Ab Initio Theory of Medium-Mass Nuclei

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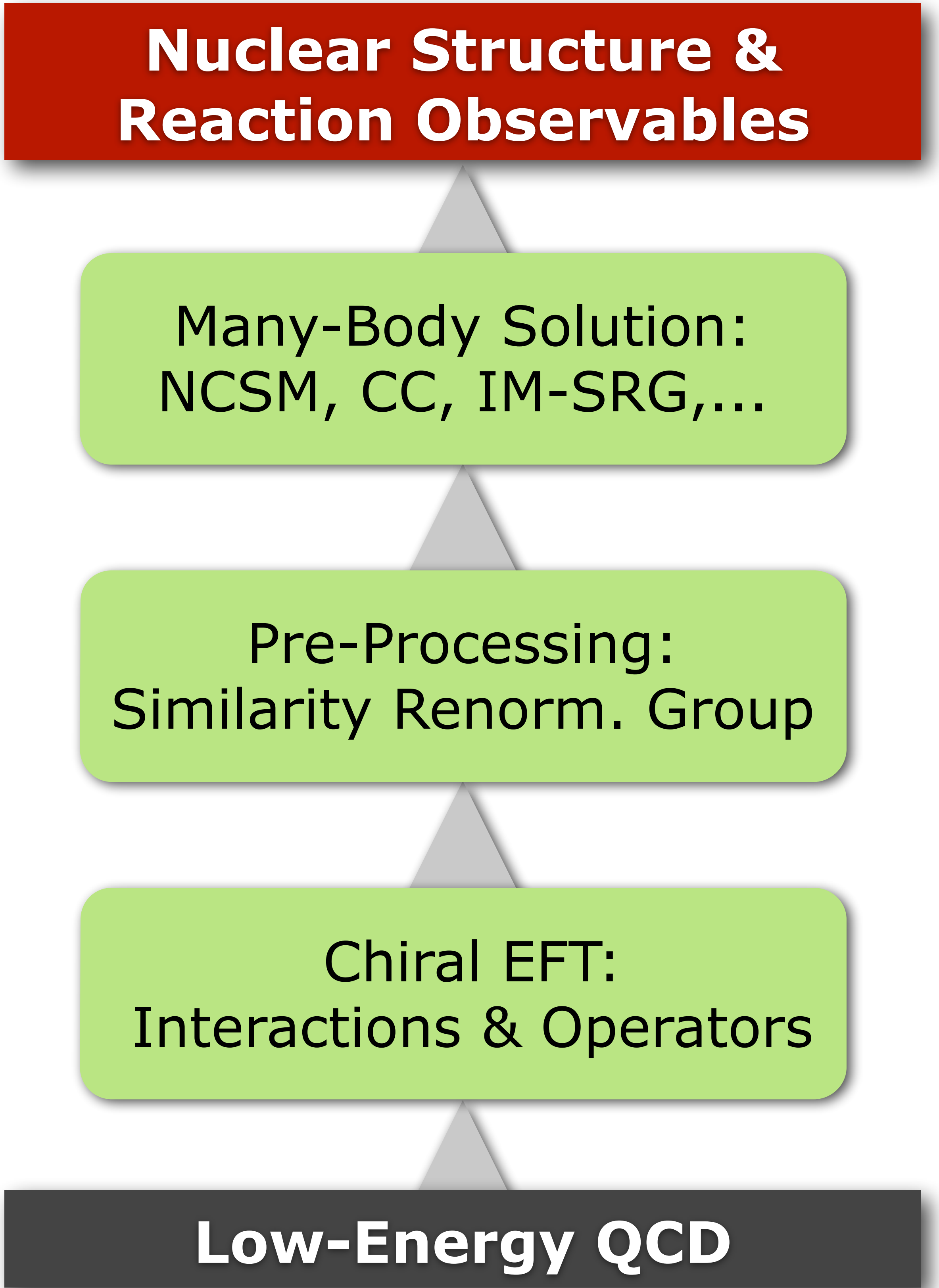
Ab Initio Workflow



Ab Initio Workflow

Nuclear Structure & Reaction Observables

↑

Many-Body Solution:
NCSM, CC, IM-SRG,...

↑

Pre-Processing:
Similarity Renorm. Group

↑

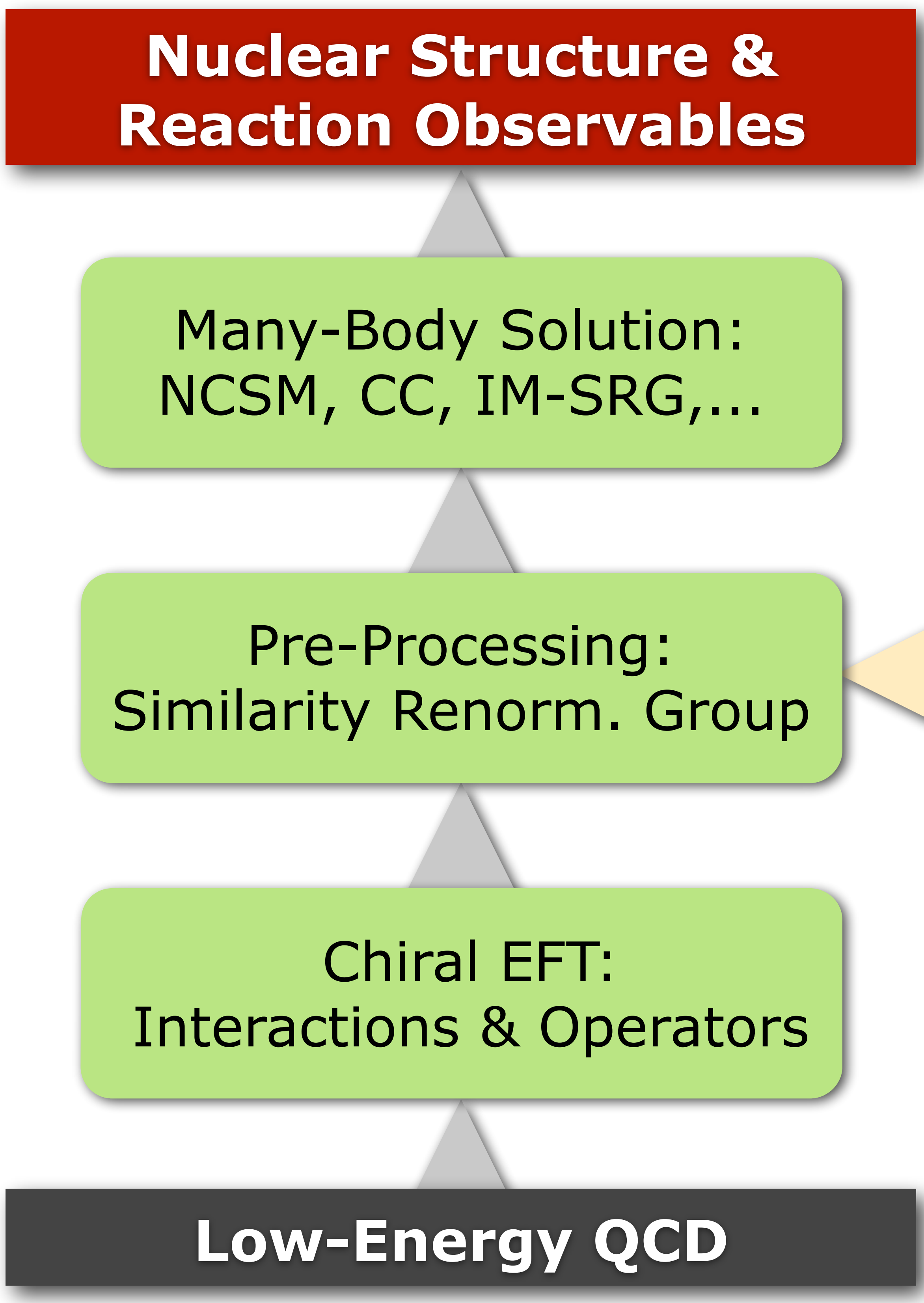
Chiral EFT:
Interactions & Operators

↑

Low-Energy QCD

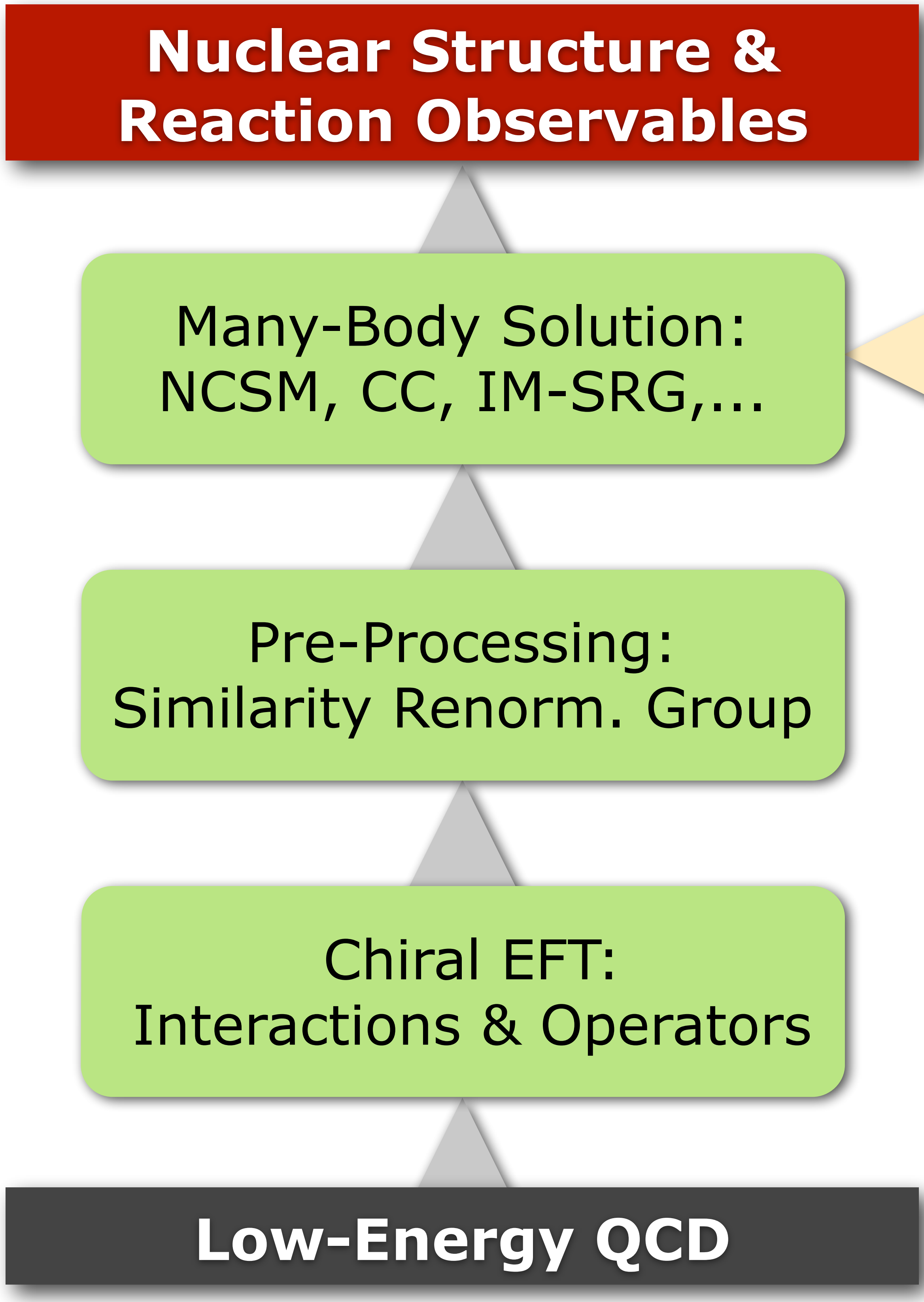
- systematic and improvable with quantified uncertainties
- only "selected" chiral interactions used in nuclear structure so far
- improved chiral EFT interactions offer opportunity to quantify uncertainties systematically

Ab Initio Workflow



- drastically improves convergence of many-body calculation
- induces many-body interactions which can be sizeable
- challenge: include or suppress induced many-body contributions

Ab Initio Workflow



- different many-body methods for different mass regimes and different observables
- present frontiers: continuum & open-shell medium-mass nuclei

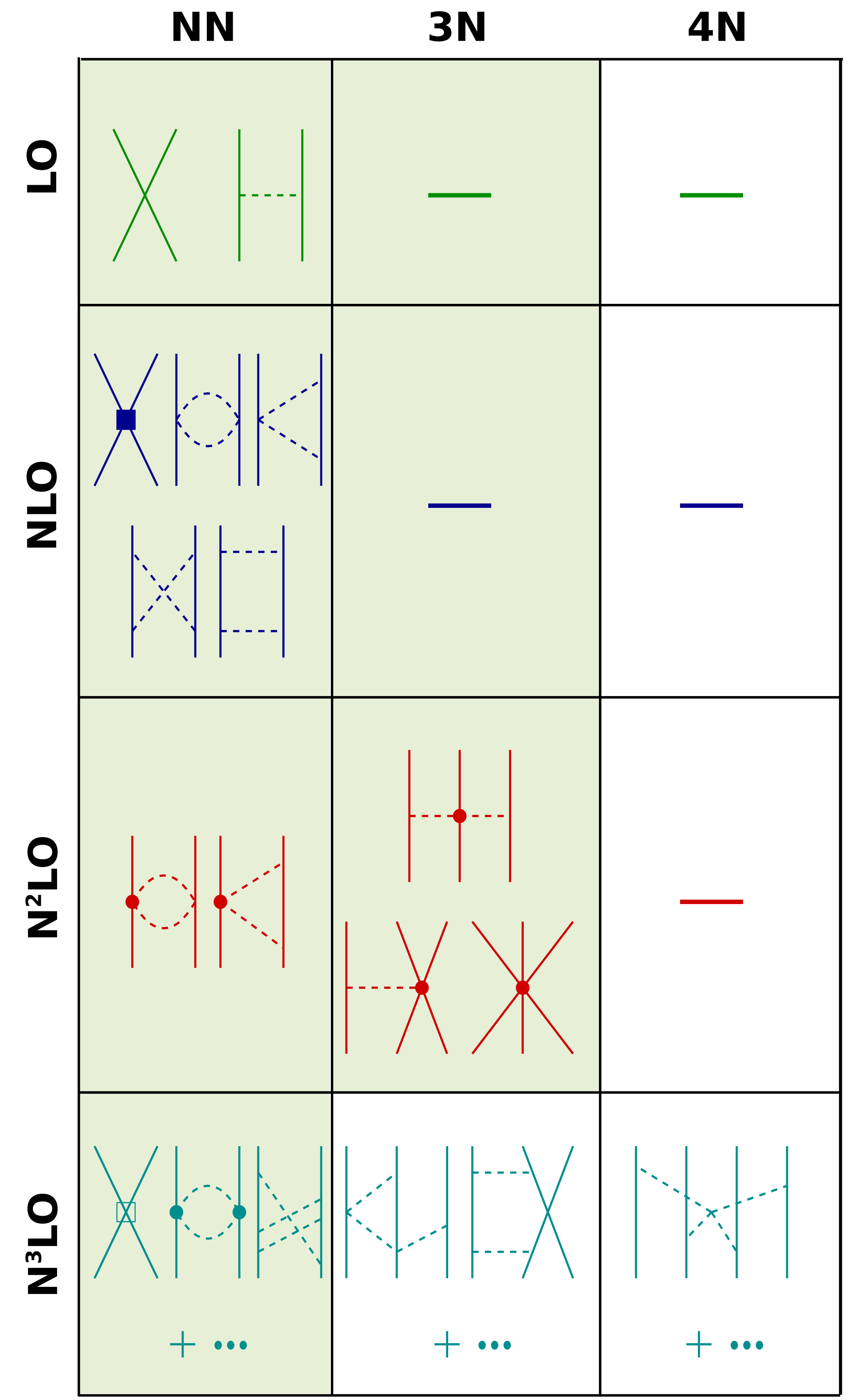
Hamiltonian

Chiral EFT for Nuclear Interactions

Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs, Bernard,...

- nuclear structure practitioners have used selected chiral NN+3N interactions
  - standard Hamiltonian
    NN @ N3LO: Entem & Machleidt, cutoff 500 MeV
    3N @ N2LO: local, cutoff 400 or 500 MeV
  - N2LO-opt, N2LO-sat,...
    purpose-build N2LO interactions utilizing extended fitting strategies
- no investigation of order-by-order convergence or regularization scheme and scale dependence of nuclear structure observables
- LENPIC: systematic propagation of chiral EFT uncertainties to nuclear observables

(talk by H. Krebs)



Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...

continuous unitary transformation driving Hamiltonian towards diagonal form

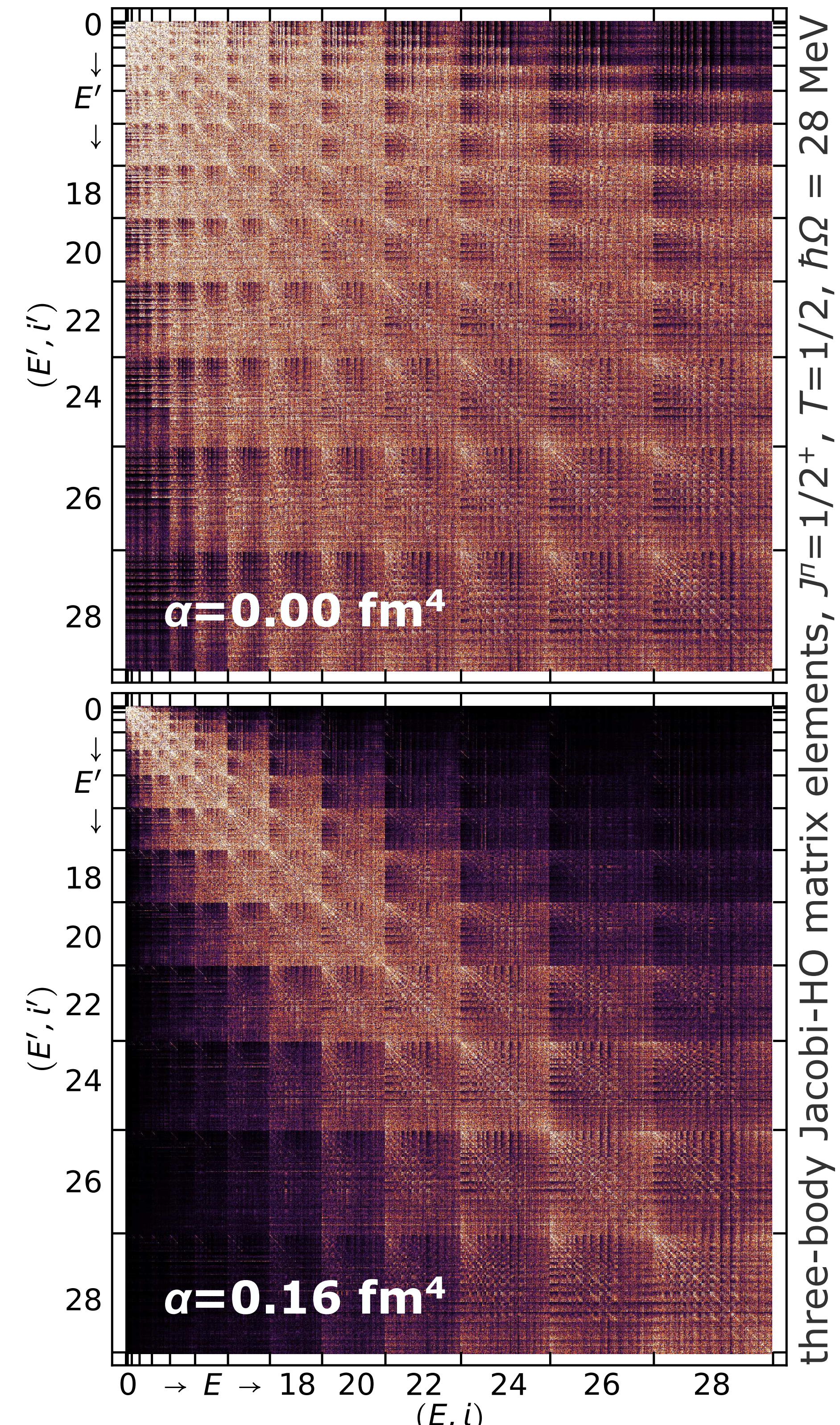
- unitary transformation via flow equation

$$H_\alpha = U_\alpha^\dagger H_0 \, U_\alpha \qquad \rightarrow \qquad \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha]$$

- dynamic generator determines physics of transformation

$$\eta_\alpha = (2\mu)^2 \, [T_{\text{int}}, H_\alpha]$$

- solve flow equation using matrix representation in two- and three-body space
- flow parameter α determines how far to go



Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...

pro:
improves convergence of many-body calculations

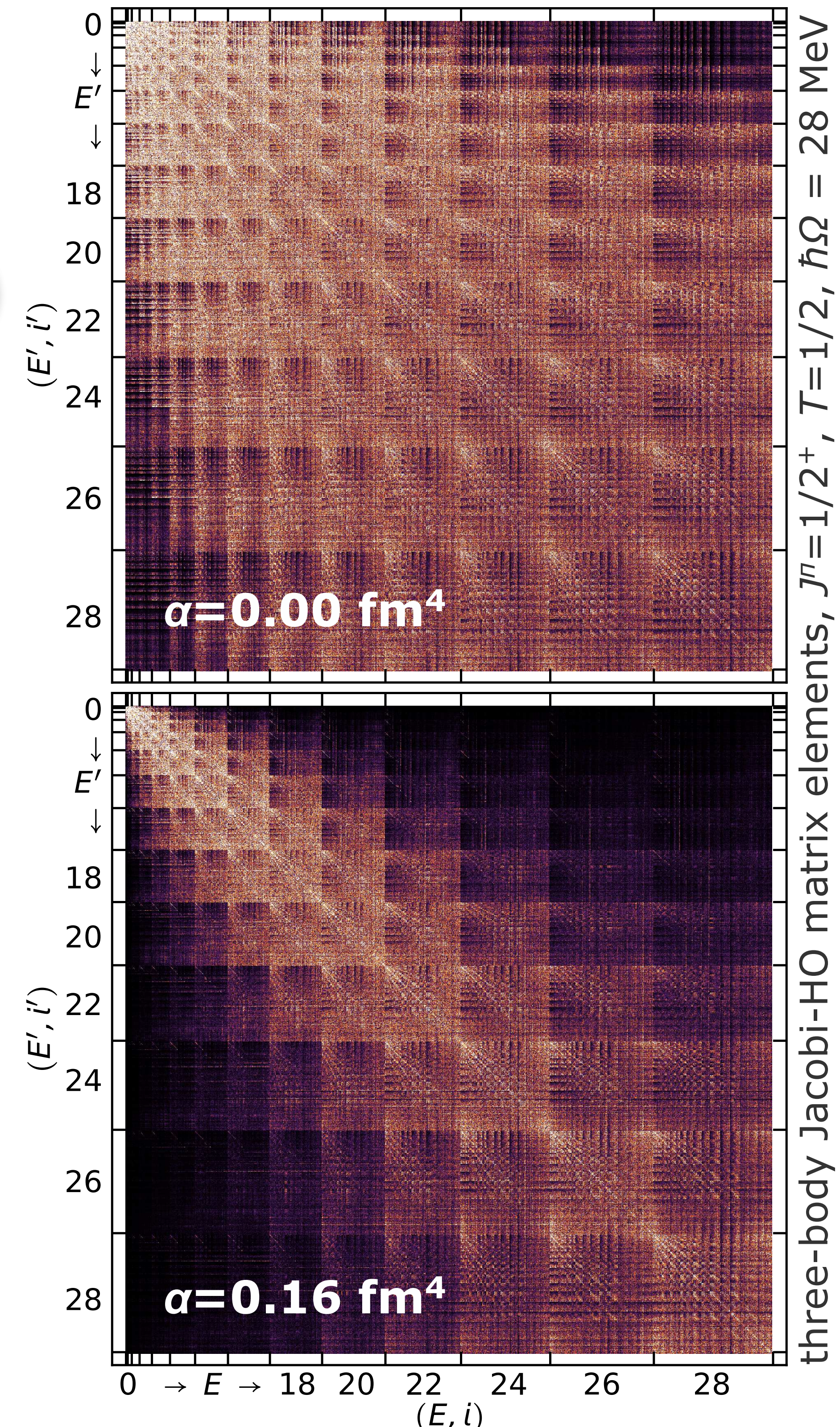
con:
induces many-body interactions

- need to truncate evolved Hamiltonian

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + \cdots$$

- variation of flow parameter provides diagnostic for omitted many-body terms

- truncations used in the following:
  - **NN+3N$_{\text{ind}}$**
    use initial NN, keep evolved NN+3N
  - **NN+3N$_{\text{full}}$**
    use initial NN+3N, keep evolved NN+3N



Light Nuclei

No-Core Shell Model & Friends

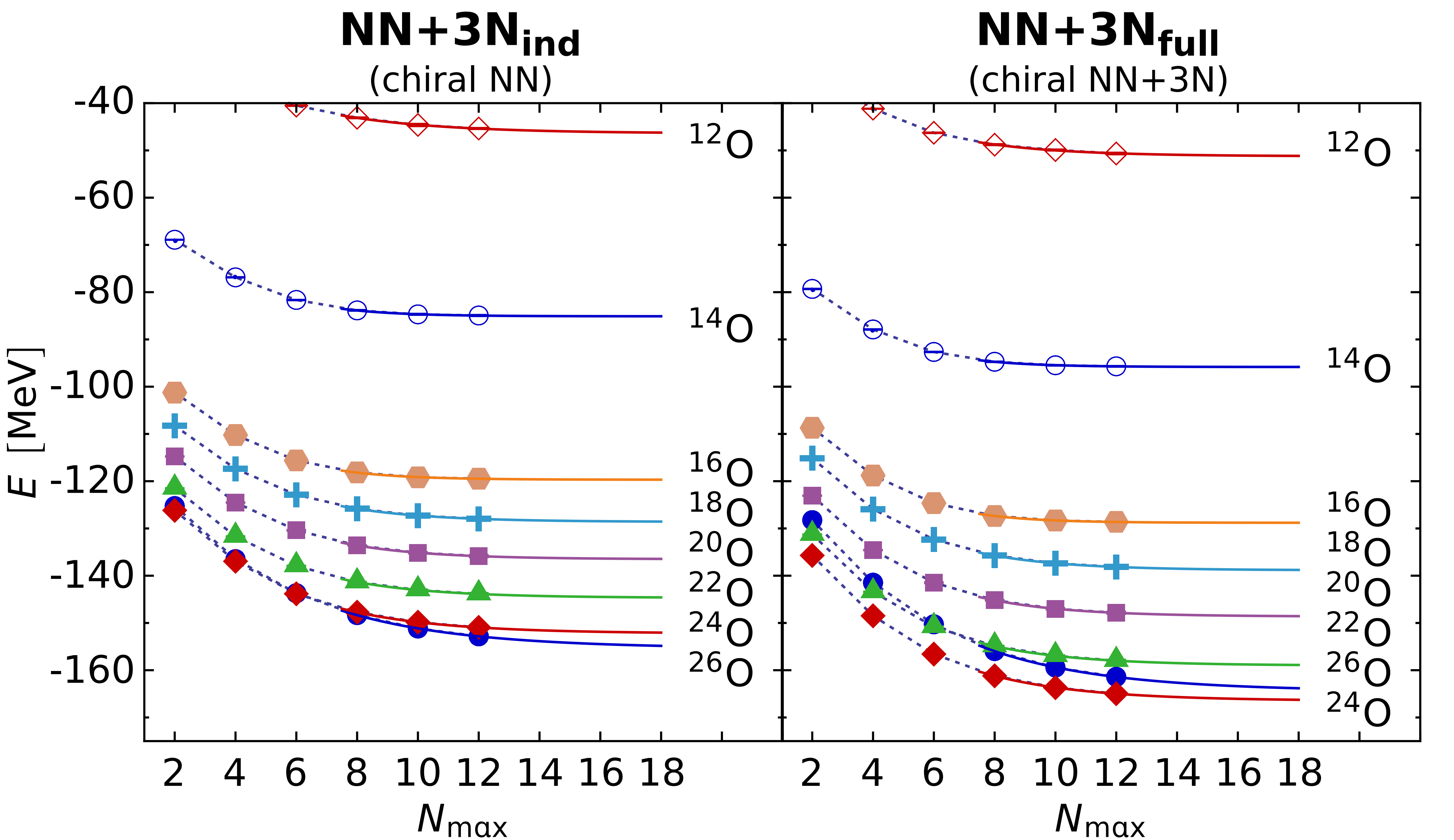
Barrett, Vary, Navrátil, Maris, Nogga, Roth,...

NCSM-type approaches are the most powerful and universal ab initio methods for the p- and lower sd-shell

- **NCSM**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
  - convergence of observables w.r.t. $N_{\max}$ is the only limitation and source of uncertainty
- **Importance-Truncated NCSM**: reduce NCSM model space to physically relevant basis states and extrapolate to full space a posteriori
  - increases the range of applicability of NCSM significantly
- **NCSM with Continuum**: merge NCSM for description of clusters with Resonating Group Method for description of their relative motion
  - explicitly includes continuum degrees of freedom
- more: Gamow NCSM, Symplectic NCSM, ...

Ground States of Oxygen Isotopes

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



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

Ground States of Oxygen Isotopes

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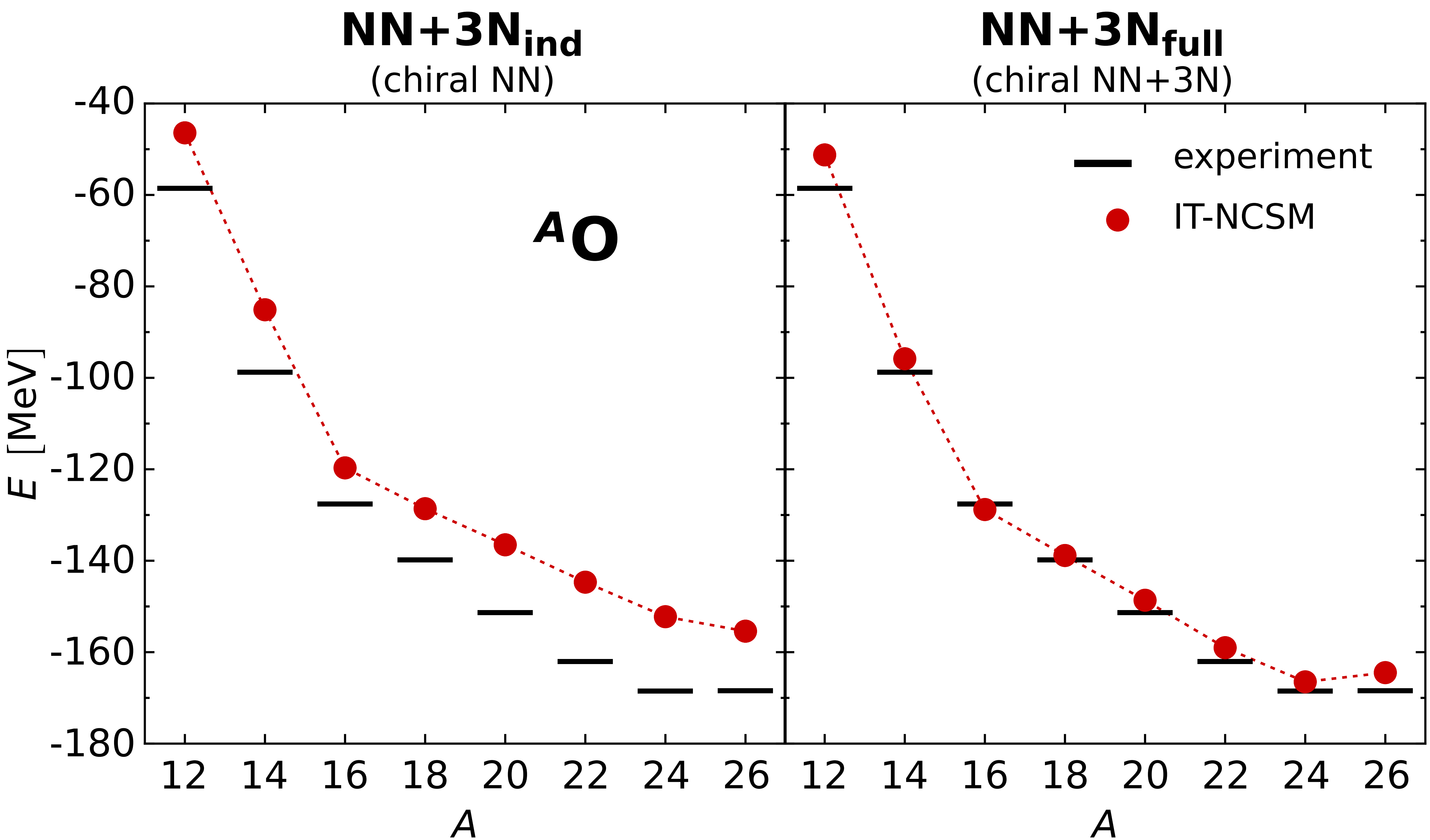

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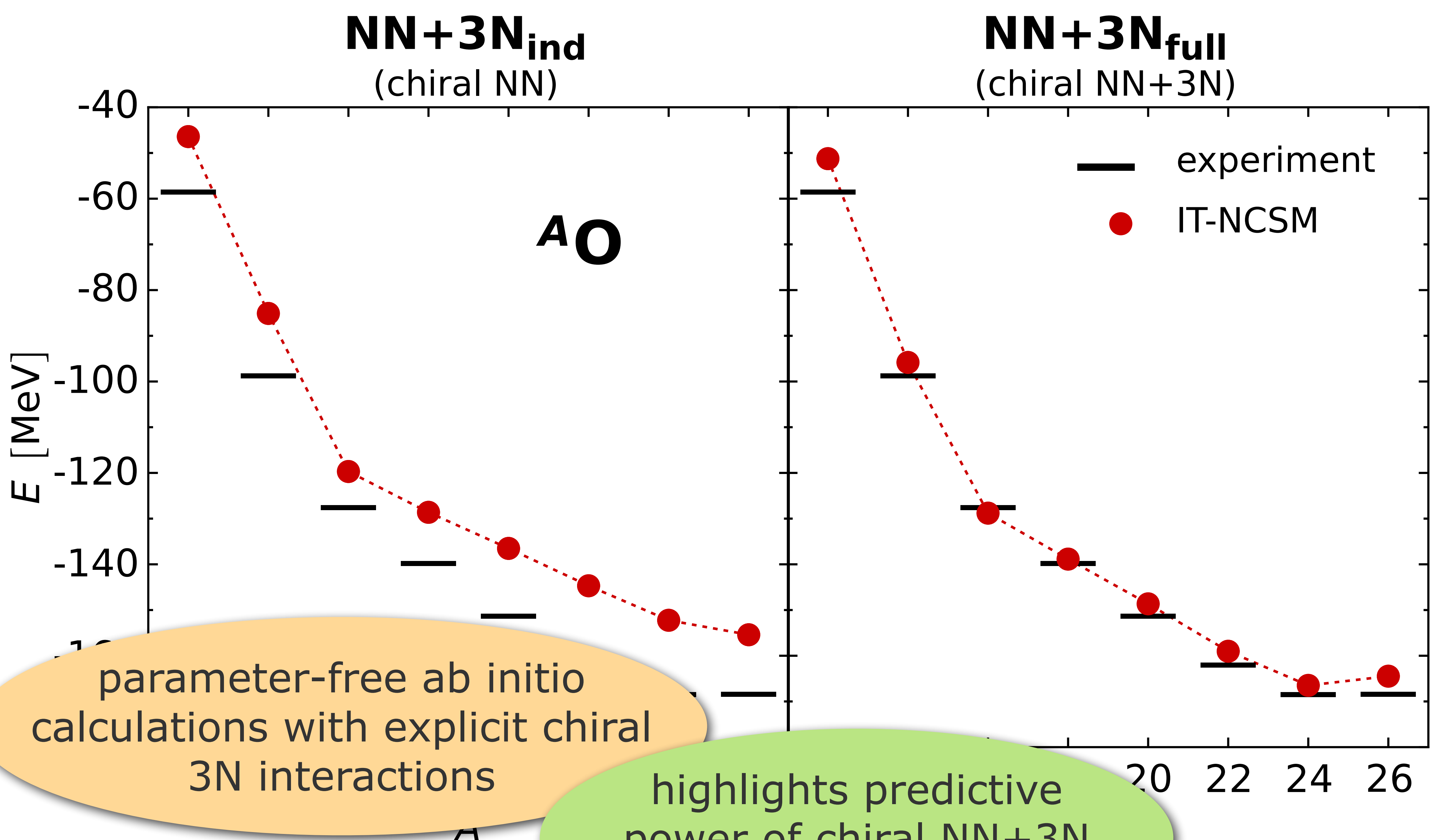


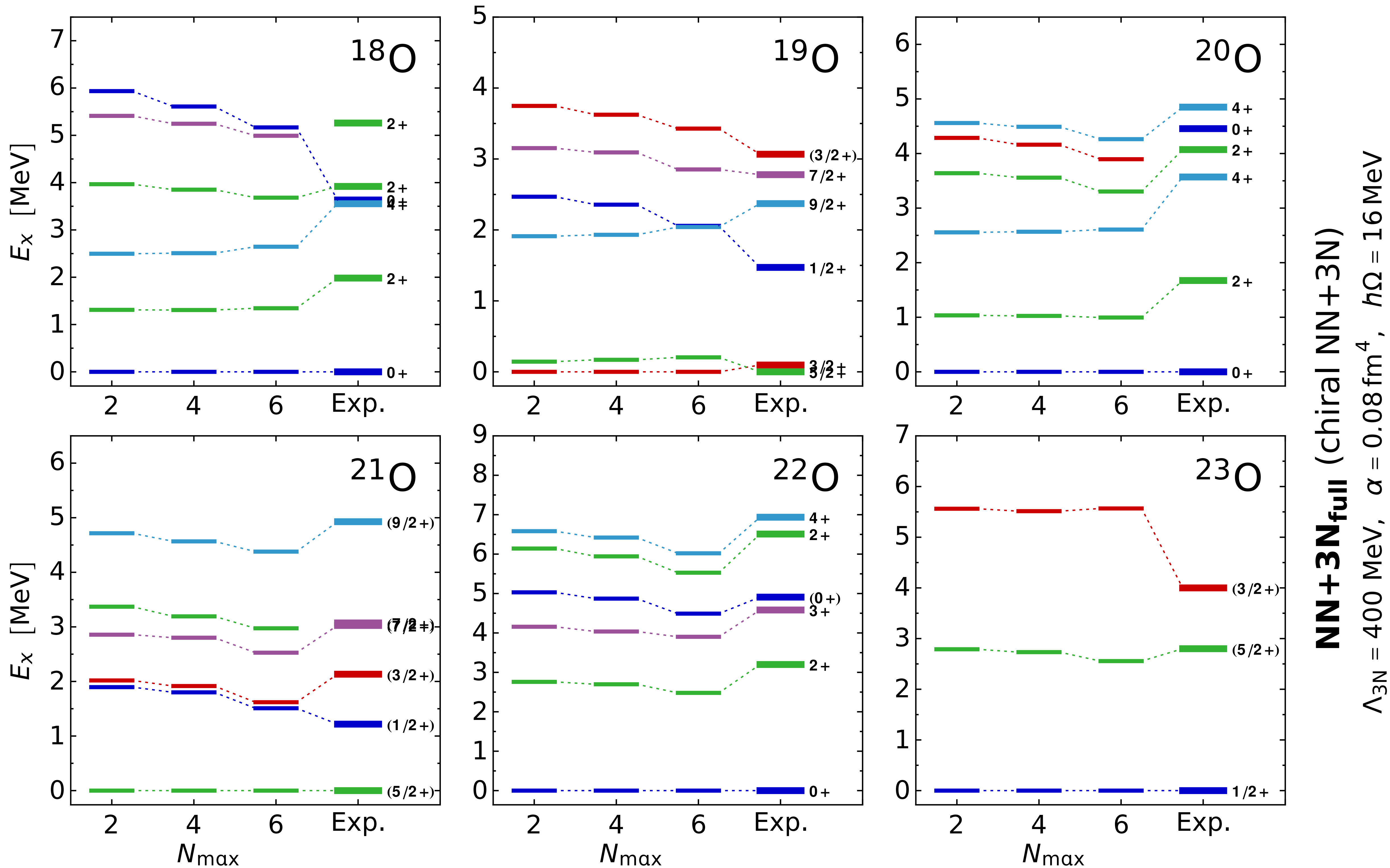
parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

Λ_{3N} = 400 MeV, α = ... optimal $\hbar\Omega$

Spectra of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013) & in prep.



Medium-Mass Nuclei

Medium-Mass Approaches

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 exponential wave operator applied to single-determinant reference state
  - truncation at doubles level (CCSD) plus triples corrections (Λ-CCSD(T))
  - equations of motion for excited states and near-closed-shell nuclei

Bogner, Tsukiyama, Schwenk, Hergert,...

- **in-medium SRG**: complete decoupling of particle-hole excitations from many-body reference state through SRG evolution
  - normal-ordered evolving A-body Hamiltonian truncated at two-body level
  - both closed- and open-shell ground states; excitations via EOM or SM

Barbieri, Soma, Duguet,...

- self-consistent Green's function approaches and others...

Medium-Mass Approaches

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  - ... ...ell ground states; excitations via EOM or SM

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

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

Ground States of Oxygen Isotopes

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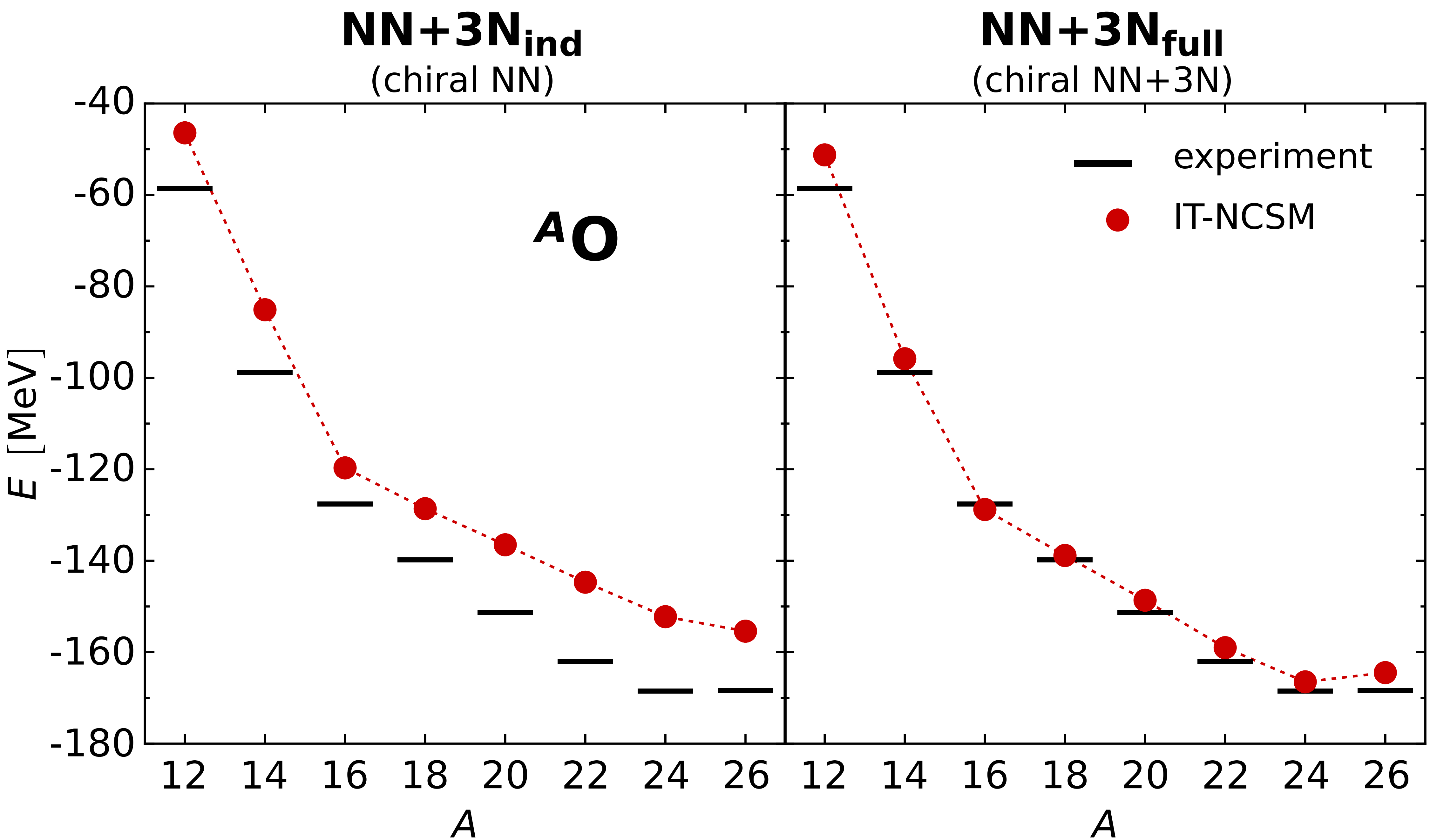

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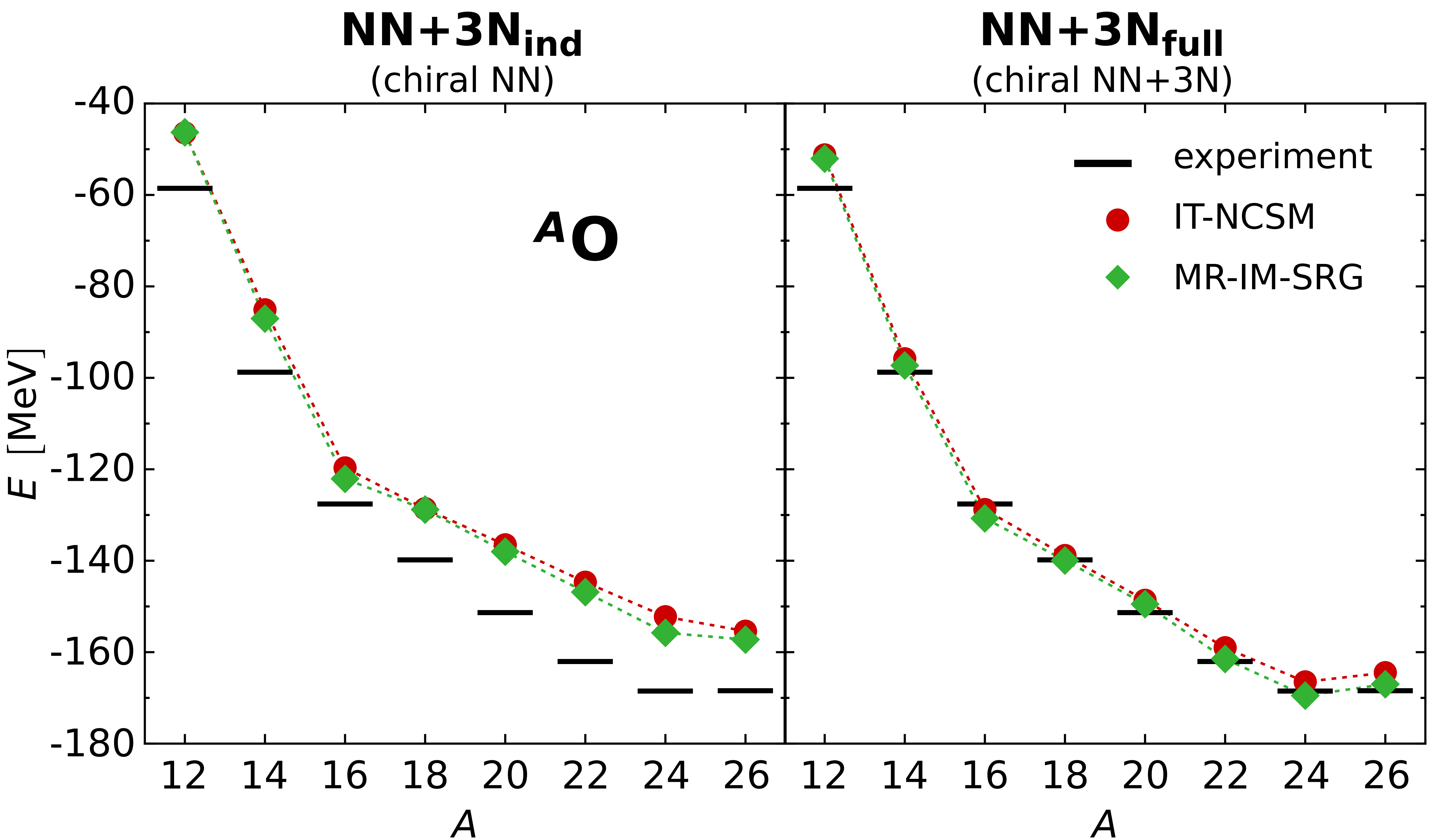

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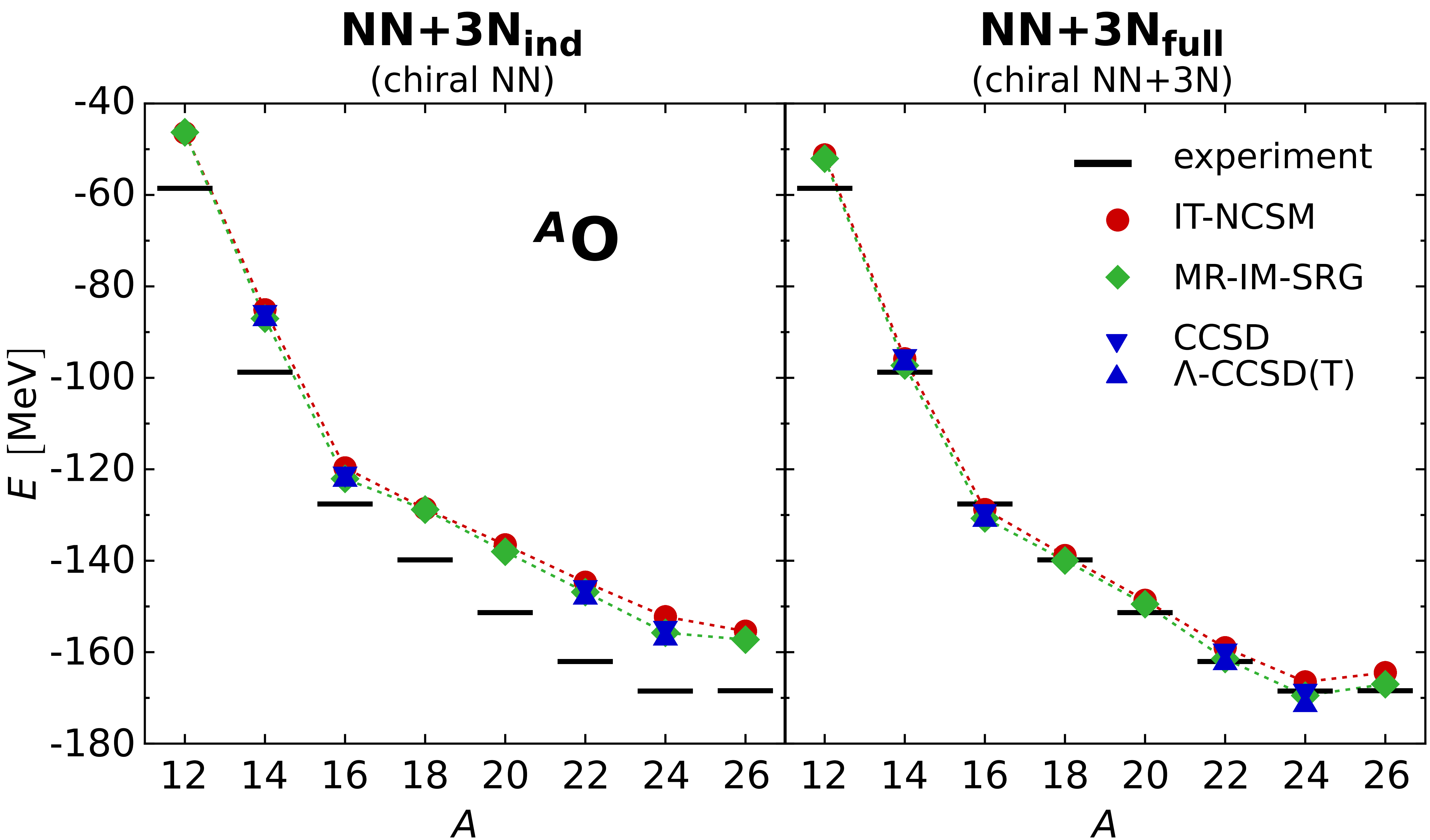

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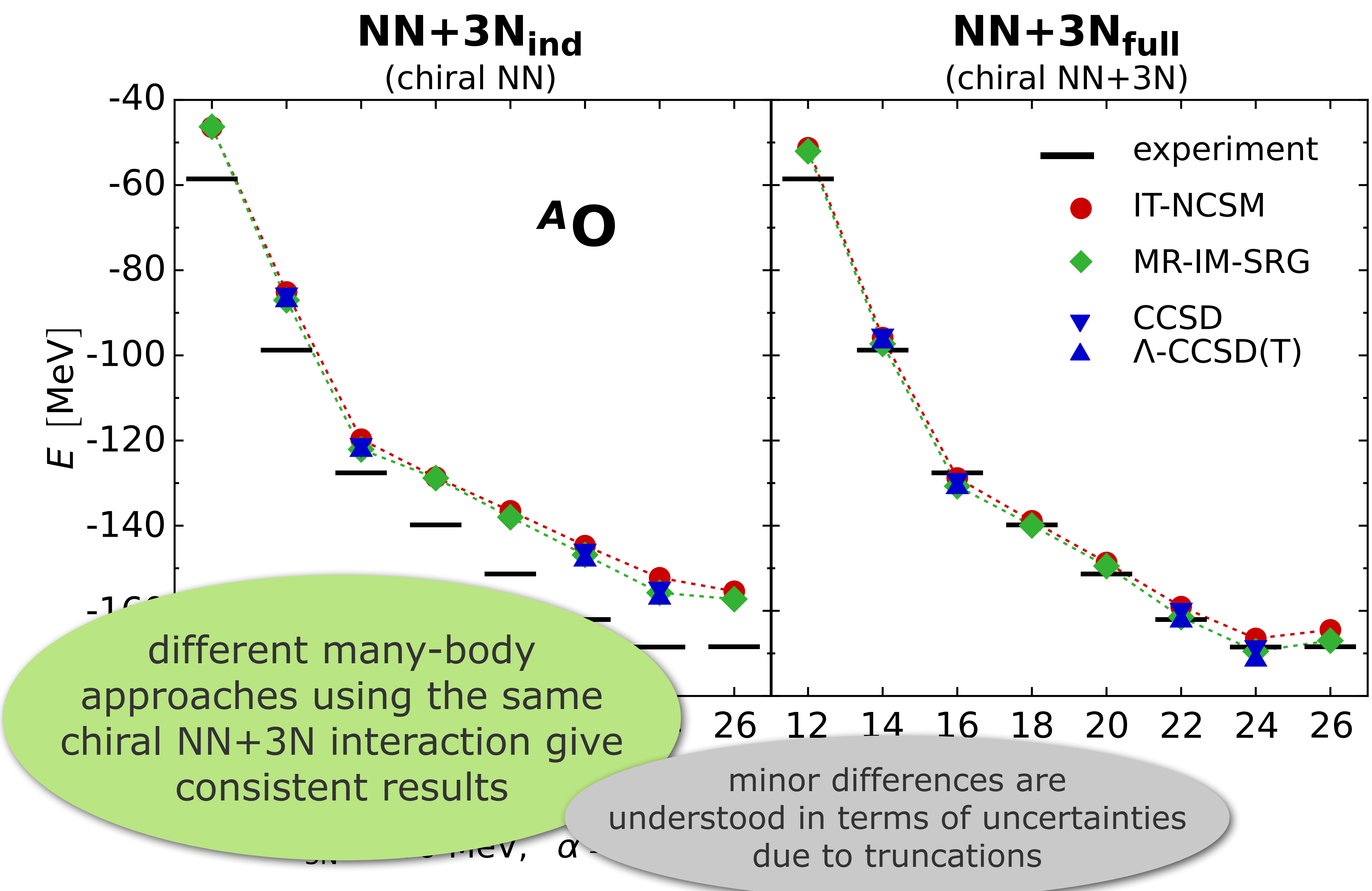
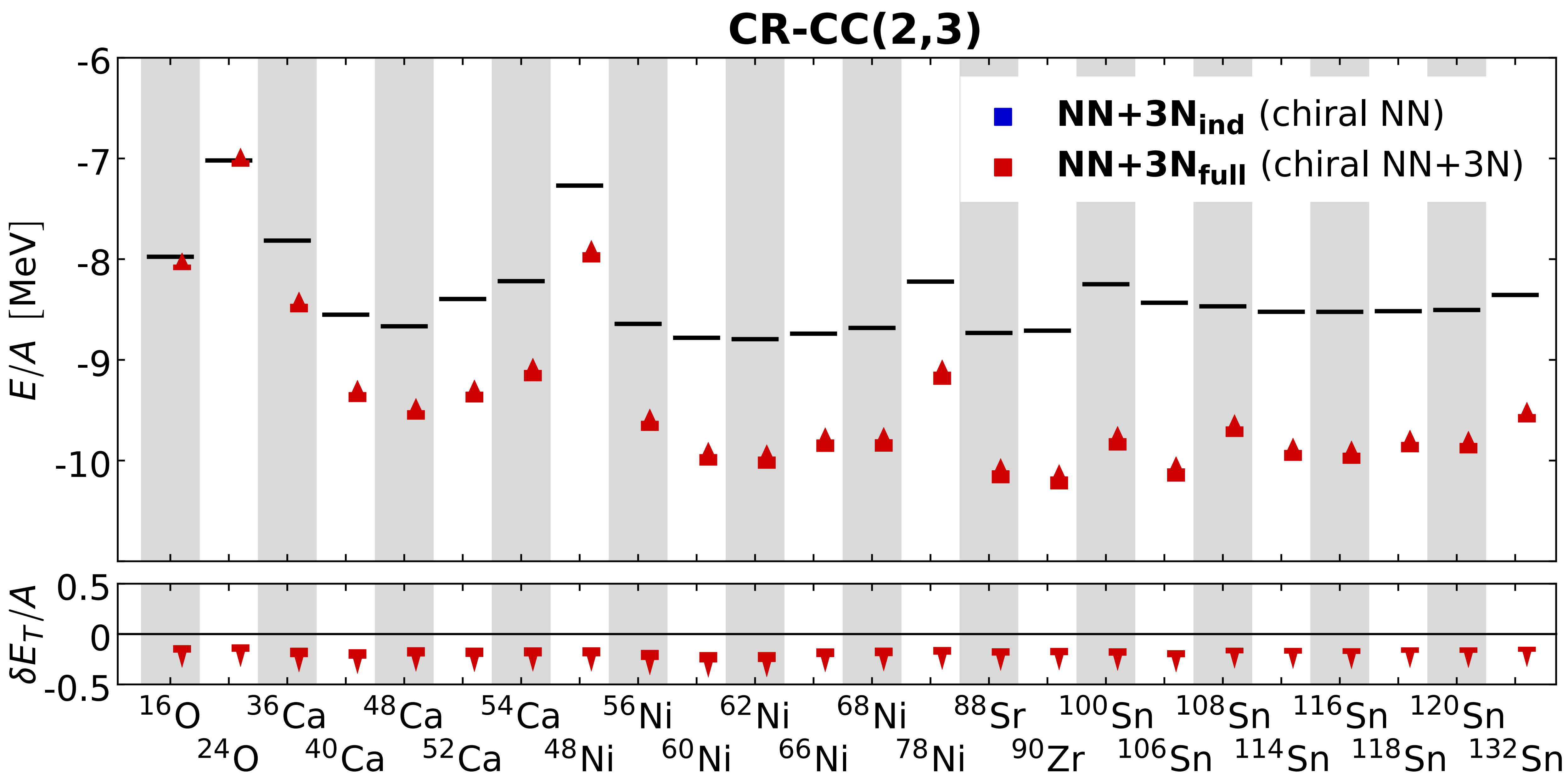


Towards Heavy Nuclei - Ab Initio

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



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

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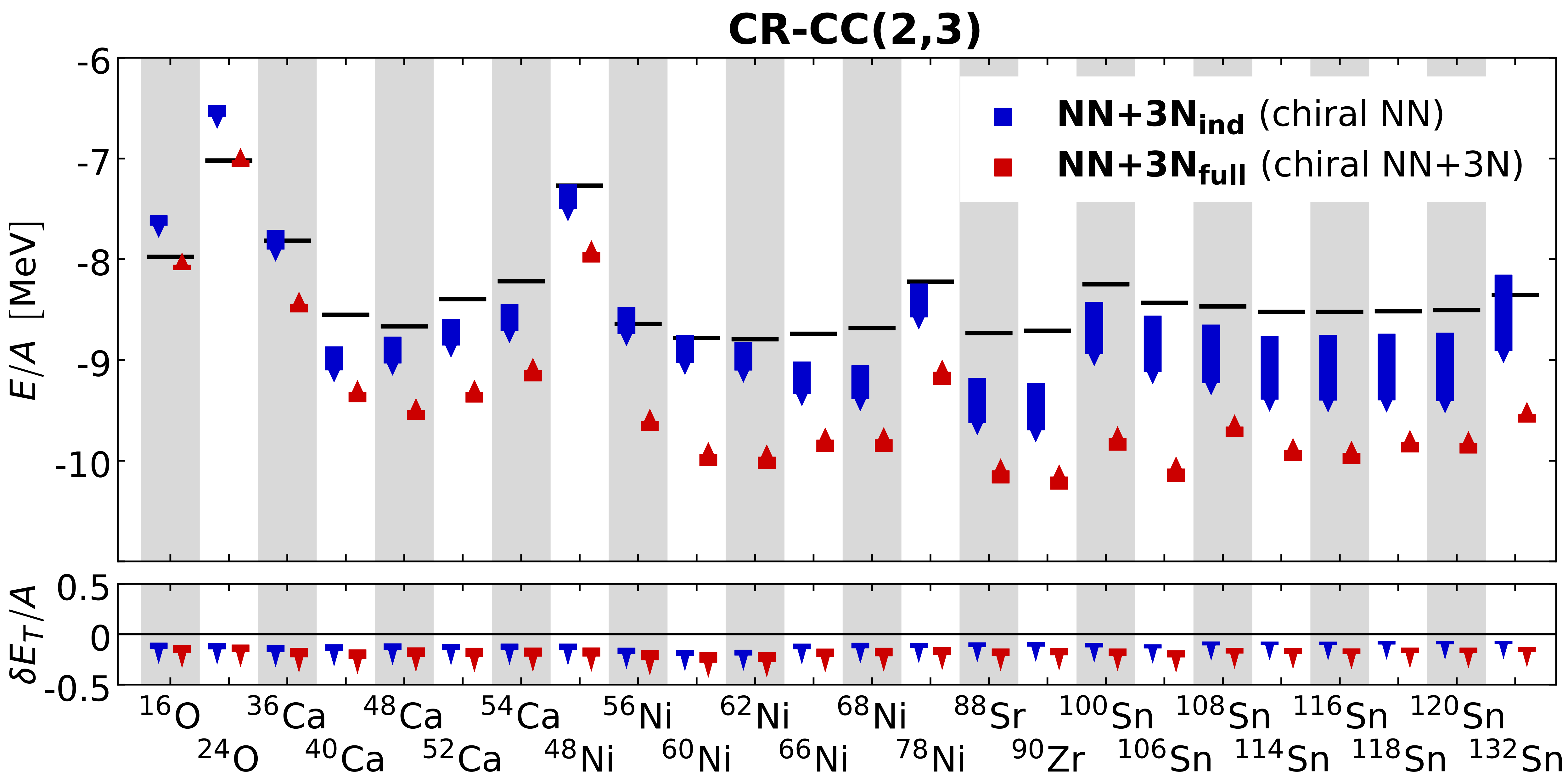

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\mathrm{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

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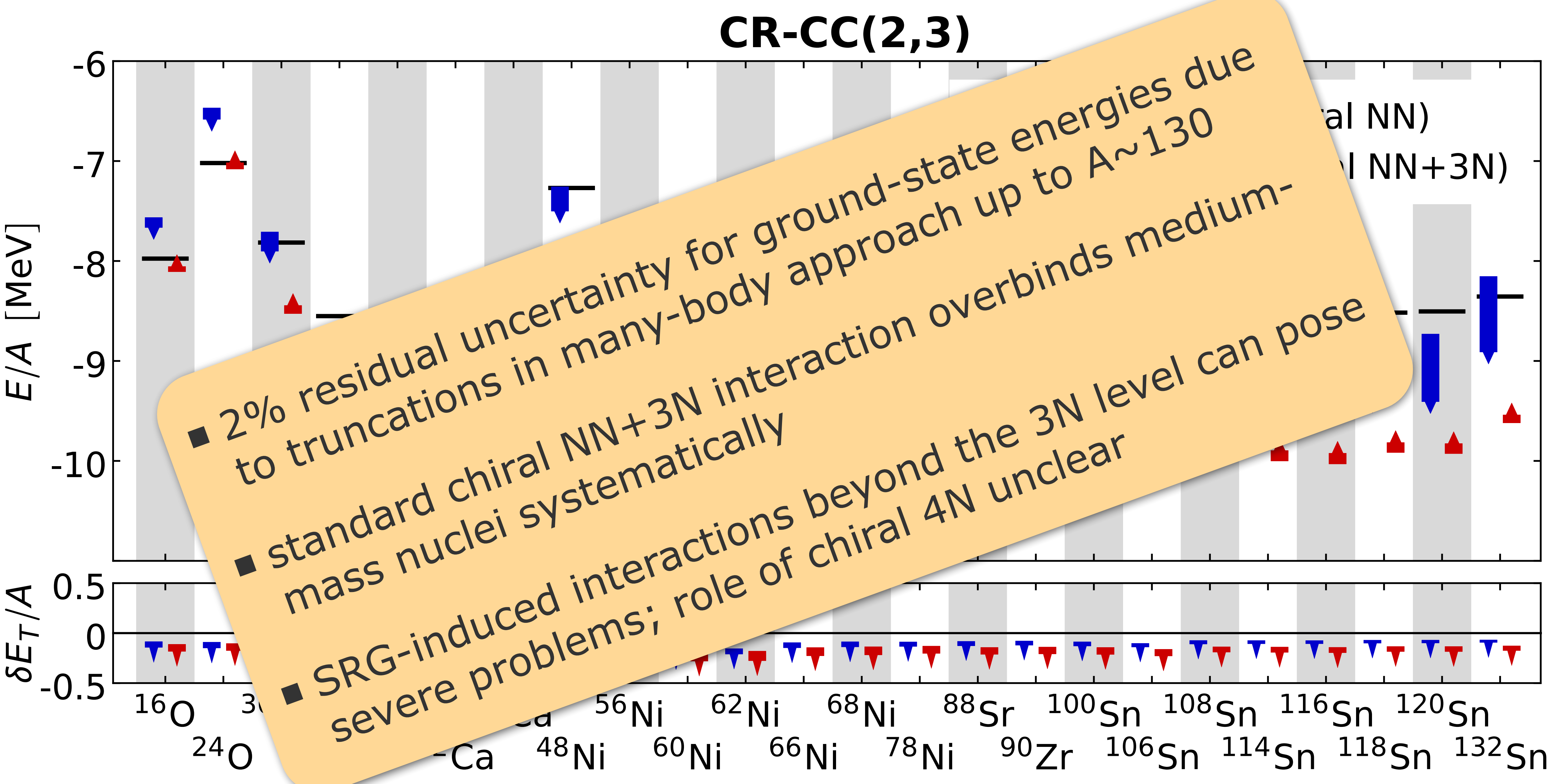
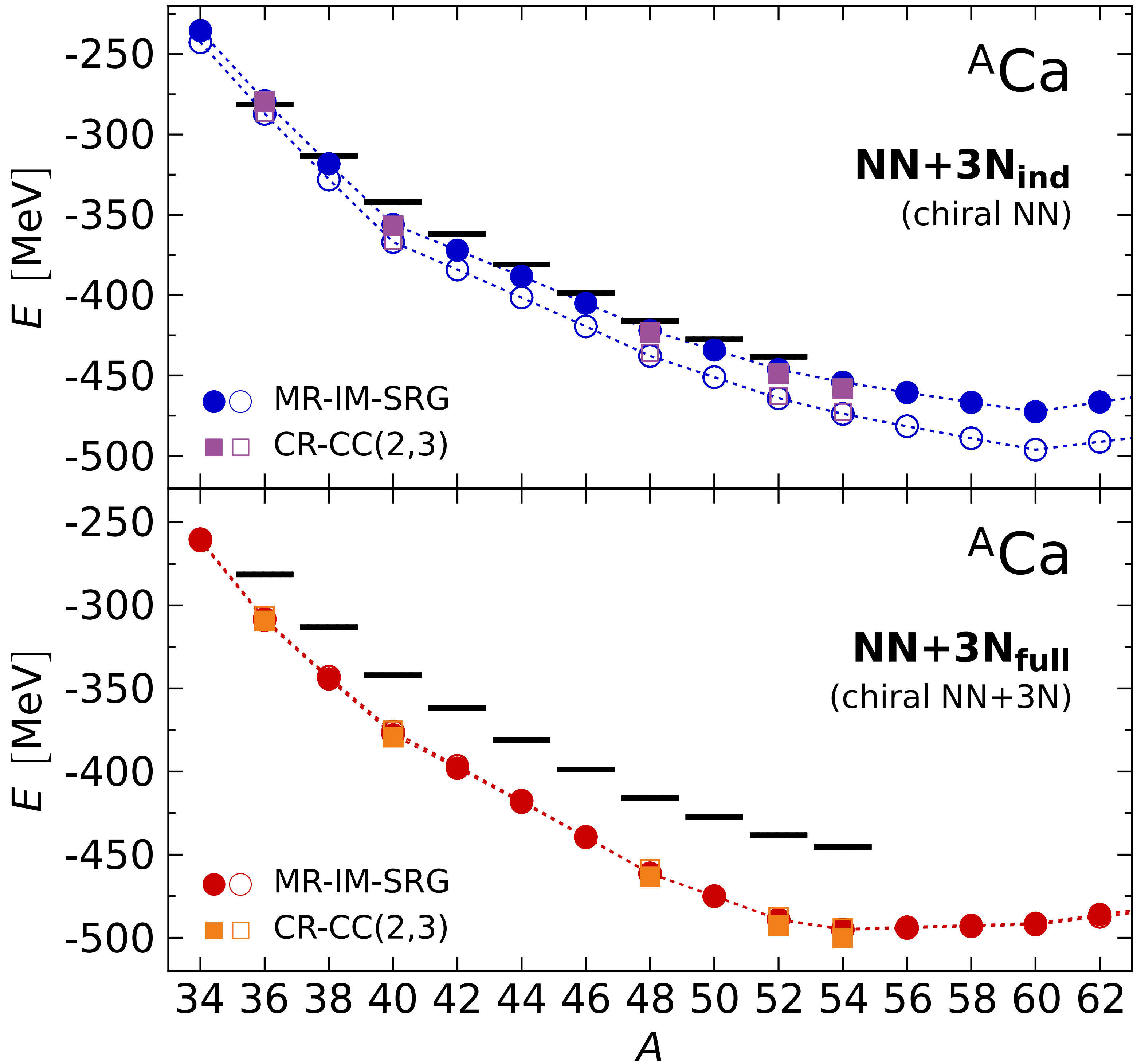


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

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

Open-Shell Medium-Mass Nuclei

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

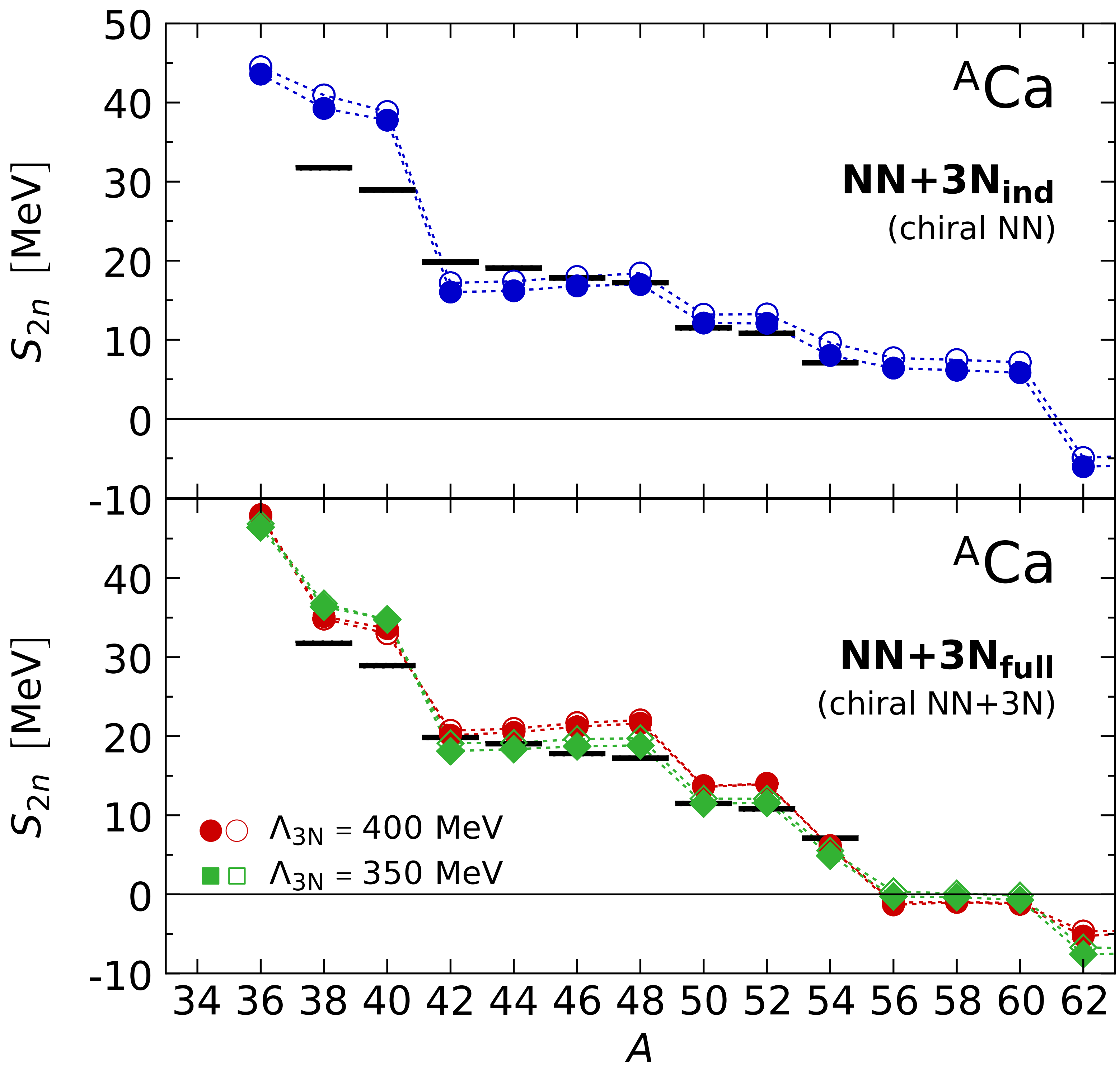


- systematic multi-reference IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

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

Next Step:

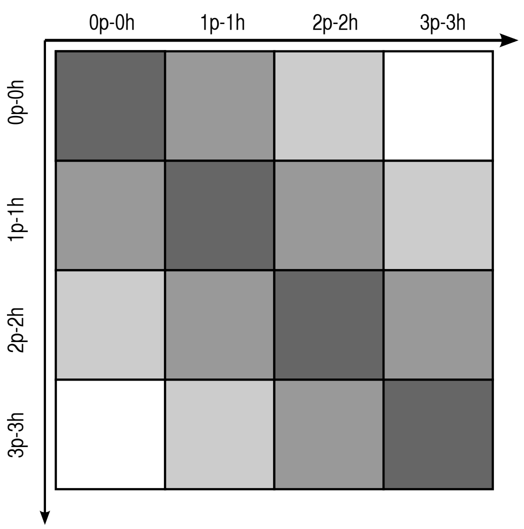
Merging NCSM and IM-SRG

with

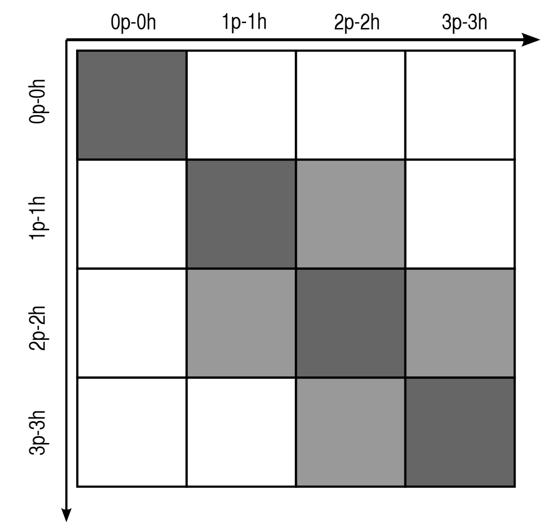
Eskendr Gebrerufael, Heiko Hergert, Klaus Vobig

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 (Kutzelnigg/Mukherjee) normal order, omitting normal-ordered 3B term

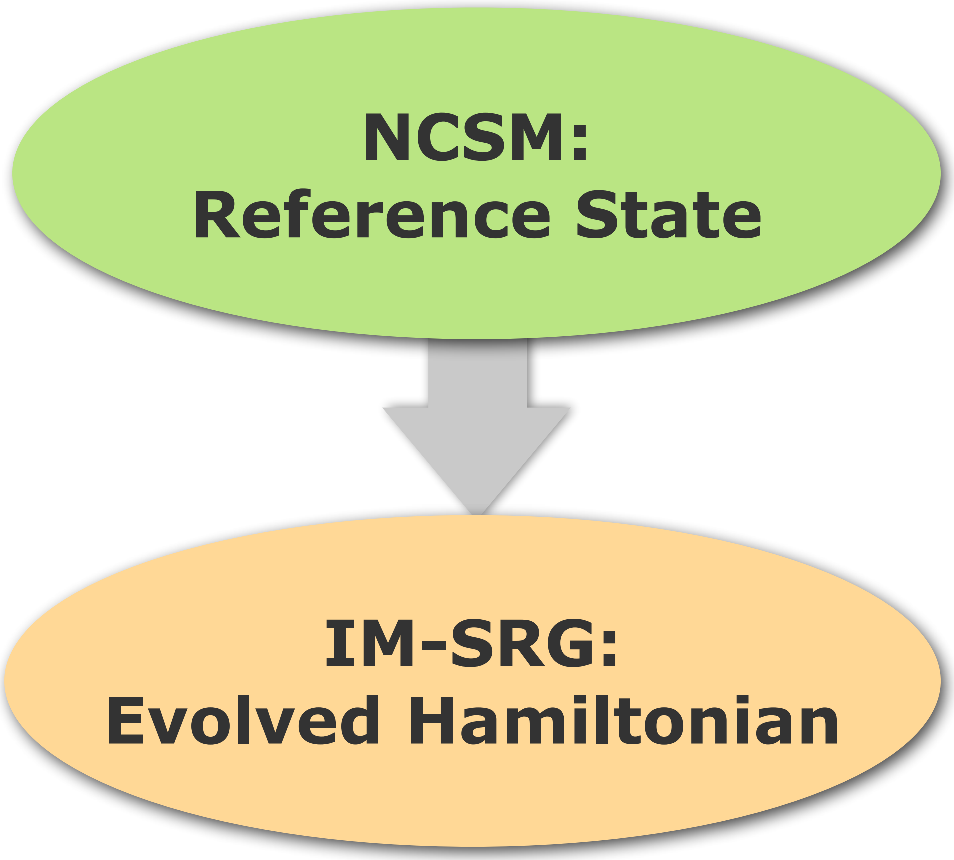
$$H(s) = E(s) + \sum_{ij} f^i_j(s)\,\tilde{A}^i_j + \frac{1}{4}\sum_{ijkl}\Gamma^{ij}_{kl}(s)\,\tilde{A}^{ij}_{kl} + \frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn}(s)\,\tilde{A}^{ijk}_{lmn}$$

Merging NCSM and IM-SRG

NCSM:
Reference State

- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- not limited to subsets of open-shell nuclei and systematically improvable

Merging NCSM and IM-SRG



- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- not limited to subsets of open-shell nuclei and systematically improvable

- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in A-body space

Merging NCSM and IM-SRG

NCSM: Reference State

- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- not limited to subsets of open-shell nuclei and systematically improvable

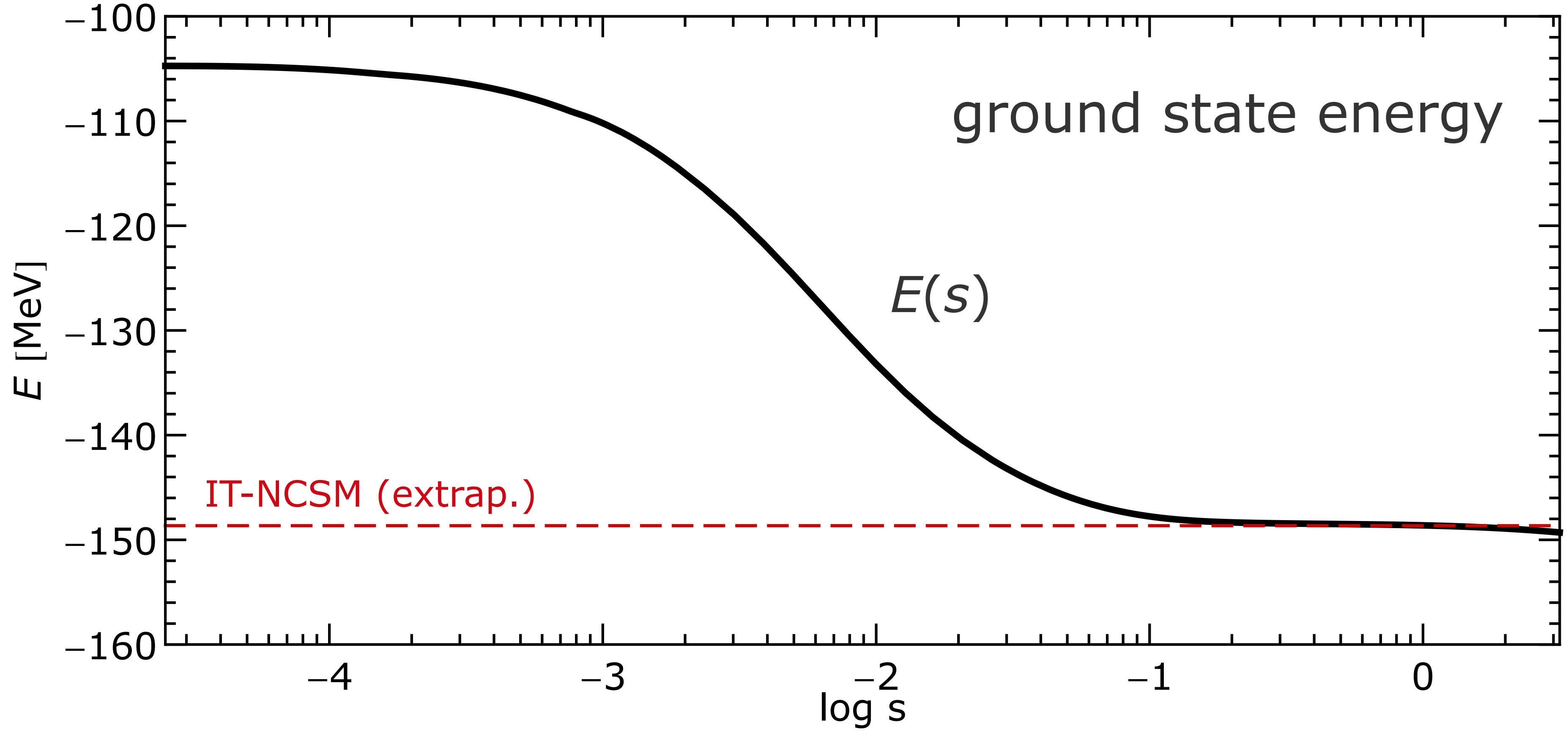
IM-SRG: Evolved Hamiltonian

- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in A-body space

NCSM: Observables

- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

^{20}O: Flowing Energy



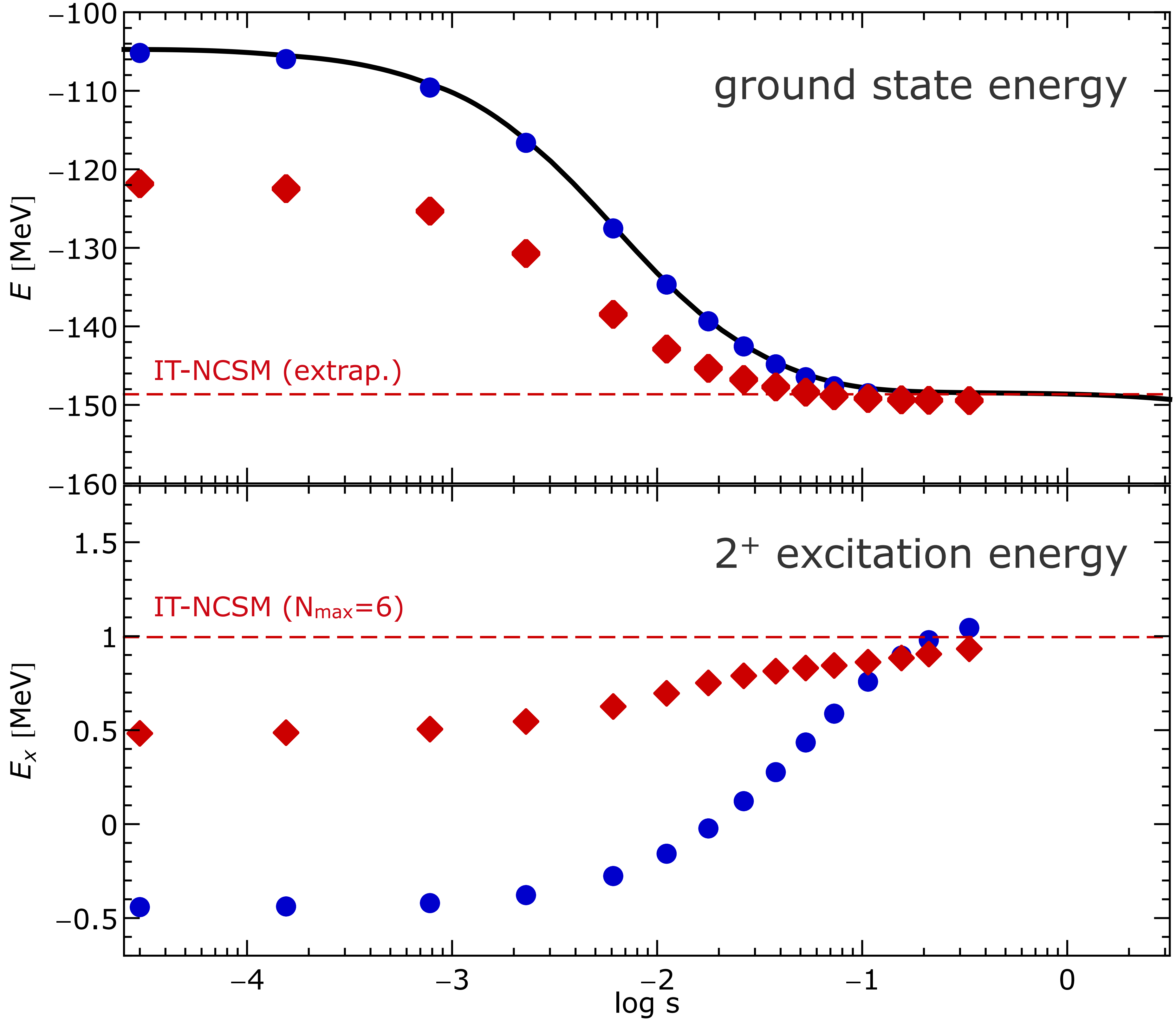
^{20}O

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV

N_{max}=0
reference state

e_{max}=10

^{20}O: Flowing Energy



^{20}O

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV

N_{max}=0
reference state

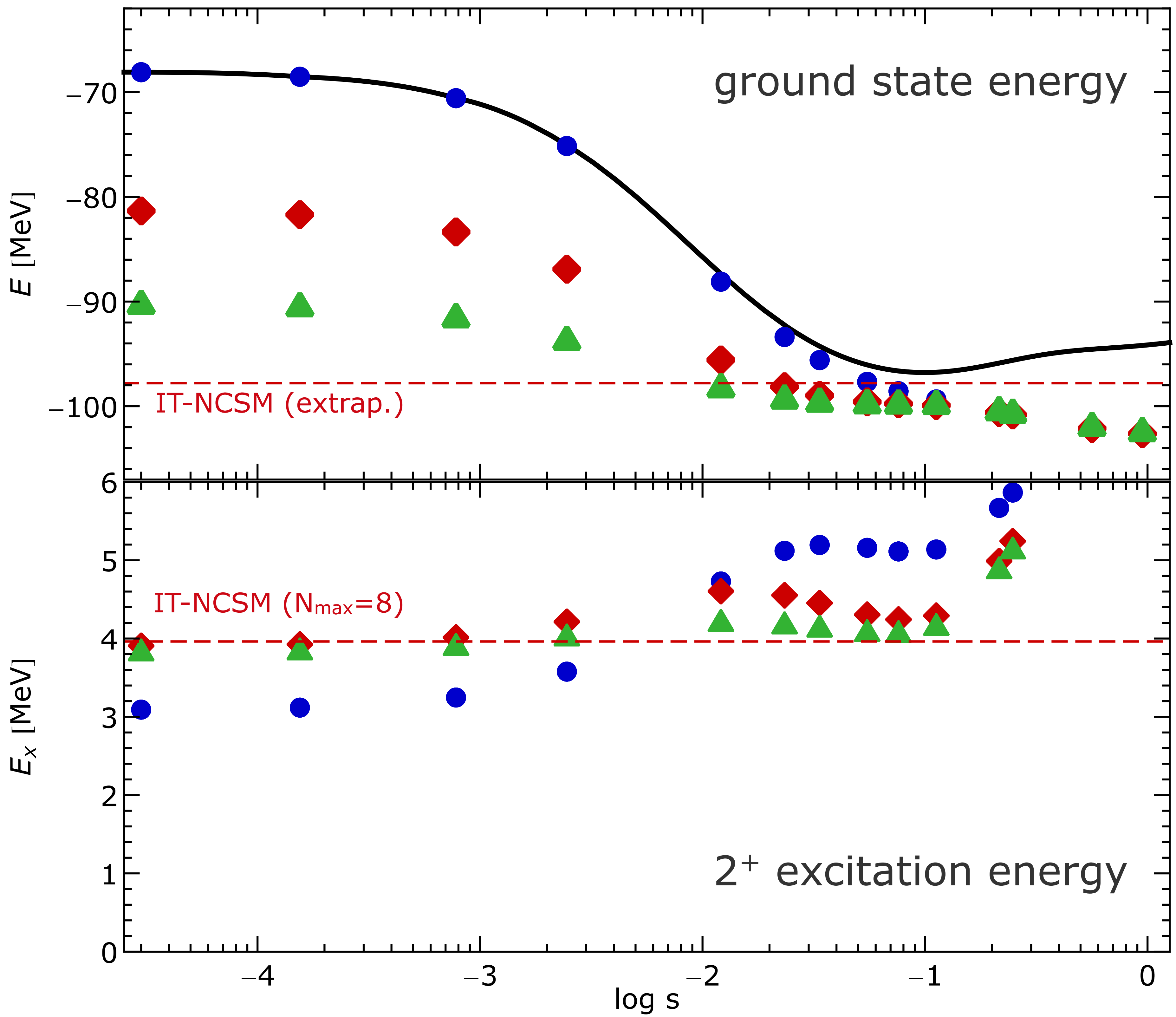
e_{max}=10

NCSM with flowing Hamiltonian

● N_{max}=0

◆ N_{max}=2

^{12}C: Flowing Energy



^{12}C

chiral NN+3N
Λ_{3N}=500 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV

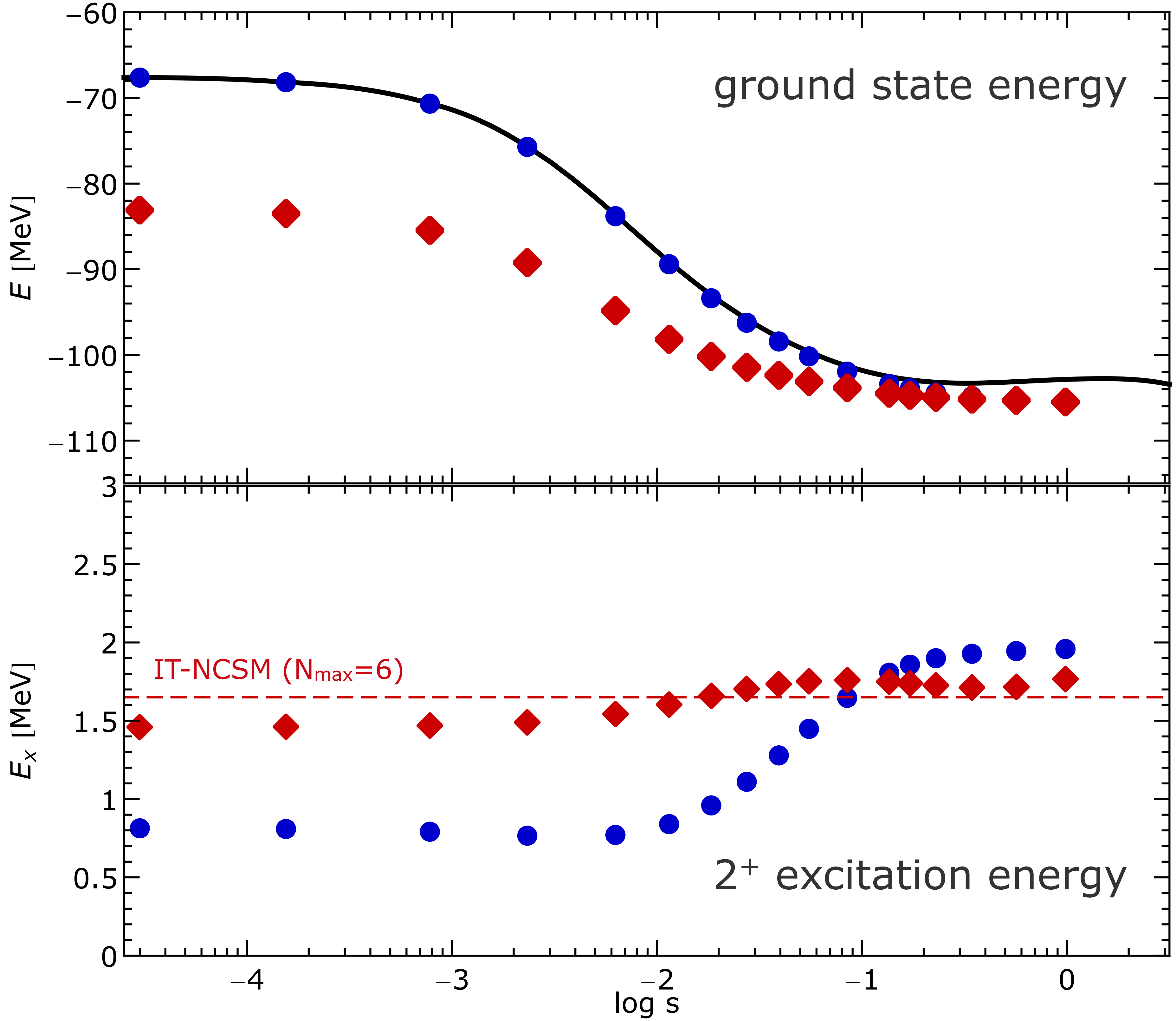
N_{max}=0
reference state

e_{max}=10

NCSM with flowing Hamiltonian

- N_{max}=0
- N_{max}=2
- N_{max}=4

^{16}C: Flowing Energy



^{16}C

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV

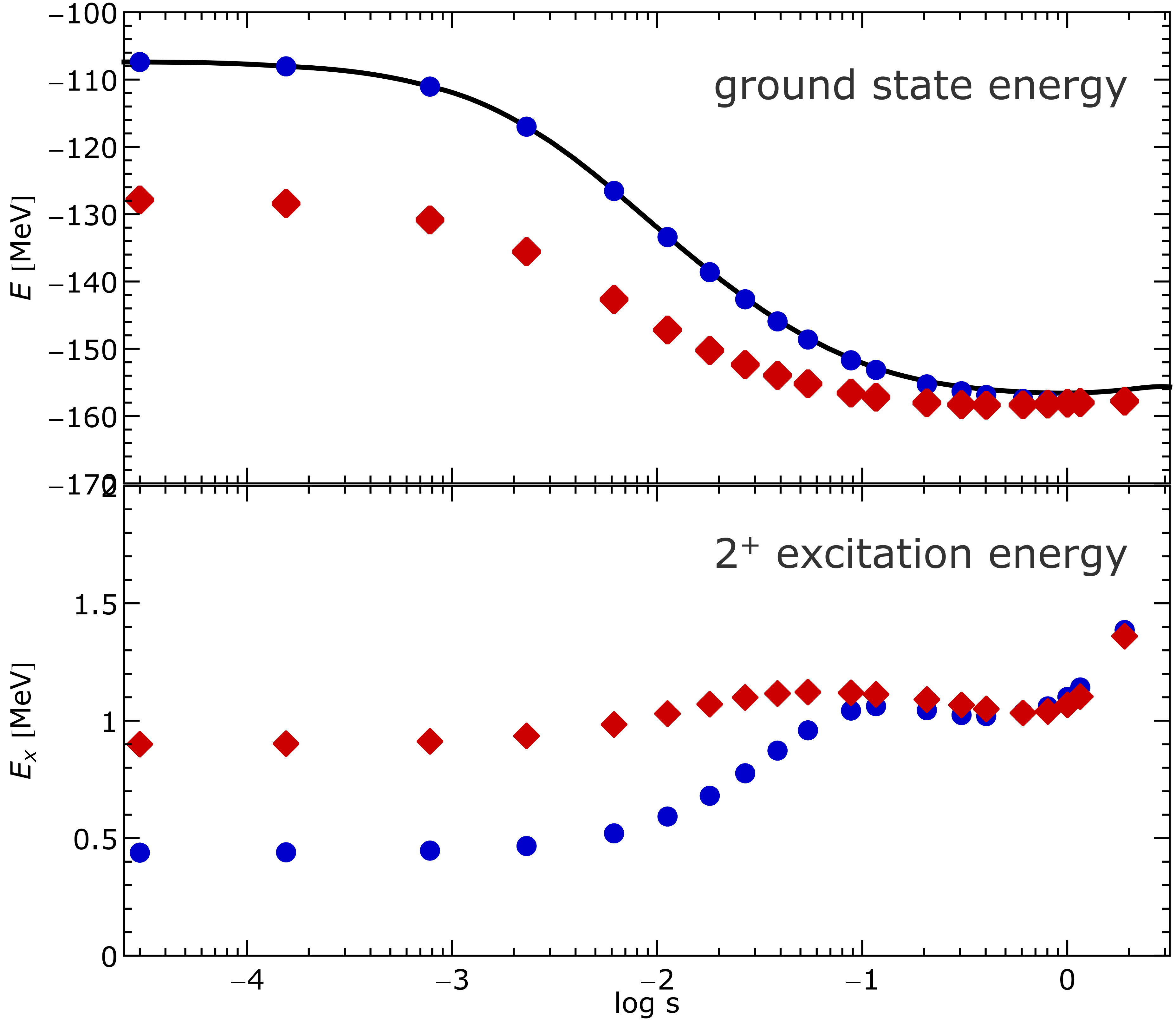
N_{max}=0
reference state

e_{max}=10

NCSM with flowing Hamiltonian

- N_{max}=0
- N_{max}=2

^{20}Ne: Flowing Energy



^{20}Ne

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
ħΩ=20 MeV

N_{max}=0
reference state

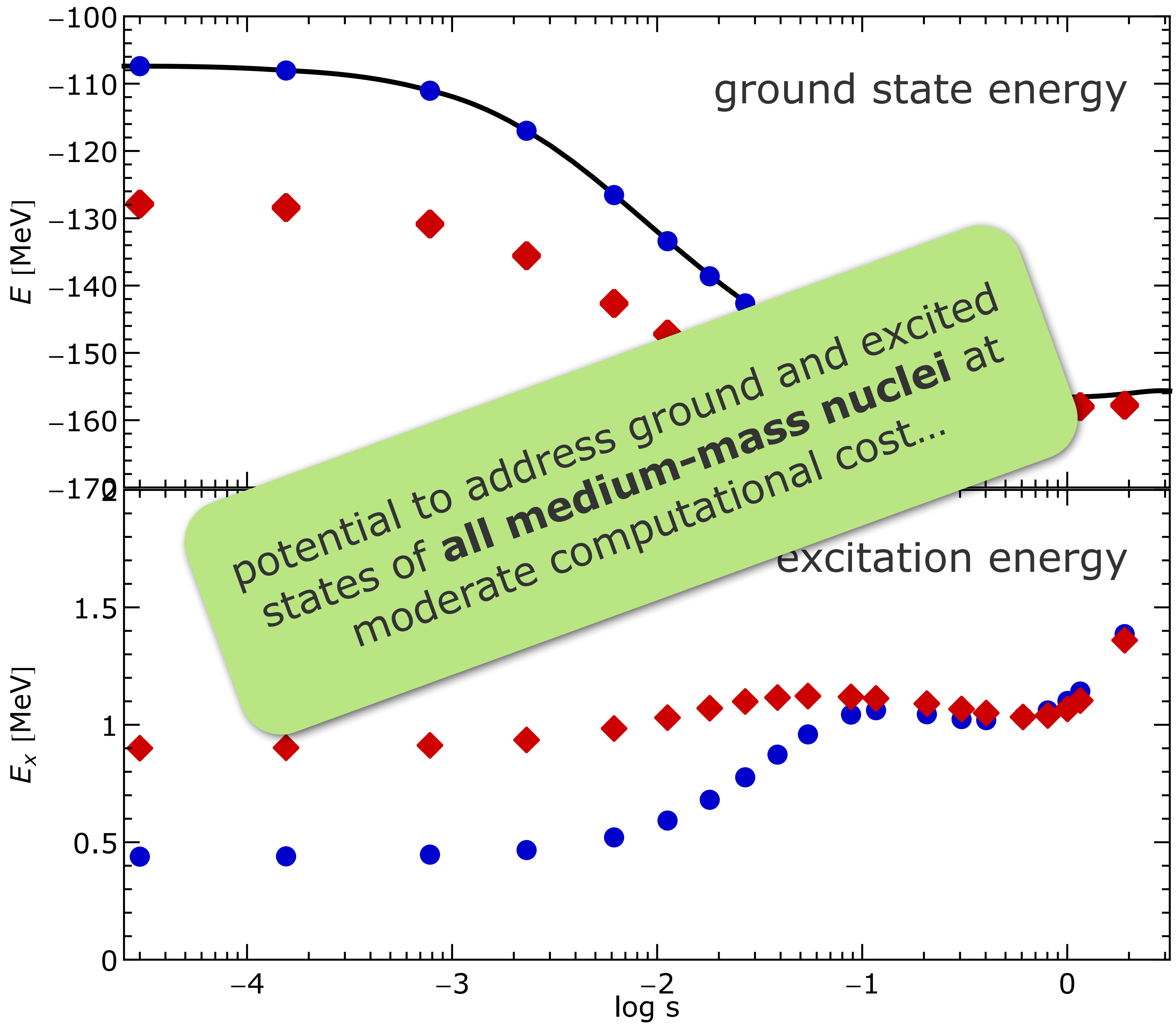
e_{max}=10

NCSM with flowing Hamiltonian

● N_{max}=0

◆ N_{max}=2

^{20}Ne: Flowing Energy



potential to address ground and excited states of **all medium-mass nuclei** at moderate computational cost...

^{20}Ne

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV

N_{max}=0
reference state

e_{max}=10

NCSM with flowing Hamiltonian

● N_{max}=0
◆ N_{max}=2

Conclusions

A Look Back…

- past few years have seen dramatic progress in ab initio many-body methods for nuclear structure (and reactions)

  ...extensions of NCSM, coupled-cluster theory, in-medium SRG, self-consistent Green's function, many-body perturbation theory,...

- a number of important developments are in progress

  ...spectroscopy of open-shell nuclei, merging NCSM and IM-SRG, derivation of valence-space interactions, broad range of observables...

- the reach of ab initio methods has grown tremendously

  ...medium-mass and heavy nuclei, continuum effects and reaction observables, hypernuclei...

A Look Ahead...

- for the next few years the focus will move towards improvements of the chiral interactions

  ...consistent higher orders, systematic study of order-by-order convergence, inclusion of consistent currents, improved fitting strategies, ...

- rigorous quantification of theoretical uncertainties will play an important role

  ...propagation of uncertainties from chiral EFT inputs to nuclear structure observables, full quantification of many-body uncertainties, …

- lots of relevant physics predictions...

Epilogue

- **thanks to my group and my collaborators**
  - S. Alexa, J. Braun, E. Gebrerufael, T. Hüther, S. Schulz, H. Spiess, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
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    Iowa State University
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JUROPA — JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC — 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

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