Ab Initio Approaches to Light Nuclei

Lecture 4: Beyond Light Nuclei

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Overview

- **Lecture 1: Fundamentals**

  Prelude • Many-Body Quantum Mechanics

- **Lecture 1': Nuclear Hamiltonian**

  Nuclear Interactions • Matrix Elements

- **Lecture 2: Correlations**

  Two-Body Problem • Unitary Transformations • Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Configuration Interaction • No-Core Shell Model • Importance Truncation

- **Lecture 4: Beyond Light Nuclei**

  Coupled-Cluster Theory • In-Medium Similarity Renormalization Group

Ab Initio Beyond Light Nuclei

advent of novel ab initio many-body approaches
gives access to the medium-mass regime

Hagen, Papenbrock, Dean, Piecuch, Binder,...

- **coupled-cluster theory**: ground-state parametrized by expon[...]ial wave operator applied to single-determinant reference st[...]
  - truncation at doubles level (CCSD) plus triples co[...]
  - equations of motion for excited states an[...]

[...]sukiyama, Schwenk, Hergert,...

- **in-medium SRG**: com[...] [...]hole excitations from many-body refe[...] [...]olution
  - nor[...] [...]amiltonian truncated at two-body level
  - [...] [...]ell ground states; excitations via EOM or SM

Barbieri, Soma, Duguet,...

- self-c[...]sistent Green's function approaches and others...

controlling and quantifying the uncertainties due to various inherent truncations is a major task

Normal Ordering

Particle-Hole Excitations

- short-hand notation for creation and annihilation operators

$$a_i = a_{\alpha_i} \qquad\qquad a_i^\dagger = a_{\alpha_i}^\dagger$$

- define an A-body **reference Slater determinant**

$$|\Phi\rangle = |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = a_1^\dagger a_2^\dagger \cdots a_A^\dagger |0\rangle$$

and construct arbitrary Slater determinants through **particle-hole excitations** on top of the reference state

$$|\Phi_a^p\rangle = a_p^\dagger a_a |\Phi\rangle$$
$$|\Phi_{ab}^{pq}\rangle = a_p^\dagger a_q^\dagger a_b a_a |\Phi\rangle$$
$$\vdots$$

index convention: $a,b,c,\ldots$: hole states, occupied in reference state
$p,q,r,\ldots$: particle states, unoccupied in reference states
$i,j,k,\ldots$: all states

Normal Ordering

- a string of creation and annihilation operators is in **normal order** with respect to a specific reference state, if all
  - creation operators are on the left
  - annihilation operators are on the right

- standard particle-hole operators are normal ordered with respect to the vacuum state as reference state

$$a_i^\dagger a_j \,, \qquad a_i^\dagger a_j^\dagger a_l a_k \,, \qquad a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \,, \ldots$$

- **normal-ordered product** of string of operators

$$\{a_n a_i^\dagger \cdots a_m a_j^\dagger\} = \text{sgn}(\pi)\, a_i^\dagger a_j^\dagger \cdots a_n a_m$$

- defining property of a normal-ordered product: **expectation value with the reference state always vanishes**

$$\langle\Phi|\,\{\ldots\}\,|\Phi\rangle = 0$$

Normal Ordering with A-Body Reference

- in particle-hole formulation with respect to an ***A*-body reference Slater determinant** things are more complicated

	particle states	hole states
creation operators	$a^\dagger_p, a^\dagger_q, \ldots$	$a_a, a_b, \ldots$
annihilation operators	$a_p, a_q, \ldots$	$a^\dagger_a, a^\dagger_b, \ldots$

- redefinition of creation and annihilation operators necessary to guarantee vanishing reference expectation value

$$\langle\Phi|\{\ldots\}|\Phi\rangle = 0$$

- starting from an operator string in vacuum normal order one has to **reorder to arrive at reference normal order**
    - "brute force" using the anticommutation relations for fermionic creation and annihilation operators
    - "elegantly" using Wick's theorem and contractions…

Normal-Ordered Hamiltonian

- **second quantized Hamiltonian** in vacuum normal order

$$H = \frac{1}{4} \sum_{ijkl} \langle ij | \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{NN} | kl \rangle \, a_i^\dagger a_j^\dagger a_l a_k + \dots$$

normal-ordered two-body approximation: discard residual normal-ordered three-body part

- **normal-ordered Hamiltonian** with respect to reference sta

$$H = E + \sum_{ij} f^i_j \, \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma^{ij}_{kl} \, \{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36} \sum_{ijklmn} W^{ijk}_{lmn} \, \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$E = \frac{1}{2} \sum_{ab} \langle ab | \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{NN} | ab \rangle + \frac{1}{6} \sum_{abc} \langle abc | \mathrm{V}_{3N} | abc \rangle$$

$$f^i_j = \sum_a \langle ai | \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{NN} | aj \rangle + \frac{1}{2} \sum_{ab} \langle abi | \mathrm{V}_{3N} | abj \rangle$$

$$\Gamma^{ij}_{kl} = \langle ij | \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{NN} | kl \rangle + \sum_a \langle aij | \mathrm{V}_{3N} | akl \rangle$$

$$W^{ijk}_{lmn} = \langle ijk | \mathrm{V}_{3N} | lmn \rangle$$

Coupled-Cluster Theory

Coupled-Cluster Ansatz

- coupled-cluster ground state parametrized by **exponential of particle-hole excitation operators** acting on reference state

$$|\Psi_{CC}\rangle = \exp(T)\,|\Phi\rangle = \exp(T_1 + T_2 + \cdots T_A)\,|\Phi\rangle$$

- with the **n-particle-n-hole excitation operators** with unknown amplitudes

$$T_1 = \sum_{a,p} t_a^p \;\{a_p^\dagger a_a\}$$
$$T_2 = \sum_{ab,pq} t_{ab}^{pq} \;\{a_p^\dagger a_q^\dagger a_b a_a\}$$
$$\vdots$$

- need to **truncate the excitation operator** at some small particle-hole order, defining different levels of coupled-cluster approximations

T_1	CCS
$T_1 + T_2$	CCSD
$T_1 + T_2 + T_3$	CCSDT

Coupled-Cluster Equations

- insert the coupled-cluster ansatz into the **A-body Schrödinger equation** and manipulate

$$\mathrm{H}_{\mathrm{int}}\,|\Psi_{\mathrm{CC}}\rangle = E\,|\Psi_{\mathrm{CC}}\rangle \qquad \Rightarrow \qquad \exp(-T)\,\mathrm{H}_{\mathrm{int}}\,\exp(T)\;|\Phi\rangle = E\,|\Phi\rangle$$

  to obtain Schrödinger-like equation for a **similarity-transformed Hamiltonian**

$$\mathcal{H}\;|\Phi\rangle = E\,|\Phi\rangle \qquad \text{with} \qquad \mathcal{H} = \exp(-T)\,\mathrm{H}_{\mathrm{int}}\,\exp(T)$$

- note: this is **not a unitary transformation** and therefore the transformed Hamiltonian is non-hermitian
  - as a result approximations will be non-variational
- similarity transformation of the Hamiltonian can be expanded in a **Baker–Campbell–Hausdorff series**, which **terminates at finite order**
  - CCSD with a two-body Hamiltonian terminates after order T^4

CCSD Equations

- project the Schrödinger-like equation onto the reference state, 1p1h states, and 2p2h states to obtain **CCSD energy and amplitude equations**

$$\langle\Phi|\mathcal{H}|\Phi\rangle = E_{\text{CCSD}}$$
$$\langle\Phi_a^p|\mathcal{H}|\Phi\rangle = 0$$
$$\langle\Phi_{ab}^{pq}|\mathcal{H}|\Phi\rangle = 0$$

- after BCH-expansion these are **coupled non-linear algebraic equations** for the amplitudes t_a^p, t_{ab}^{pq} and the CCSD energy
- for large-scale calculations use **spherical formulation**, where particle-hole operators are coupled to J=0
- full CCSDT is too expensive, various **non-iterative triples corrections** are being used to include triples contributions
- coupled-cluster with **explicit 3N interactions** can be done and was used to test the NO2B approximation

Coupled Cluster: Pros & Cons

PRO

- much more efficient than ph-truncated CI
- can deal with explicit 3N interaction
- size extensive
- very mild scaling with A

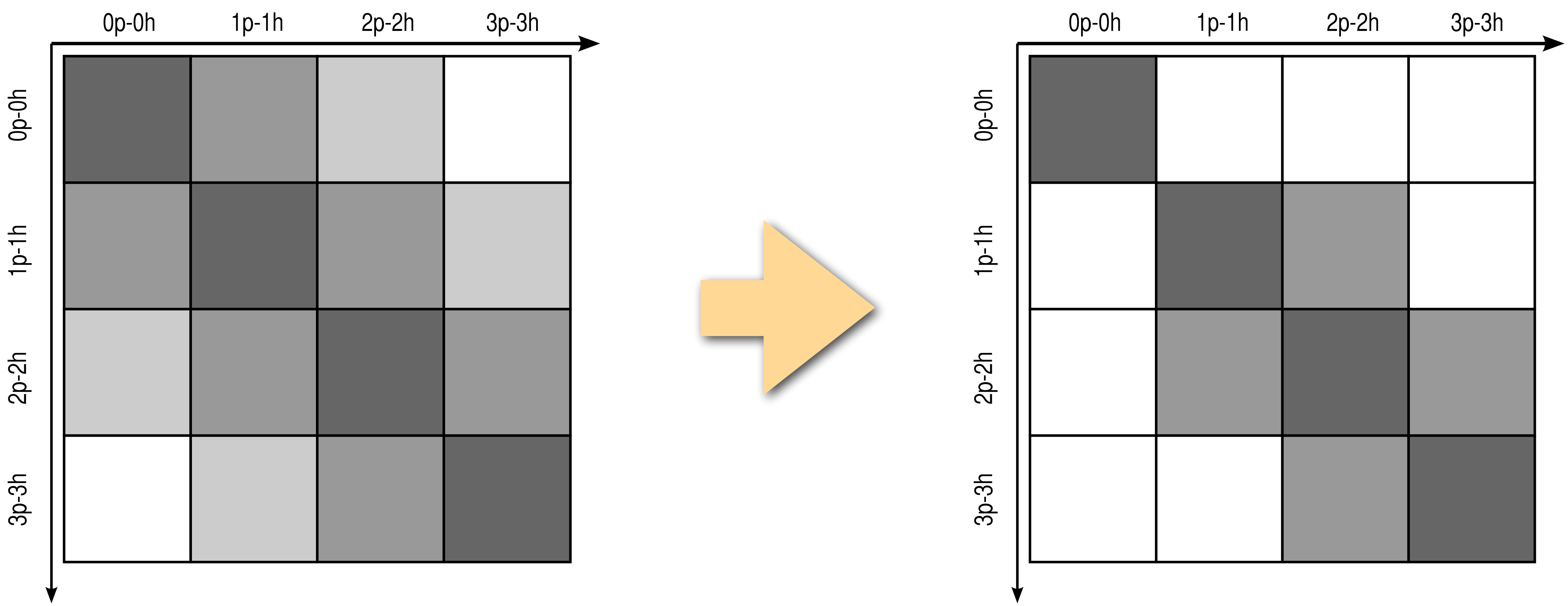
CON

- not variational
- only for closed shell nuclei *
- other observables difficult
- only for ground states *
- non-hermititan Hamiltonian

* equations of motion methods give access to near-closed-shell isotopes and excited states

In-Medium SRG

Decoupling in A-Body Space

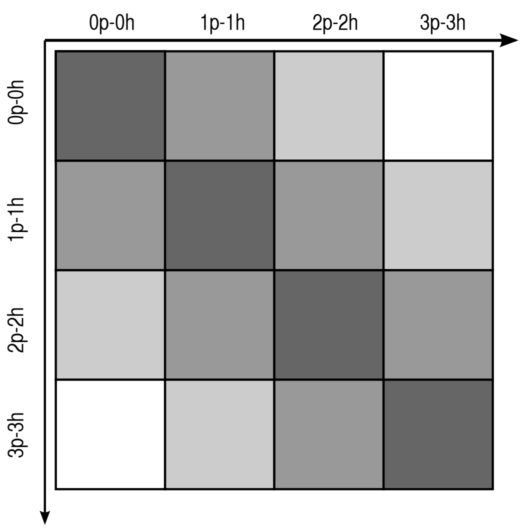


decouple reference state from all particle-hole excited states

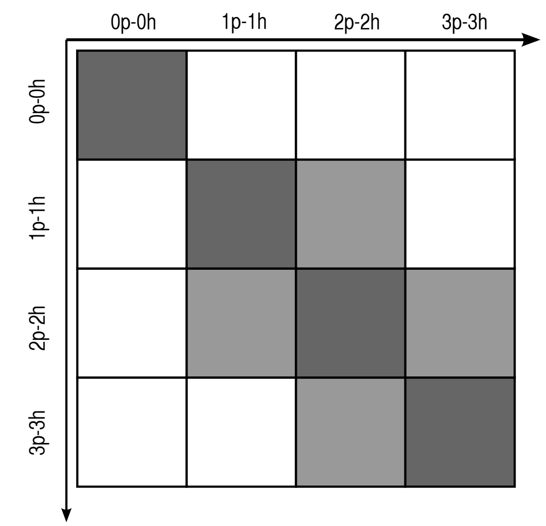
expectation value in reference state represents ground-state energy

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,…



use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations



- **flow equation** for Hamiltonian

$$\frac{d}{ds} H(s) = [\eta(s), H(s)]$$

- Hamiltonian in single-reference or multi-reference **normal order**, omitting normal-ordered 3B term

$$\mathrm{H}(s) = E(s) + \sum_{ij} f^i_j(s)\ \{a^\dagger_i a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma^{ij}_{kl}(s)\ \{a^\dagger_i a^\dagger_j a_l a_k\}$$

In-Medium SRG Generators

- **Wegner**: simple, intuitive, inefficient

$$\eta = [H_{\mathrm{d}}, H] = [H_{\mathrm{d}}, H_{\mathrm{od}}]$$

- **White**: efficient, problems with near degeneracies

$$\eta^{1}_{2} = (\Delta^{1}_{2})^{-1}\, n_1 \bar{n}_2\, f^{1}_{2} - [1 \longleftrightarrow 2]$$

$$\eta^{12}_{34} = (\Delta^{12}_{34})^{-1}\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma^{12}_{34} - [12 \longleftrightarrow 34]$$

- **Imaginary Time**: good work horse *[Morris, Bogner]*

$$\eta^{1}_{2} = \mathrm{sgn}(\Delta^{1}_{2})\, n_1 \bar{n}_2\, f^{1}_{2} - [1 \longleftrightarrow 2]$$

$$\eta^{12}_{34} = \mathrm{sgn}(\Delta^{12}_{34})\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma^{12}_{34} - [12 \longleftrightarrow 34]$$

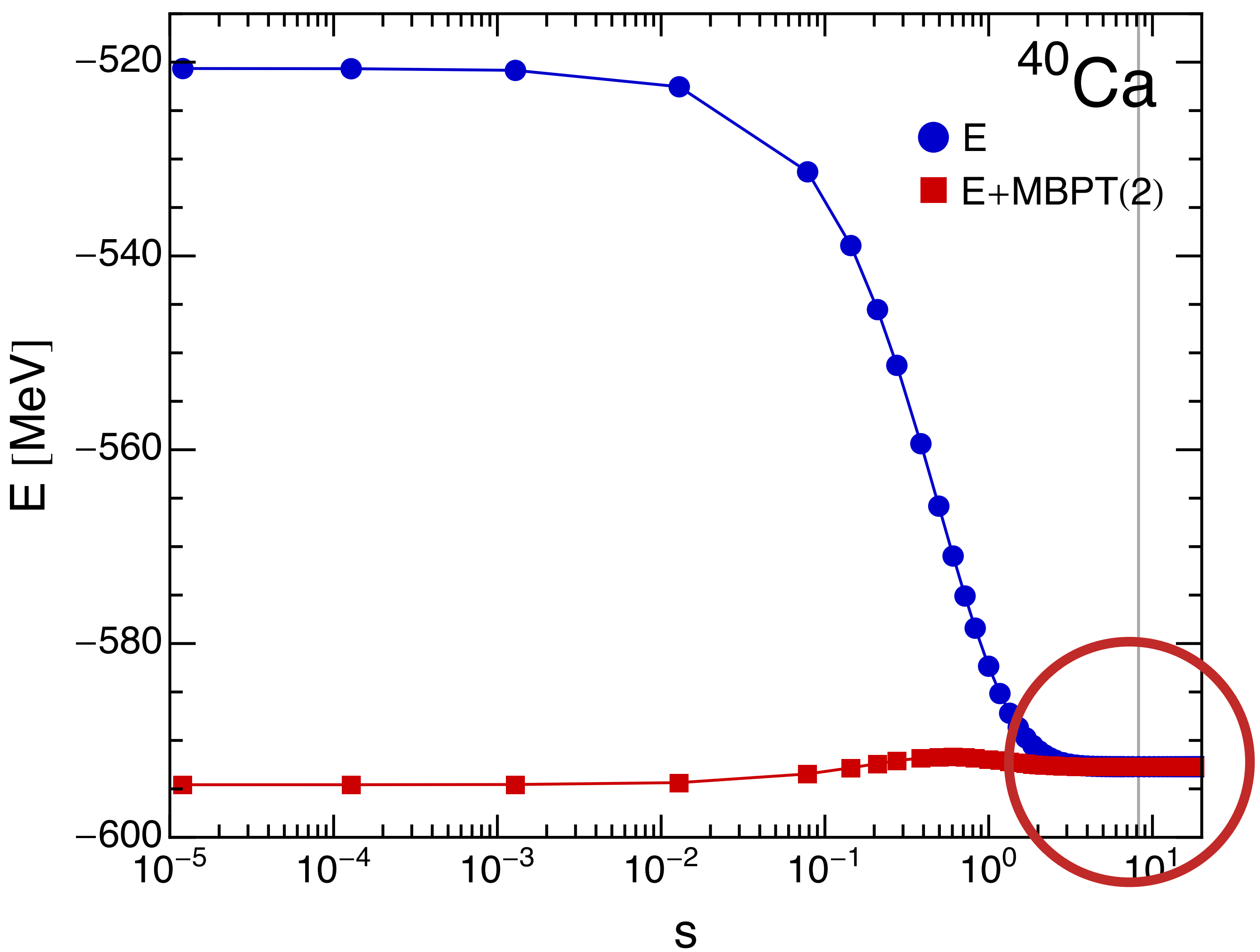
- **Brillouin**: potentially better work horse *[Hergert]*

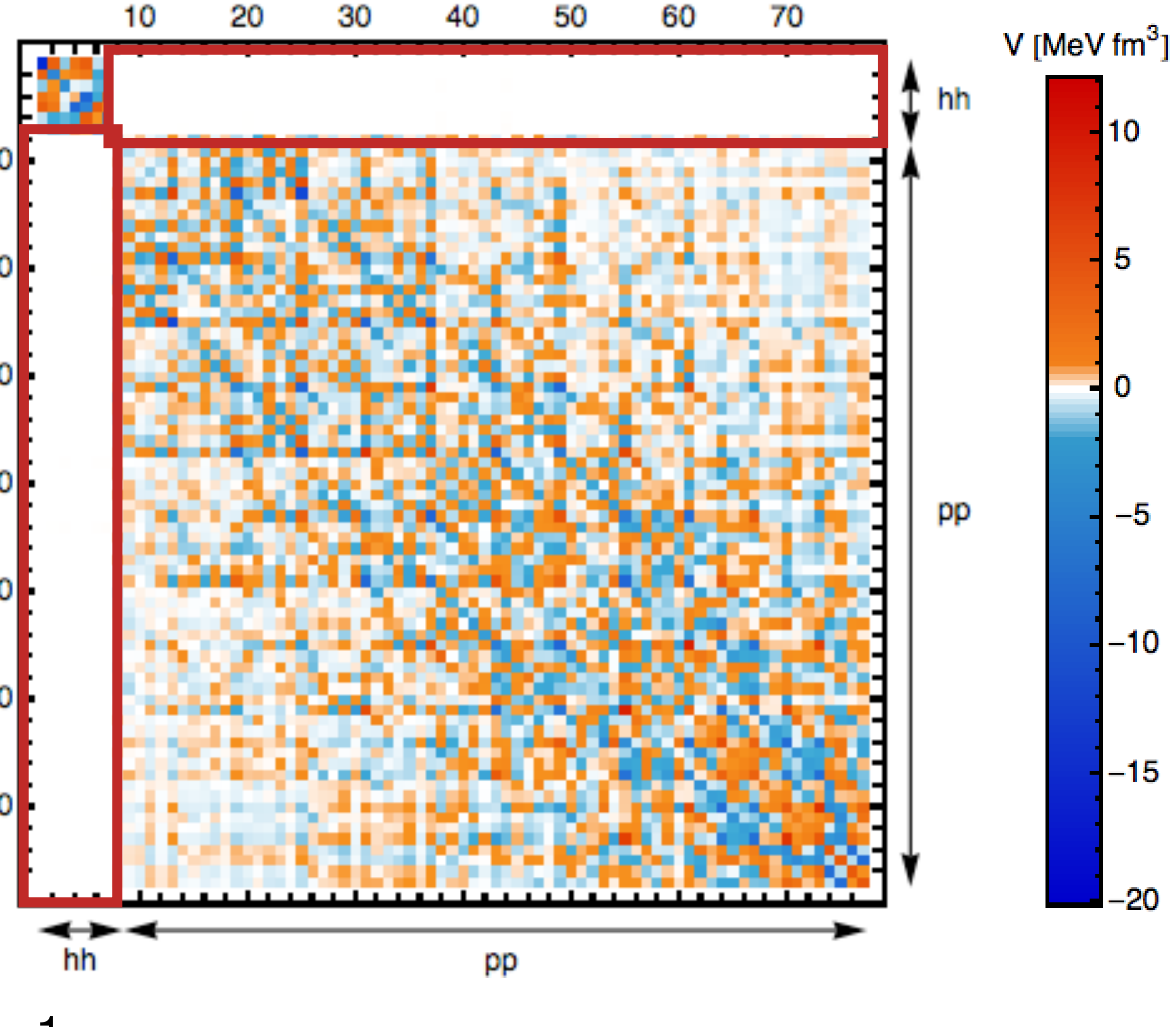
$$\eta^{1}_{2} = \langle\Phi|\,[H, \{a^{\dagger}_{1} a_2\}]\,|\Phi\rangle$$

$$\eta^{12}_{34} = \langle\Phi|\,[H, \{a^{\dagger}_{1} a^{\dagger}_{2} a_4 a_3\}]\,|\Phi\rangle$$

In-Medium SRG Evolution

H. Hergert





In-Medium SRG: Pros & Cons

PRO

- flexibility of generators
- much more efficient than ph-truncated CI
- straight-forward extension to open-shell nuclei
- size extensive
- very mild scaling with A
- hermitian Hamiltonian
- easy access to other observables
- bridge to shell model

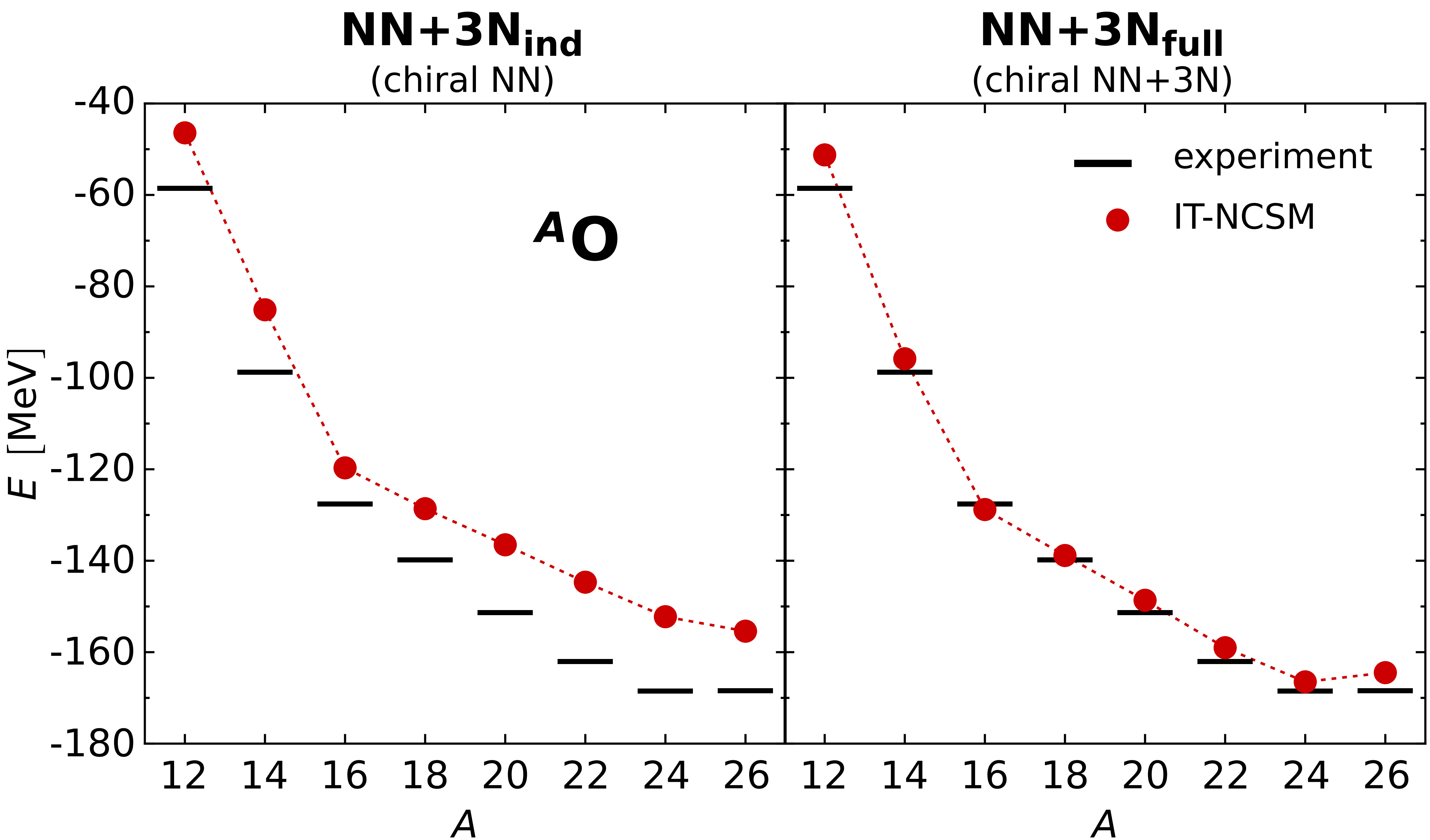
CON

- not variational
- NO3B needs some work

Applications for Medium-Mass Nuclei

Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

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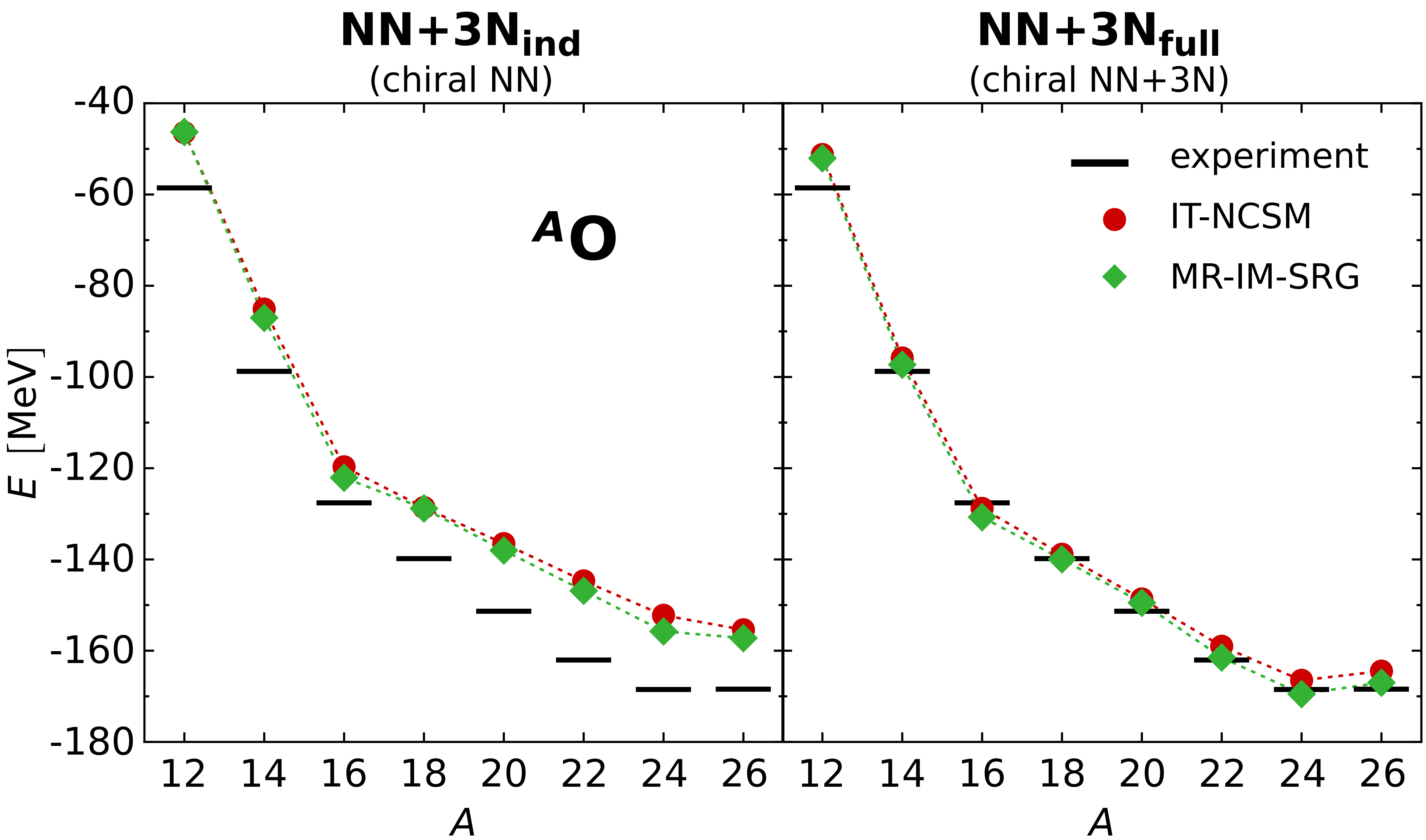

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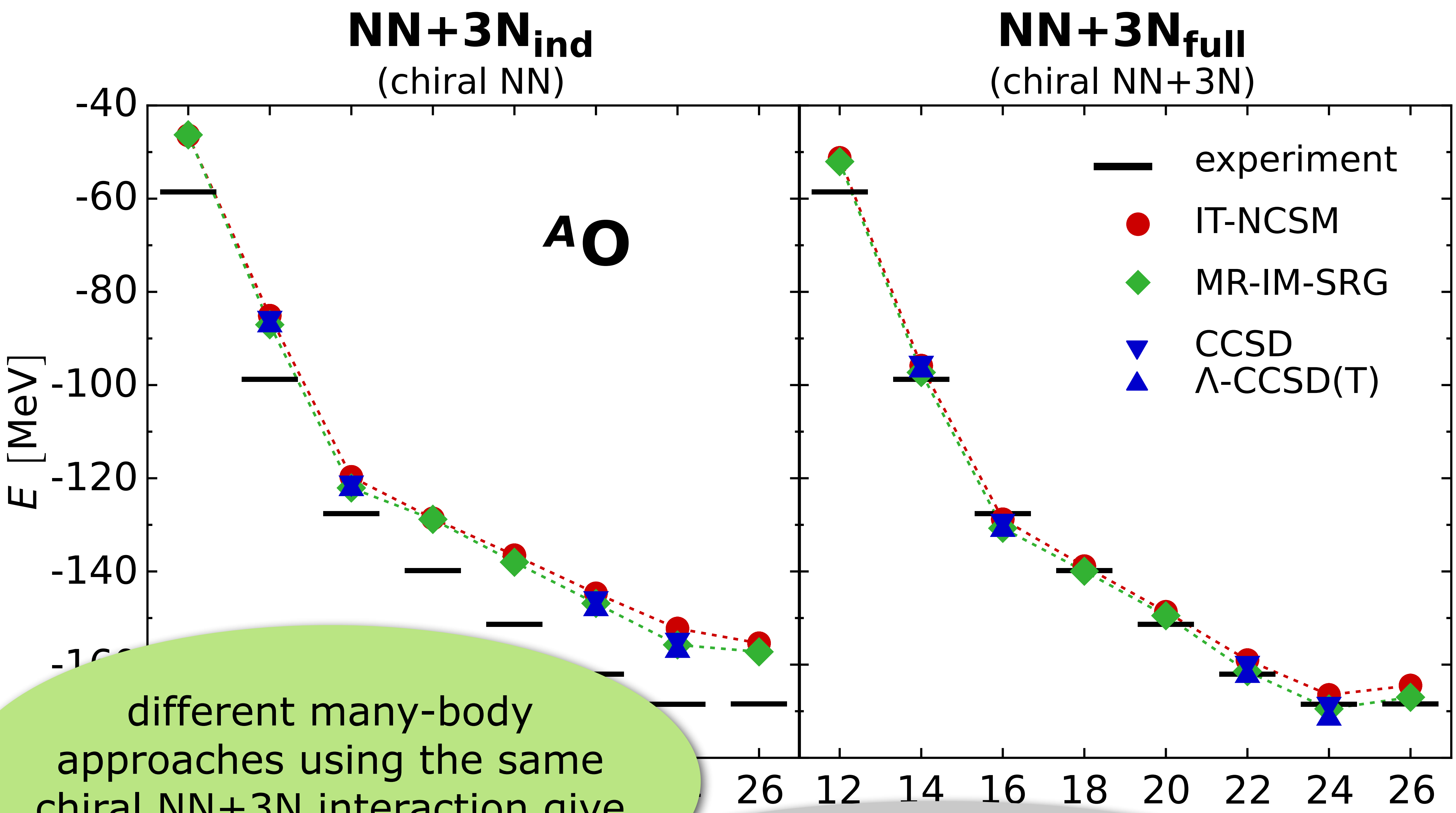
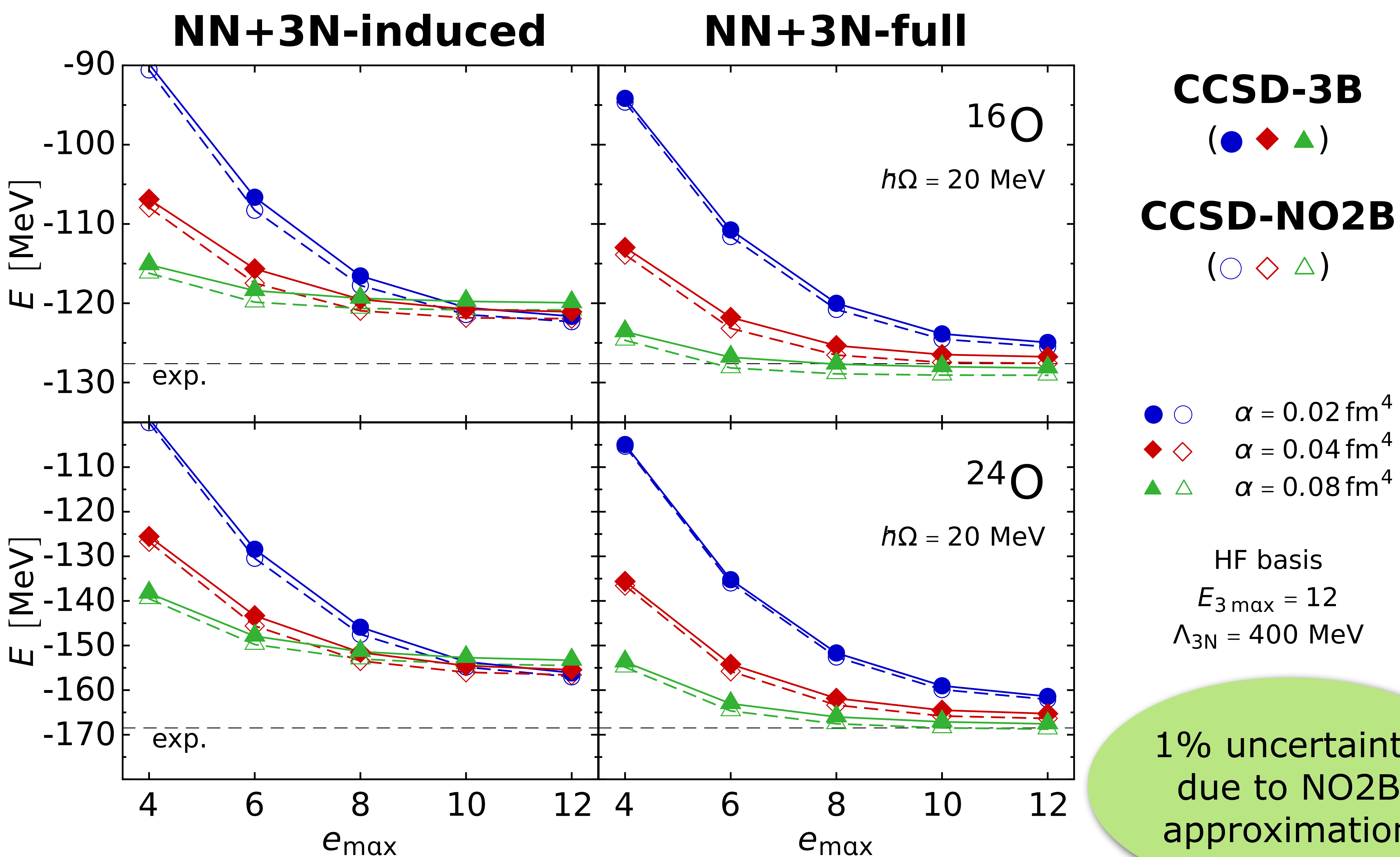


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Benchmark of NO2B Approximation

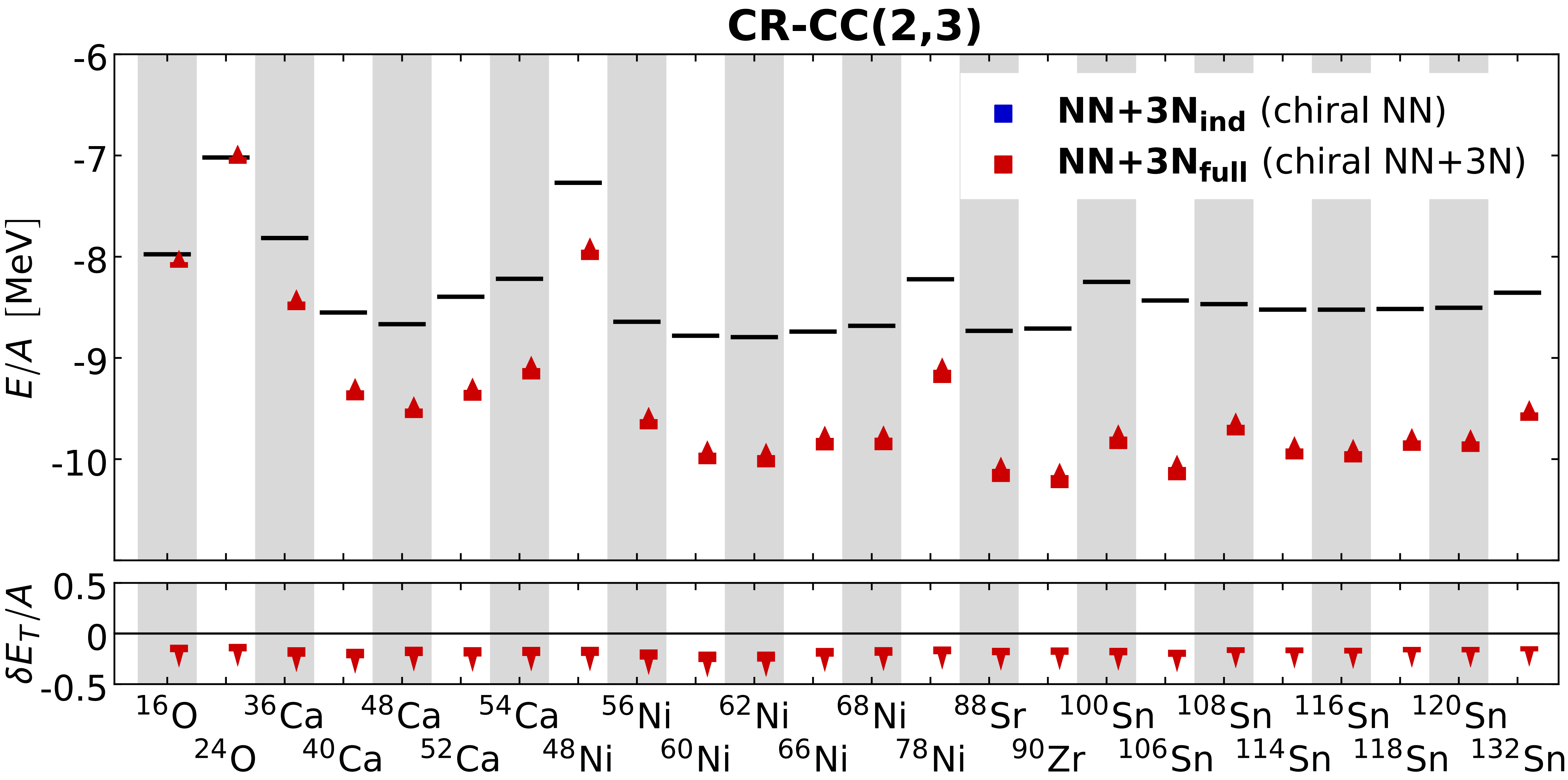
Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)



1% uncertainty due to NO2B approximation

Towards Heavy Nuclei - Ab Initio

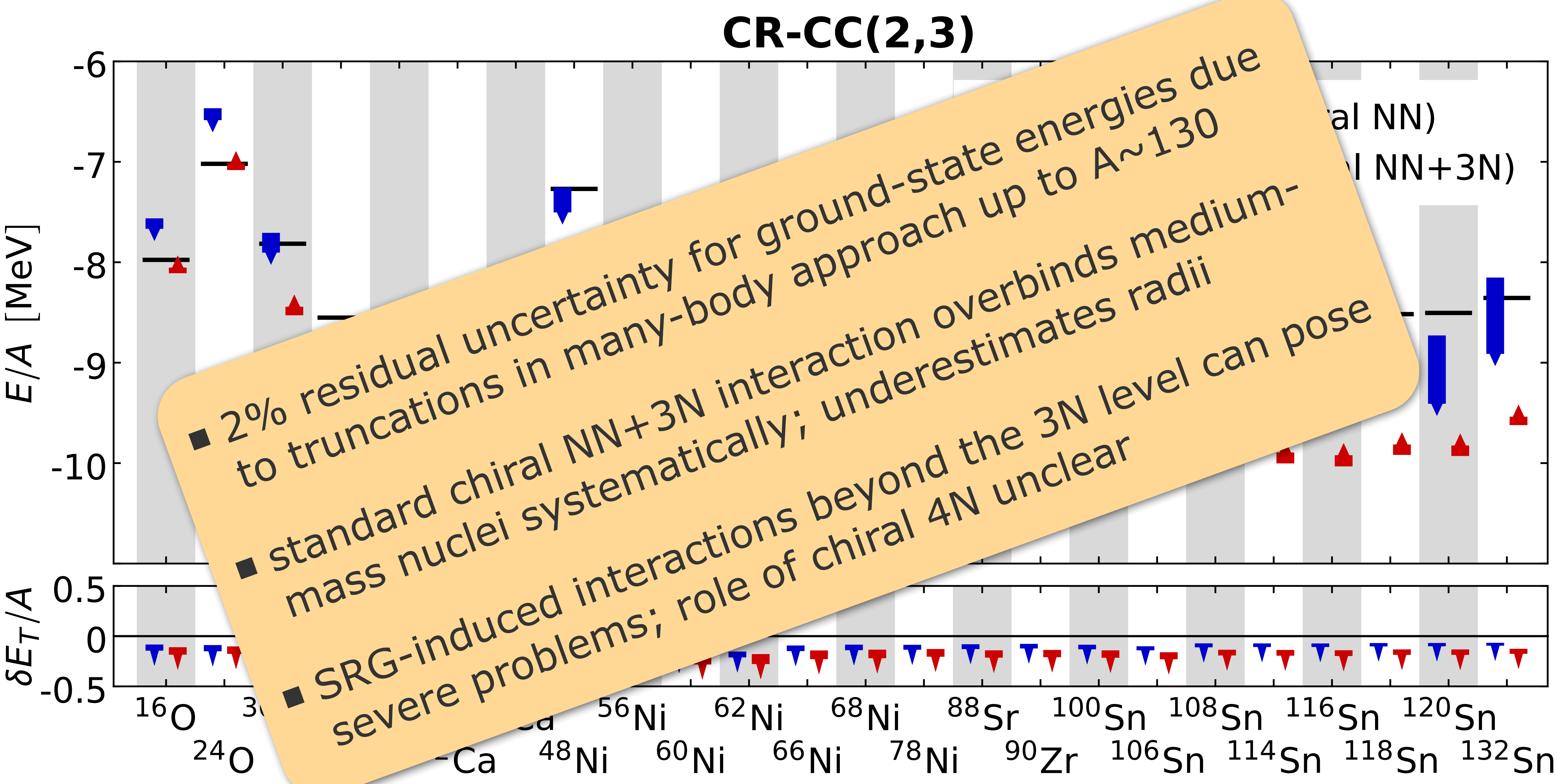
Binder et al., PLB 736, 119 (2014)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\text{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

Towards Heavy Nuclei - Ab Initio

Binder et al., PLB 736, 119 (2014)

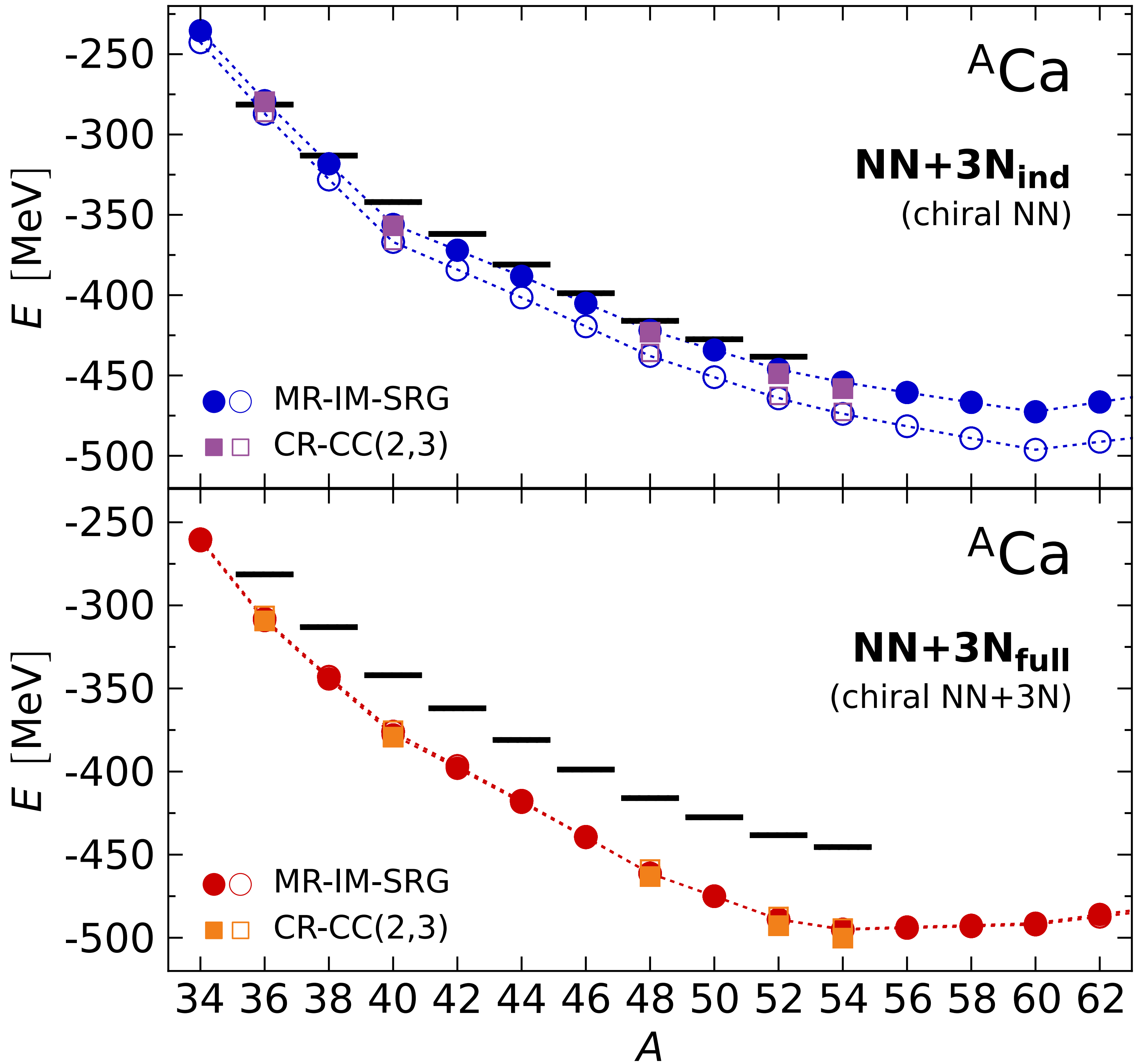


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically; underestimates radii
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\text{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

Open-Shell Medium-Mass Nuclei

Hergert et al., PRC 90, 041302(R) (2014)

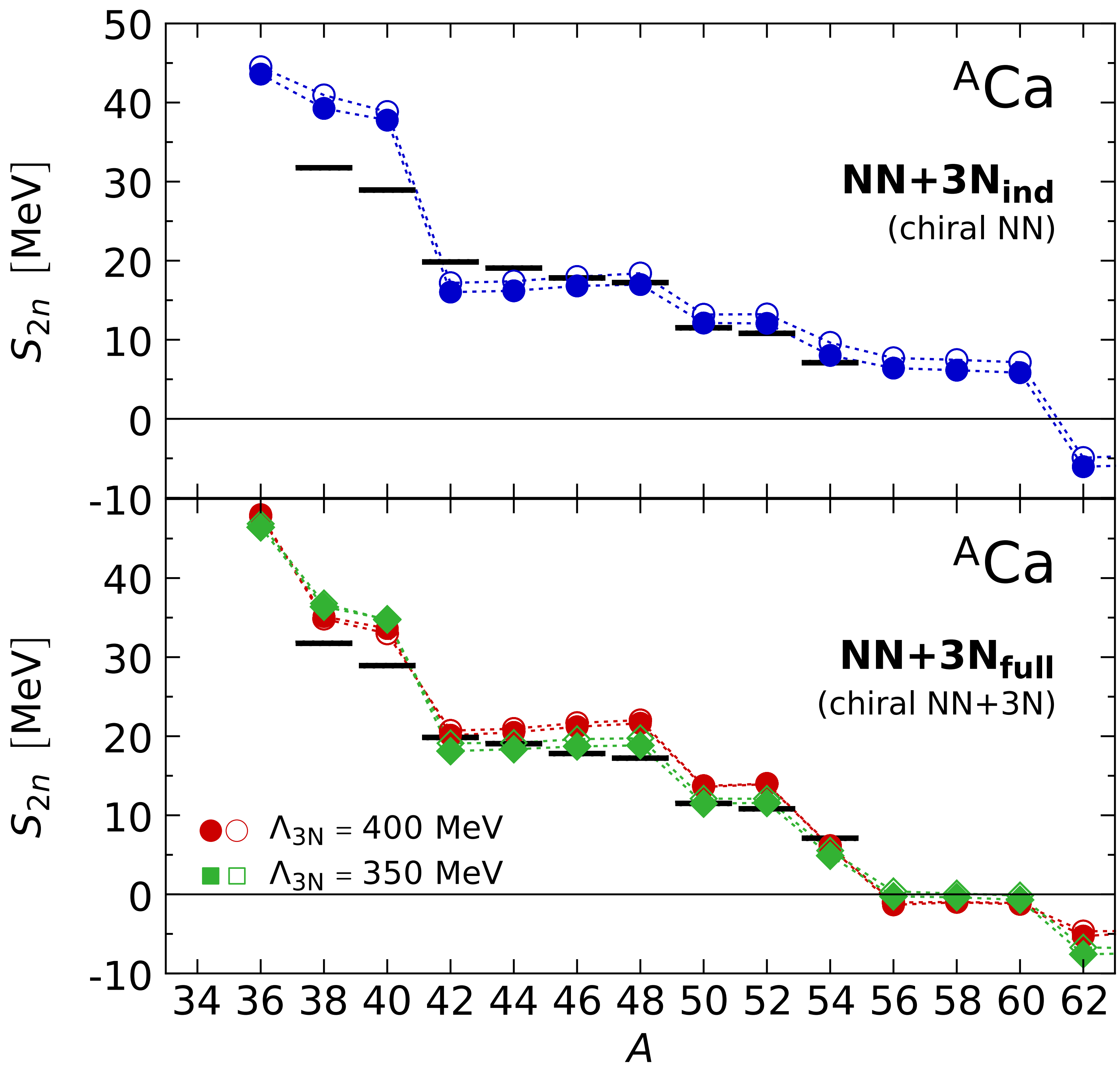


- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

Λ_{3N} = 400 MeV
α = 0.04 fm^4 (○)
0.08 fm^4 (●)
$E_{3\,max}$ = 14, 16

Open-Shell Medium-Mass Nuclei

Hergert et al., PRC 90, 041302(R) (2014)



- two-neutron separation energies hide overall energy shift
- compares well to updated Gor'kov-GF results
  [priv. comm. V. Soma]
- chiral 3N interaction predicts flat "drip-region" from ^{56}Ca to ^{60}Ca

all MR-IM-SRG

α = 0.04 fm^4 (○)
0.08 fm^4 (●)

$E_{3\,max}$ = 14, 16

Conclusions

Ab Initio Frontiers

- **ab initio theory is entering new territory...**
  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT
  - **precision frontier**
    precision spectroscopy of light nuclei, including current contributions
  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum frontier**
    include continuum effects and scattering observables consistently
  - **strangeness frontier**
    ab initio predictions for hyper-nuclear structure & spectroscopy

...providing a coherent theoretical framework for nuclear structure & reaction calculations

Epilogue

- **thanks to my group and my collaborators**
  - J. Braun, E. Gebrerufael, T. Hüther, J. Langhammer, S. Schulz, H. Spiess, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
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    Universität Bochum, ...

JUROPA — JÜLICH FORSCHUNGSZENTRUM
LOEWE-CSC — Center for Scientific Computing Frankfurt
EDISON — NERSC

COMPUTING TIME

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung