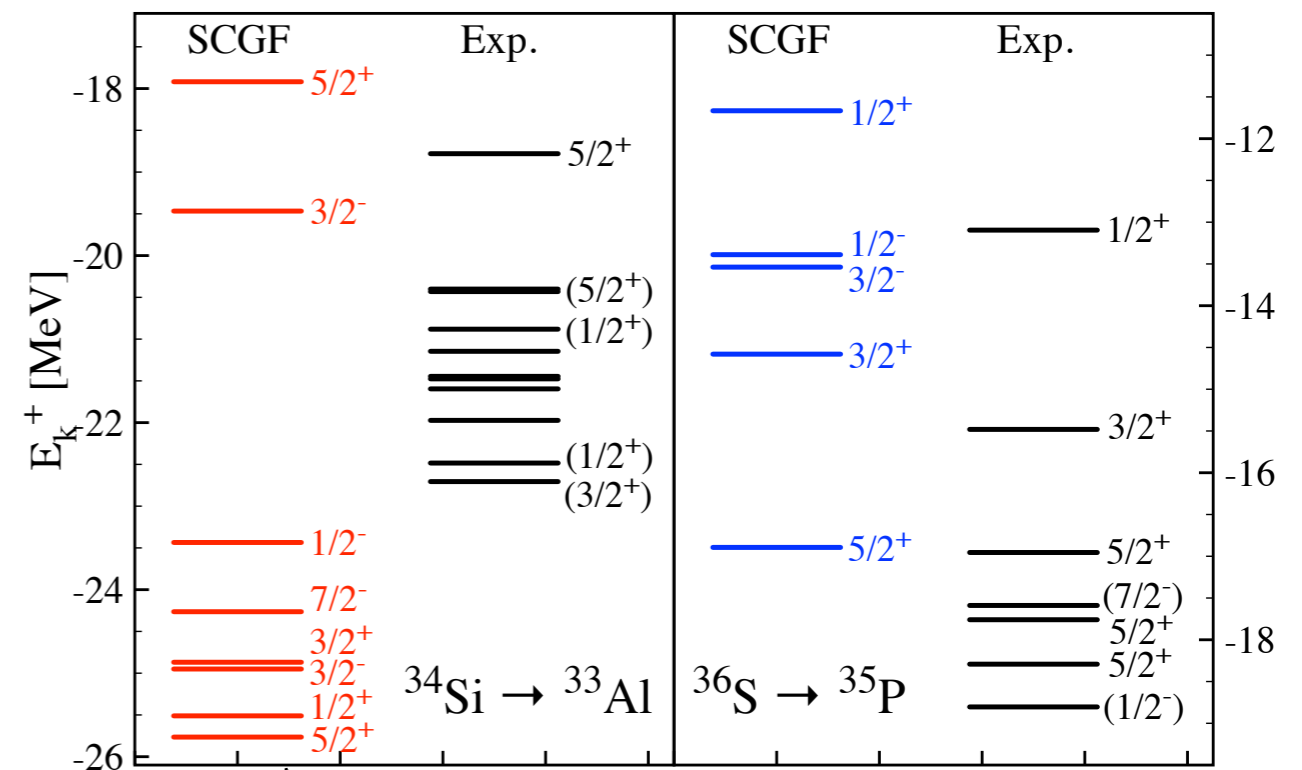[Thorn *et al.* 1984]
[Eckle *et al.* 1989]
[Burgunder *et al.* 2014]

One-proton knock-out

Exp. data:
[Khan *et al.* 1985]
[Mutschler *et al.* 2016 (PRC)]
[Mutschler *et al.* 2016 (Nature Phys.)]

[Duguet *et al.* 2017]

Reduction of $E_{1/2^-}$ - $E_{3/2^-}$ spin-orbit splitting well reproduced

Agreement gets worse for one-proton removal → deformation?

K spectra

⇨ **K spectra show interesting g.s. spin inversion and re-inversion**

Laser spectroscopy COLLAPS @ ISOLDE
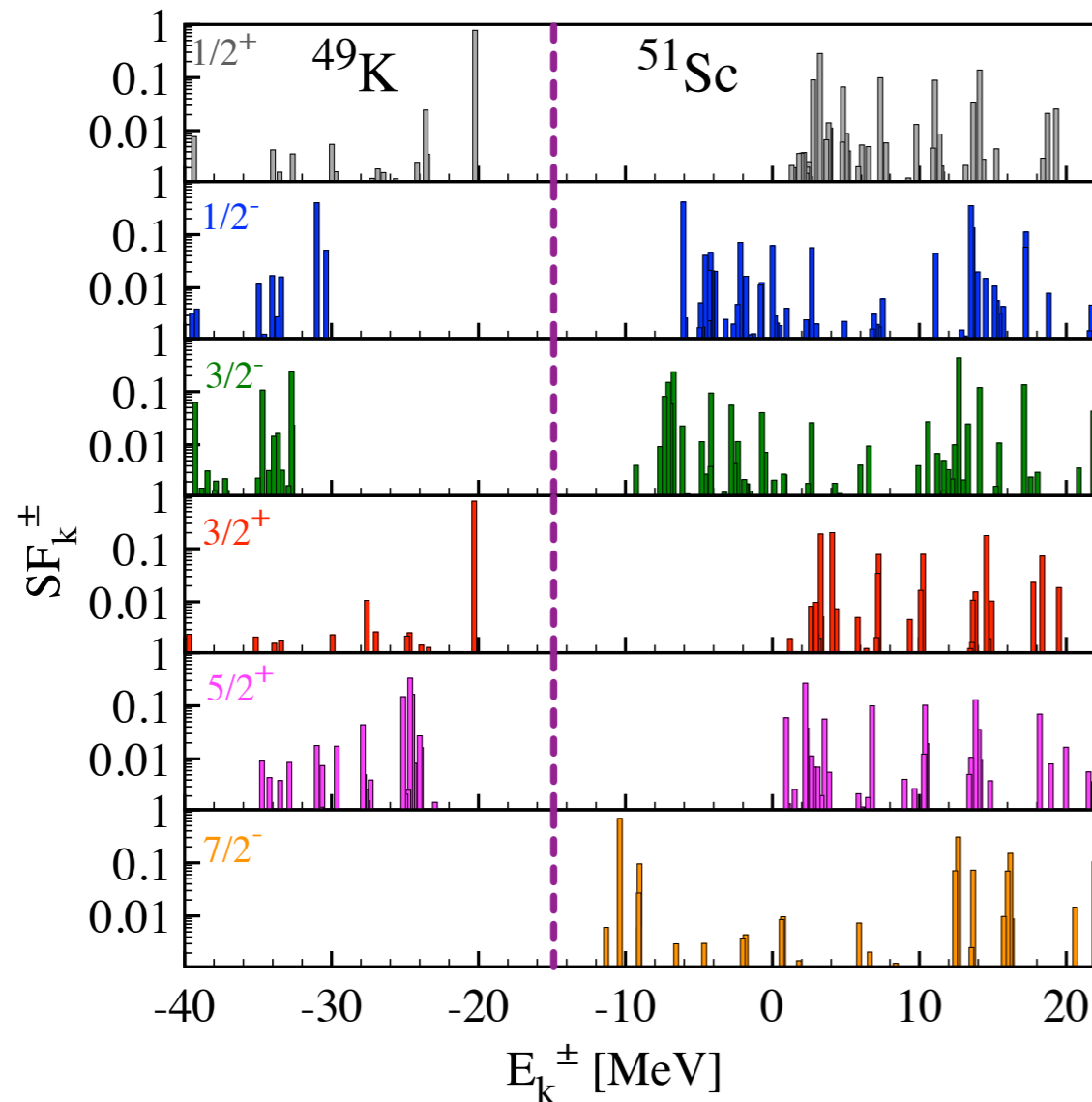
[Papuga *et al.* 2013]

One-proton addition and removal from ^{50}Ca
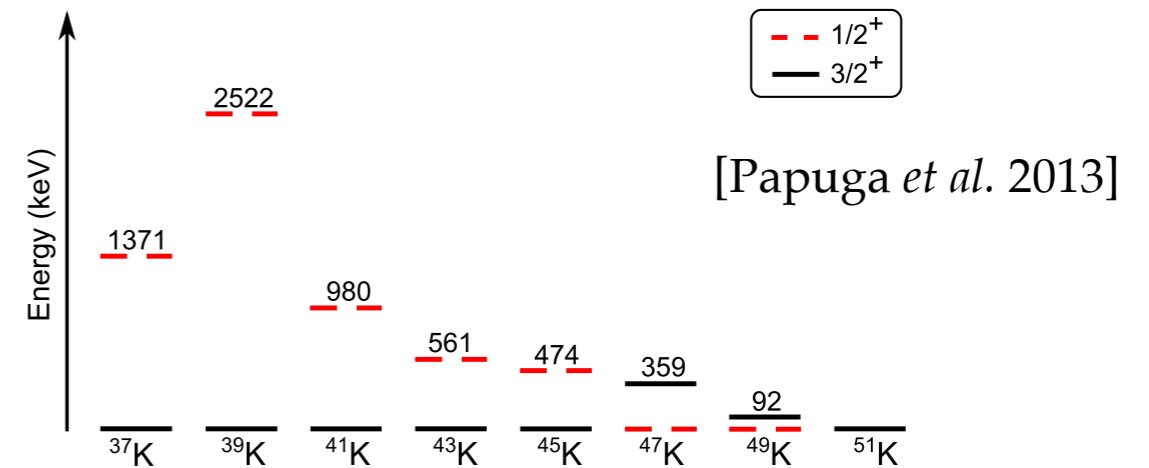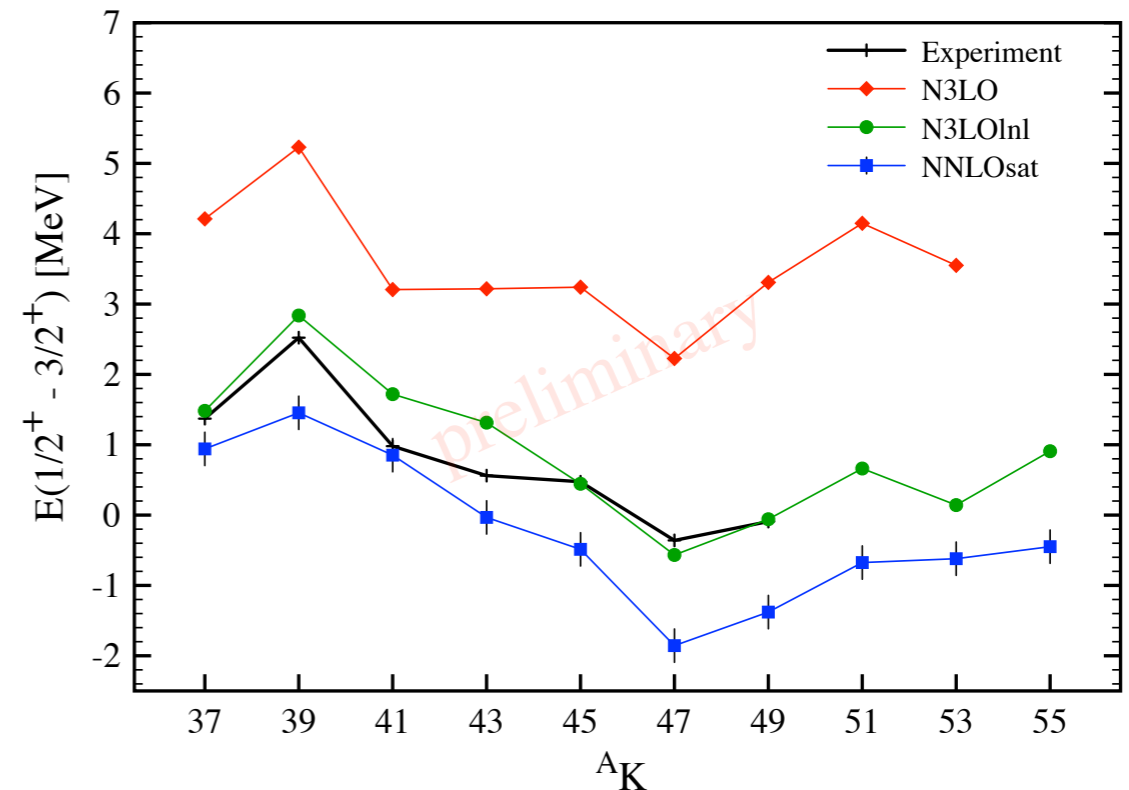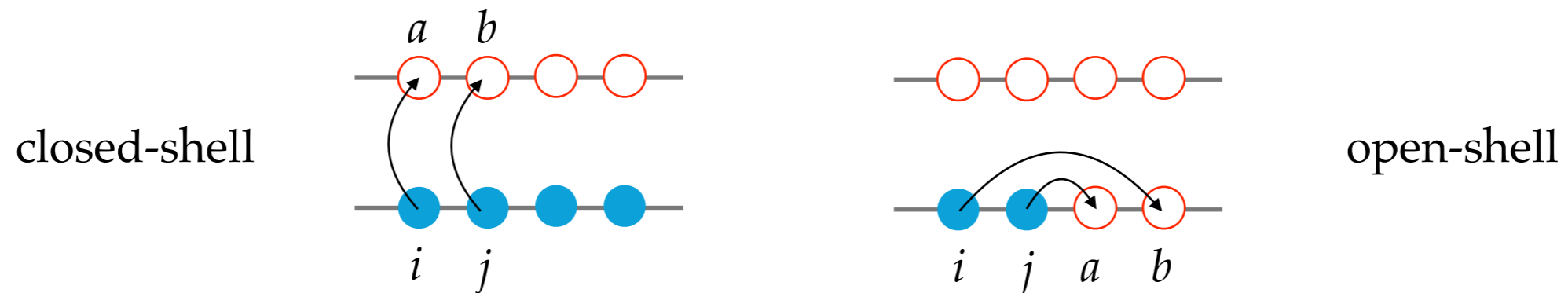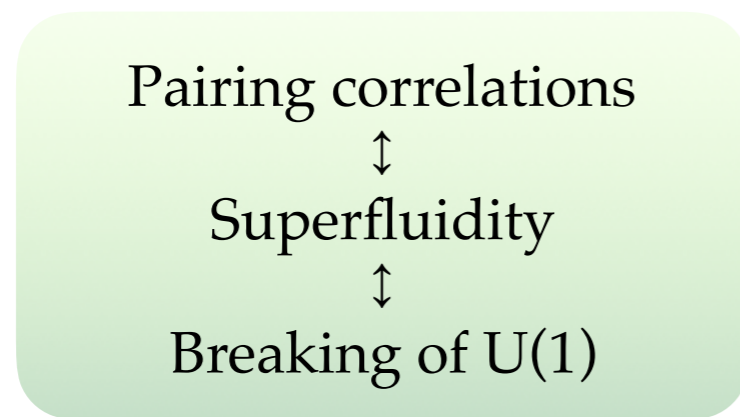
Doubly open-shell nuclei

⊙ Approximate/truncated methods capture correlations via an expansion in **ph excitations**

⊙ Open-shell nuclei are **(near-)degenerate** with respect to ph excitations

closed-shell   open-shell

⊙ Solution: multi-determinantal or **symmetry-breaking** reference state

  ○ Symmetry-breaking solution allows to **lift the degeneracy**

Pairing correlations
↕
Superfluidity
↕
Breaking of U(1)

Quadrupole correlations
↕
Deformation
↕
Breaking of SU(2)

↓   ↓

Singly open-shells   **Doubly** open-shells
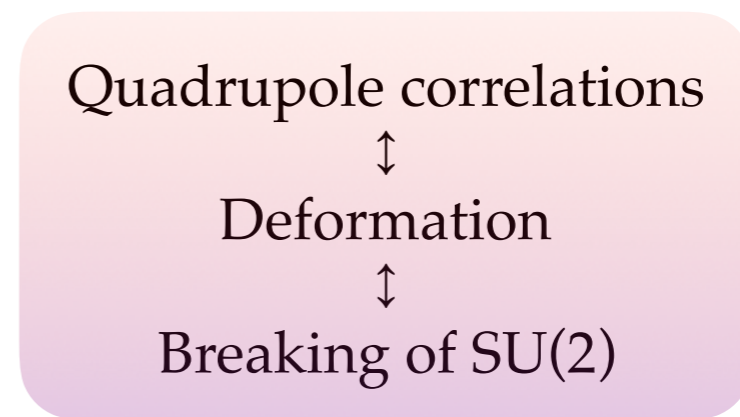
Developed and implemented   To be developed and implemented

Tensor decomposition of many-body formalism
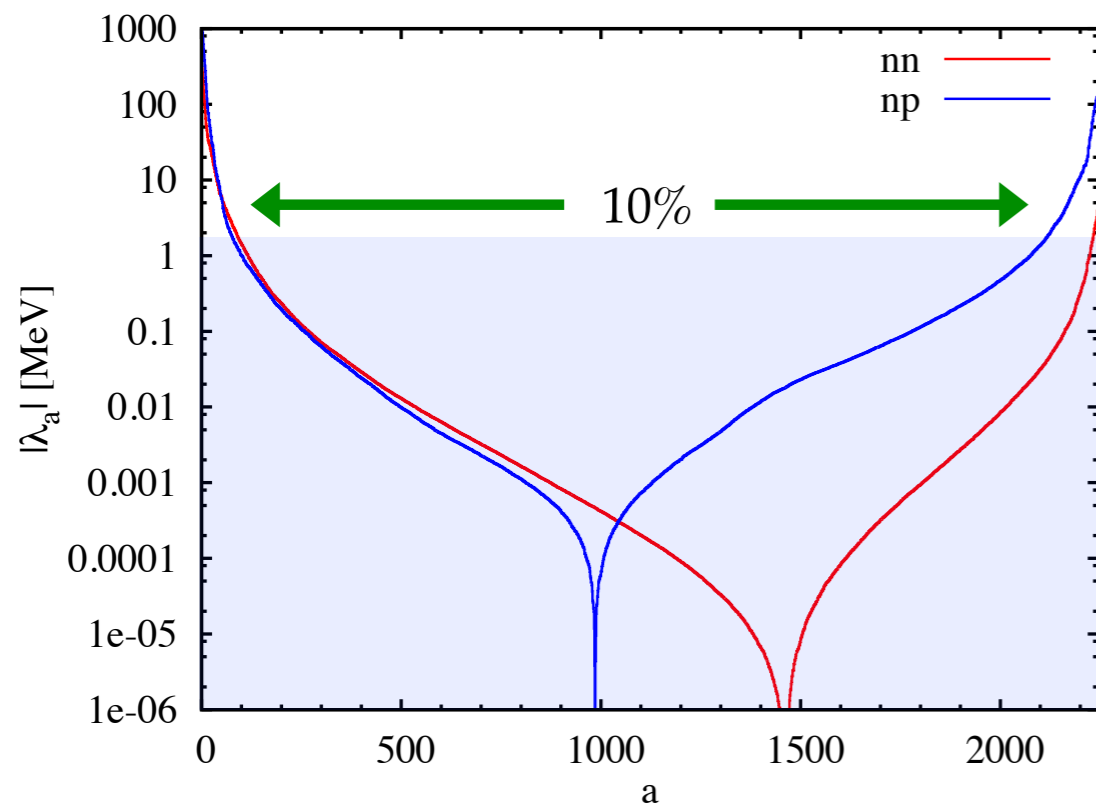
⇨ Many-body methods require the handling (computation & storage) of **large tensors**

⇨ **Matrix elements of 3-body interaction** represent current memory bottleneck

Use **tensor decomposition techniques**

⊙ **Two-body forces** can be factorised as $v_{ijkl} = \sum_a \lambda_a \, g_{ik}^a \, g_{jl}^a$ ($\rightarrow$ Singular Value Decomposition)

[Lesinski 2013]

Gain #1: **size** ($\rightarrow$ storage and memory needs)

$$\sum_{kl} v_{ijkl} = \sum_a \lambda_a \sum_k g_{ik}^a \sum_l g_{jl}^a$$

$$\mathbf{N^2} \qquad \mathrm{m} \qquad (\mathrm{N} \; + \; \mathrm{N}) \quad = \quad \mathbf{mN}$$

Gain #2: **CPU speed-up**

HF test: $\rightarrow$ **0.003% error** and **factor 10 speed-up**

⊙ **Higher-order tensors:** exploit techniques from applied maths (e.g. tensor hypercontraction)

Conclusions

- **Not so good news**

  - Renormalisable approach → still a long way to go?
  - Fix-cutoff approach → few issues hinder full phenomenological success

- **Good news**

  - Many-body methods mature for applications in medium-mass nuclei
  - Promising ideas for extension to heavy nuclei

- **Extension of ab initio simulations to heavy nuclei**

  - Extension to doubly open shell requires new formal developments
  - Computational challenges ahead: work in progress and more smart ideas needed