Ab Initio Theory of Medium-Mass Nuclei

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Ab Initio Nuclear Structure - Drivers

- **QCD at low energies**

  improved understanding of nuclear interactions through effective field theories and lattice simulations

- **quantum many-body methods**

  advances in ab initio treatment of nuclear many-body problem

- **computing & algorithms**

  increase of computational resources and development of algorithms

- **experimental reach**

  exciting perspectives for detailed experimental insights far-off stability

Ab Initio Nuclear Structure - Definition

solve nuclear many-body problem
based on realistic interactions
using controlled and improvable truncations
with quantified theoretical uncertainties

Ab Initio Nuclear Structure - Tools

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 input for all ab initio calculations
- only "selected" chiral interactions used in nuclear structure so far
- next-generation chiral EFT interactions give opportunity to quantify uncertainties

Ab Initio Nuclear Structure - Tools

Nuclear Structure & Reaction Observables

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

Pre-Processing:
Similarity Renorm. Group

Chiral EFT:
Interactions & Operators

Low-Energy QCD

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

Ab Initio Nuclear Structure - Tools

Nuclear Structure & Reaction Observables

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

Pre-Processing: Similarity Renorm. Group

Chiral EFT: Interactions & Operators

Low-Energy QCD

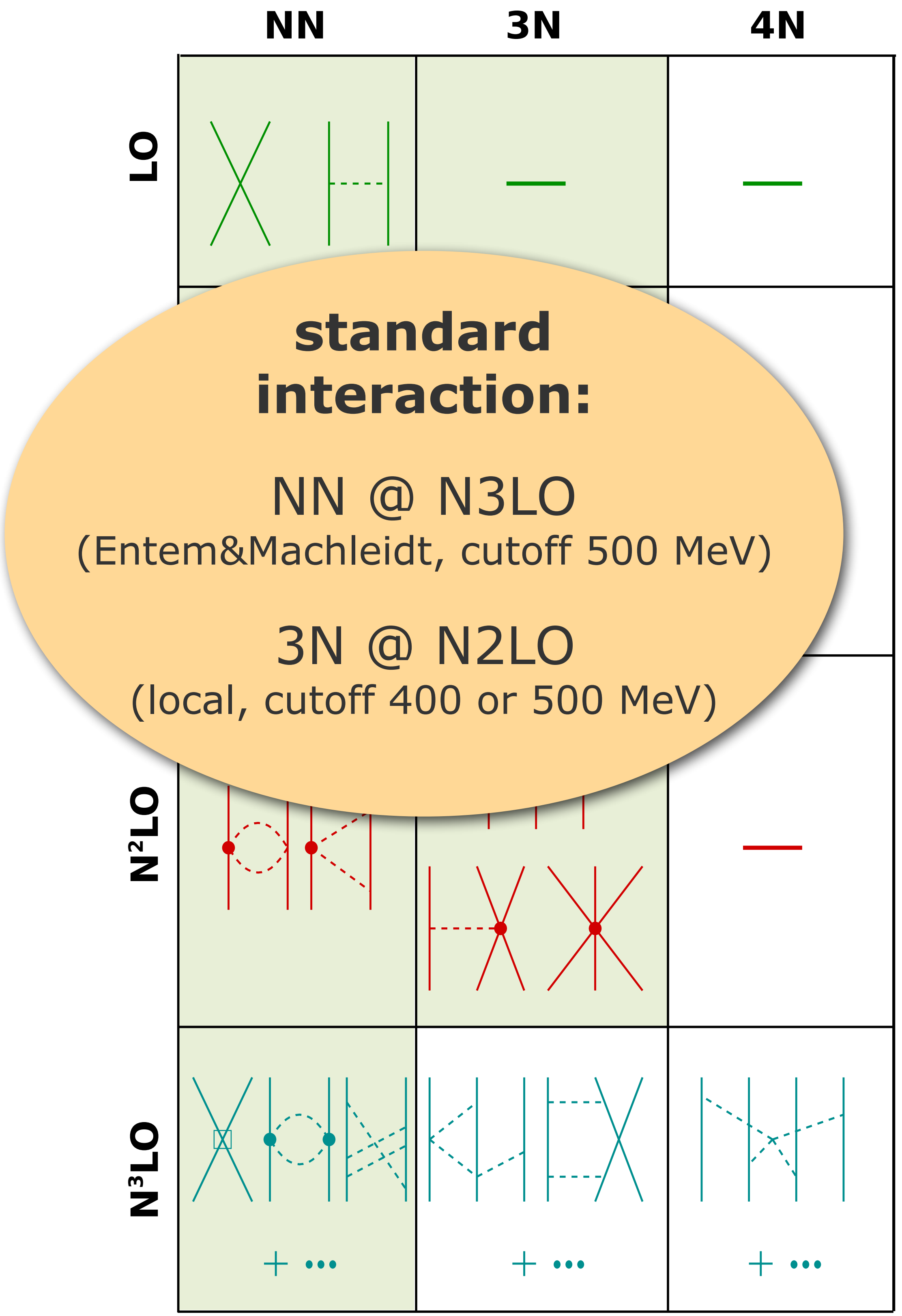
- different many-body methods for different mass regions and different observables
- present frontiers: continuum & open-shell medium-mass nuclei

Hamiltonian

Chiral EFT for Nuclear Interactions

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

- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- hierarchy of **consistent NN, 3N, 4N,...** interactions and exchange currents
- many **ongoing developments**
  - improved NN up to N4LO
  - 3N interaction up to N3LO
  - 4N interaction at N3LO
  - improved fits and error analysis
  - order-by-order uncertainty quantification



Similarity Renormalization Group

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

continuous unitary transformation driving Hamiltonian towards diagonal form

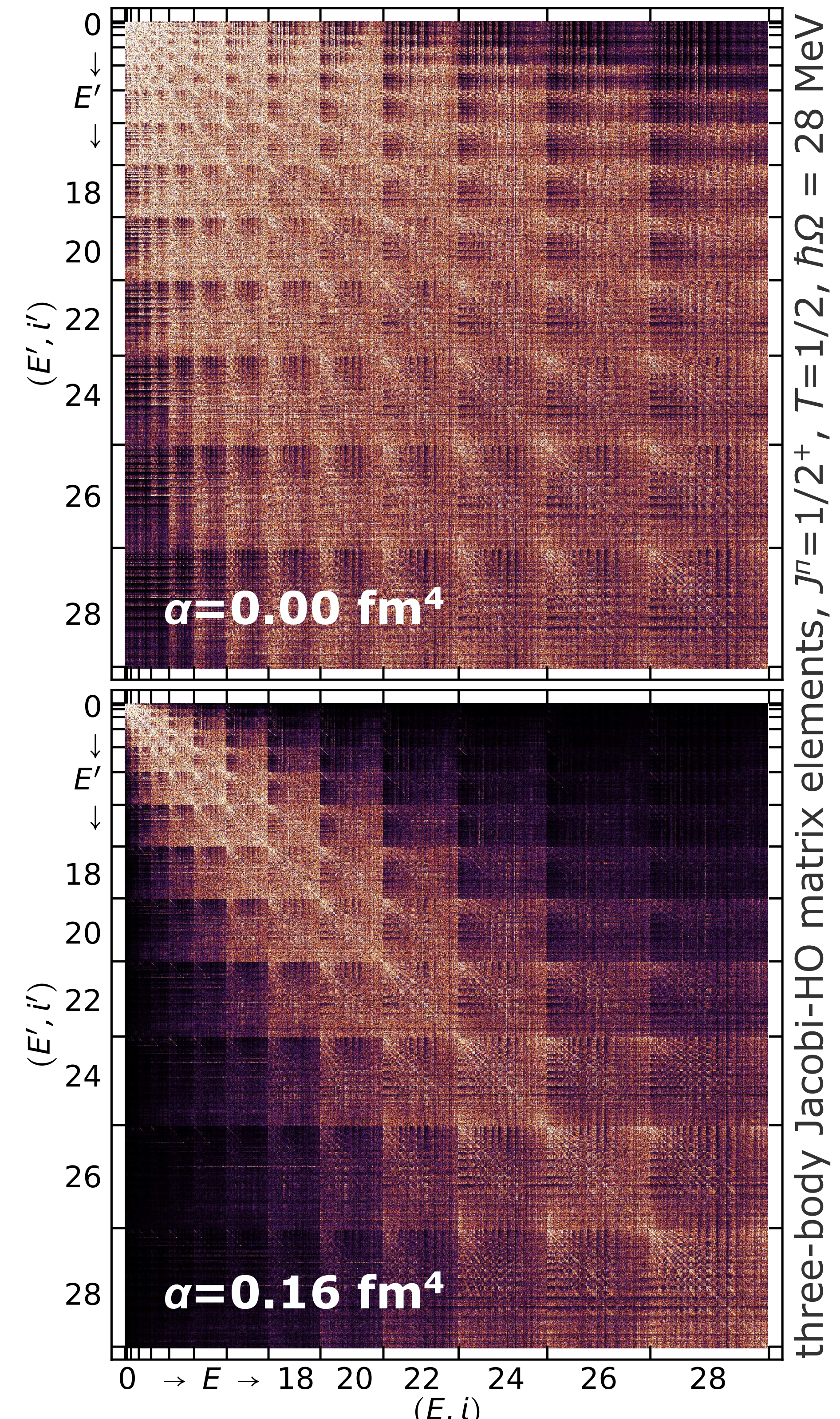
- unitary transformation via flow equation

$$\mathrm{H}_\alpha = \mathrm{U}_\alpha^\dagger \mathrm{H}_0\, \mathrm{U}_\alpha \quad \rightarrow \quad \frac{d}{d\alpha}\mathrm{H}_\alpha = [\eta_\alpha, \mathrm{H}_\alpha]$$

- dynamic generator determines physics of transformation

$$\eta_\alpha = (2\mu)^2\, [\mathrm{T}_{\mathrm{int}}, \mathrm{H}_\alpha]$$

- 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

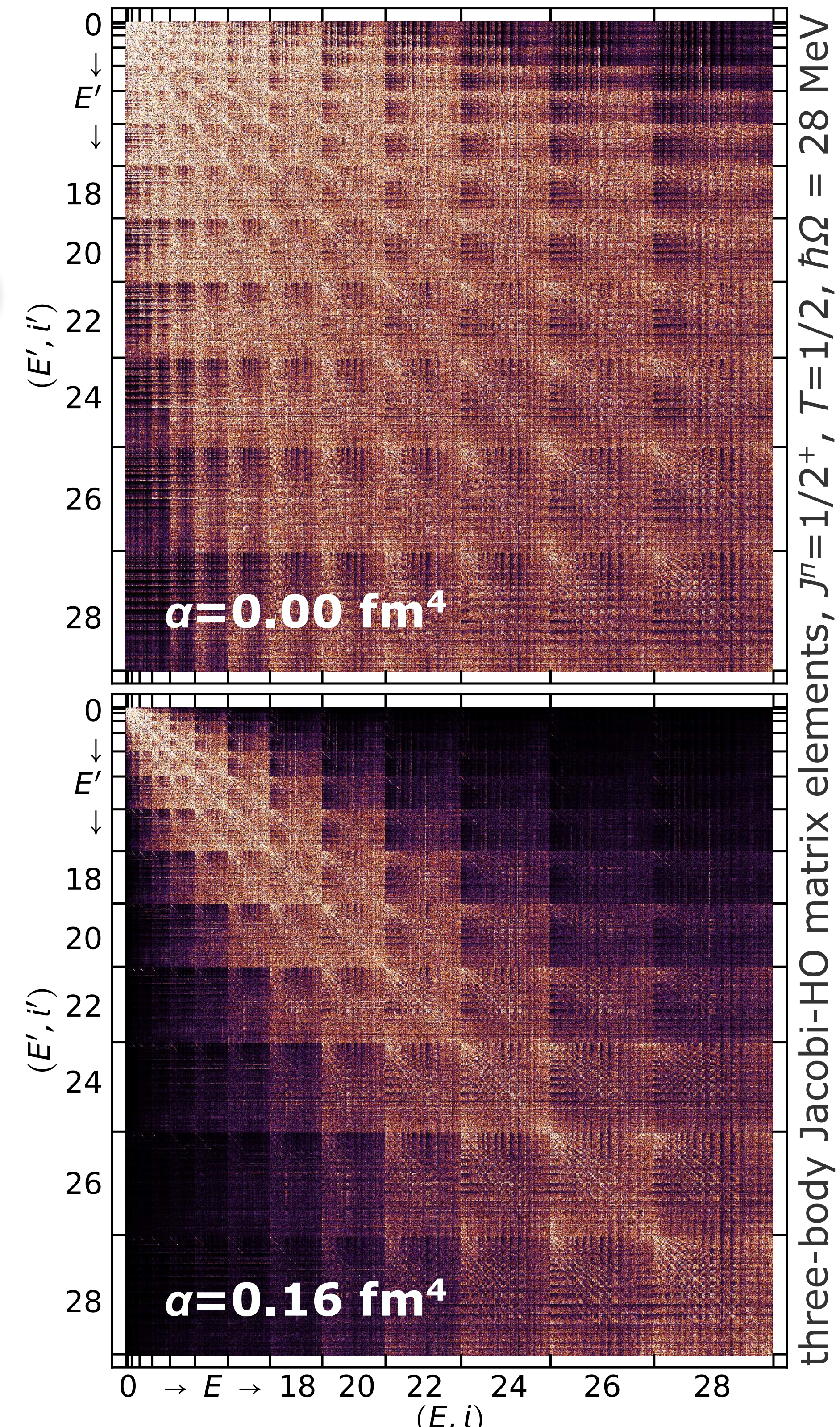
con:
induces many-body interactions

- 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:
  - **$NN+3N_{ind}$**
    use initial NN, keep evolved NN+3N
  - **$NN+3N_{full}$**
    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, ...

Oxygen Isotopes

- **oxygen isotopic chain** has received significant attention and documents the **rapid progress** over the past years

Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL 105, 032501 (2010)

- 2010: **shell-model calculations** with 3N effects highlighting the role of 3N interaction for drip line physics

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, PRL 108, 242501 (2012)

- 2012: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

Hergert, Binder, Calci, Langhammer, Roth, PRL 110, 242501 (2013)

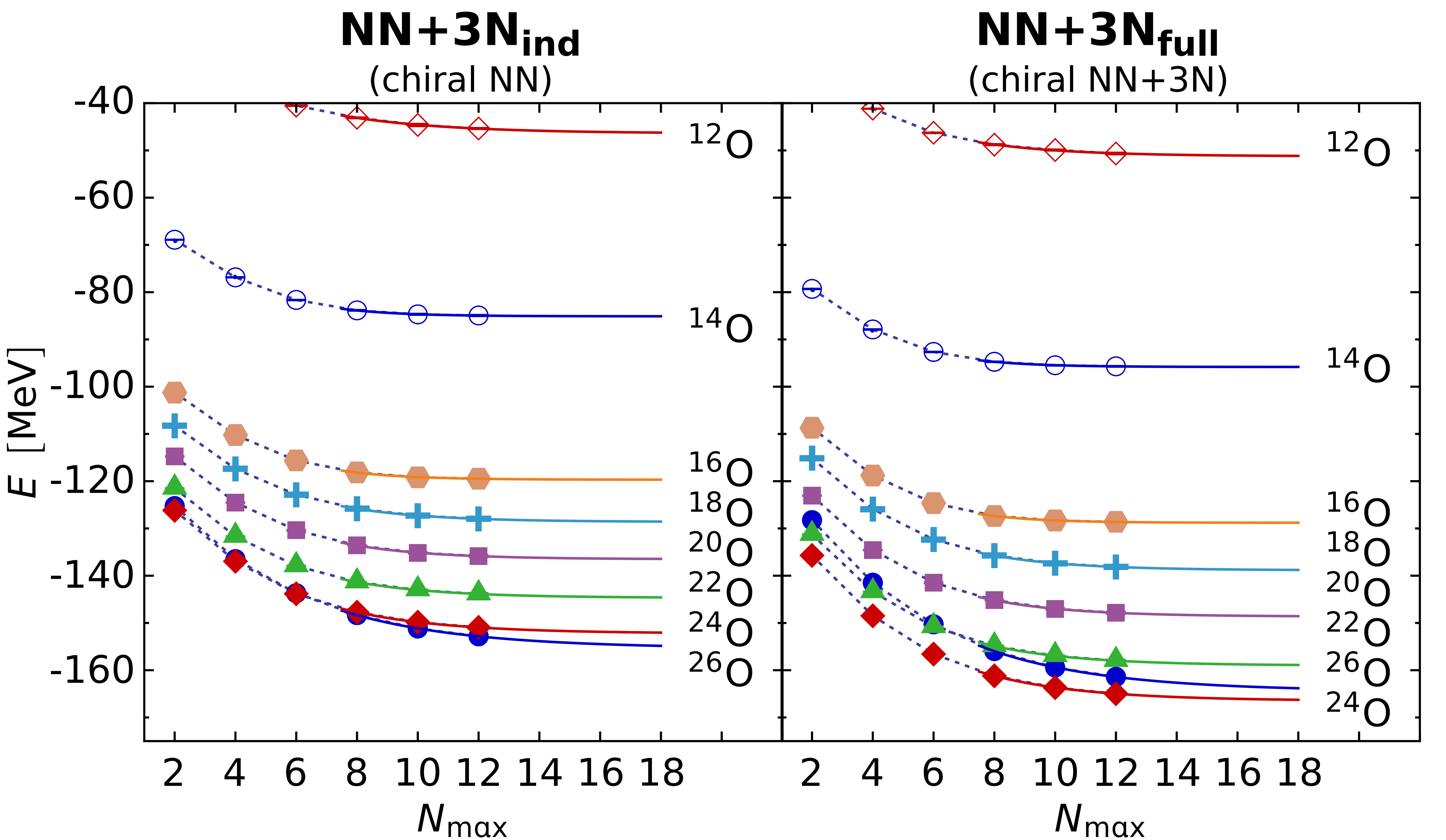
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

Cipollone, Barbieri, Navrátil, PRL 111, 062501 (2013)
Bogner, Hergert, Holt, Schwenk, Binder, Calci, Langhammer, Roth, PRL 113, 142501 (2014)
Jansen, Engel, Hagen, Navratil, Signoracci, PRL 113, 142502 (2014)

- since: self-consistent Green's function, shell model with valence-space interactions from in-medium SRG or Lee-Suzuki,...

Ground States of Oxygen Isotopes

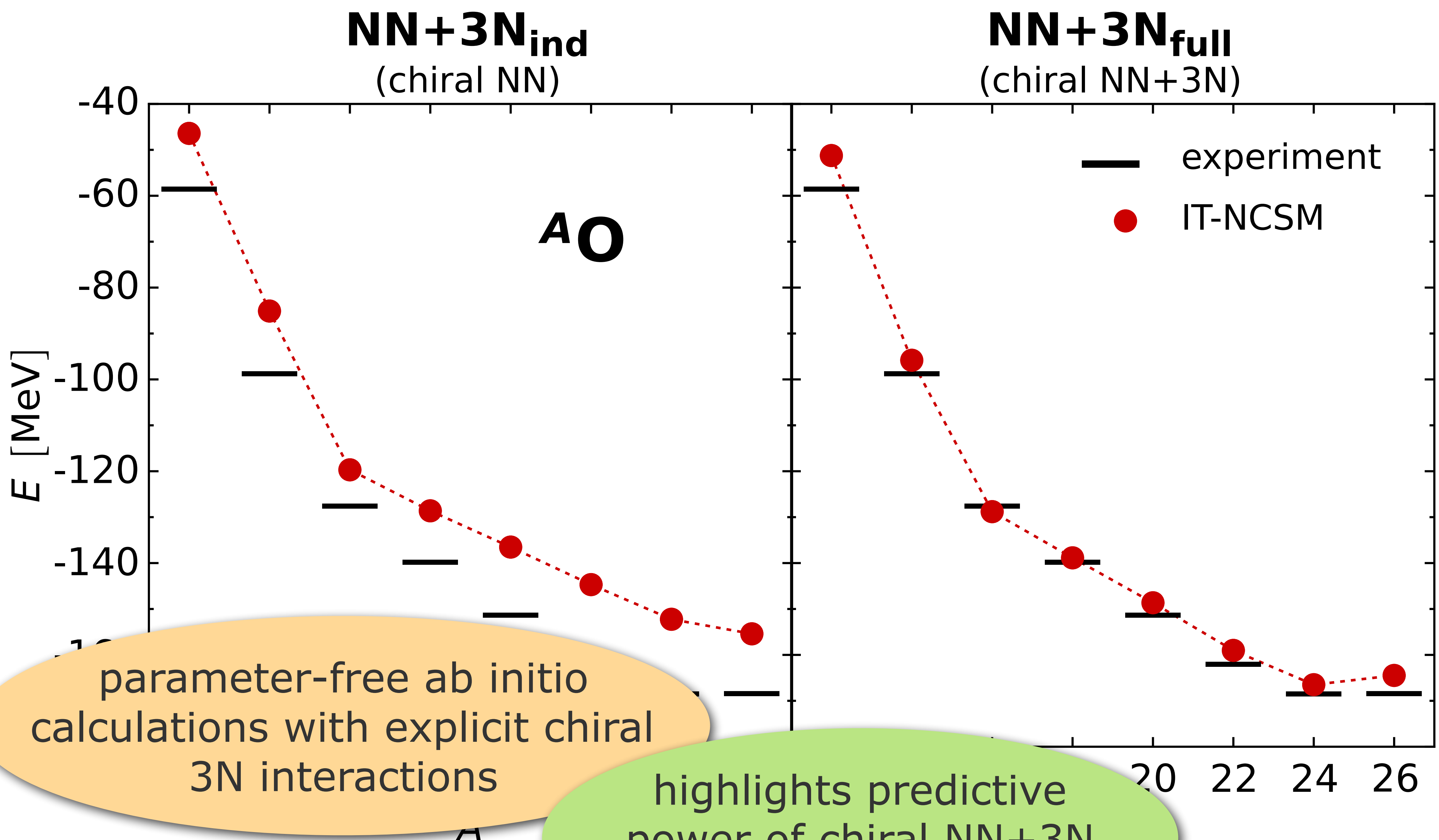
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



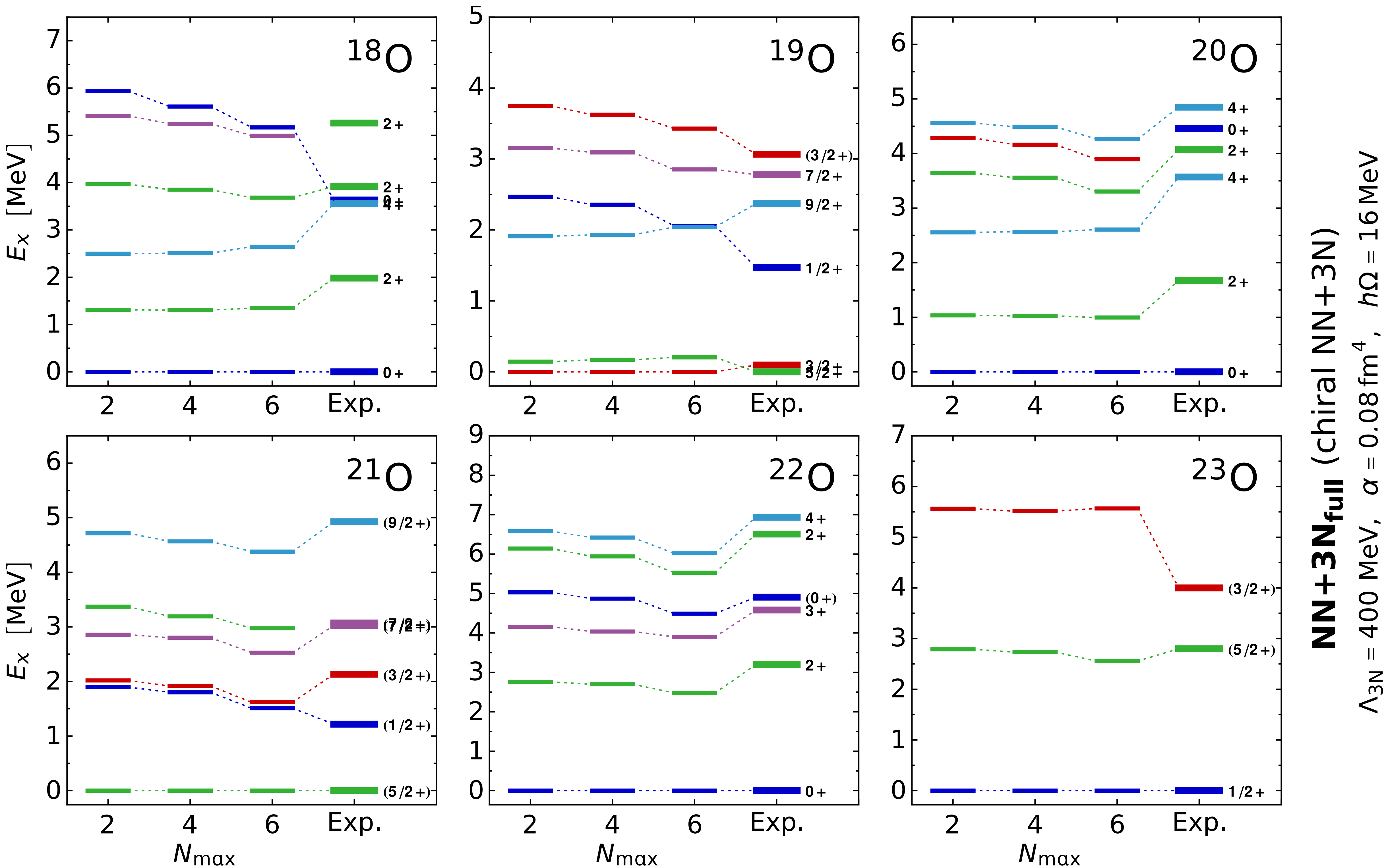
parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

Λ_{3N} = 400 MeV, α = 0... 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 expon... ial wave operator applied to single-determinant reference sta...
  - 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

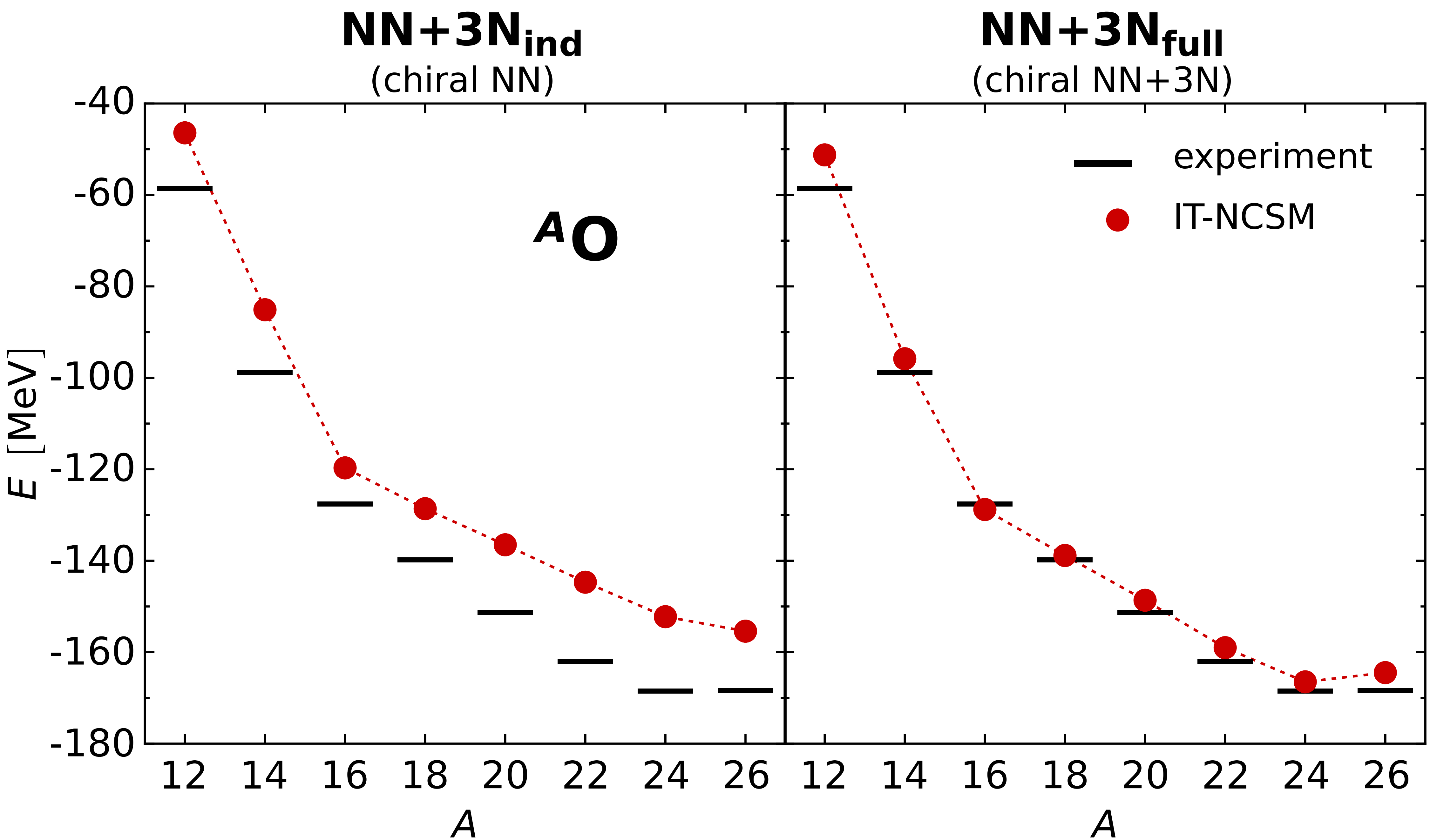
Barbieri, Soma, Duguet,...

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

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

Ground States of Oxygen Isotopes

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



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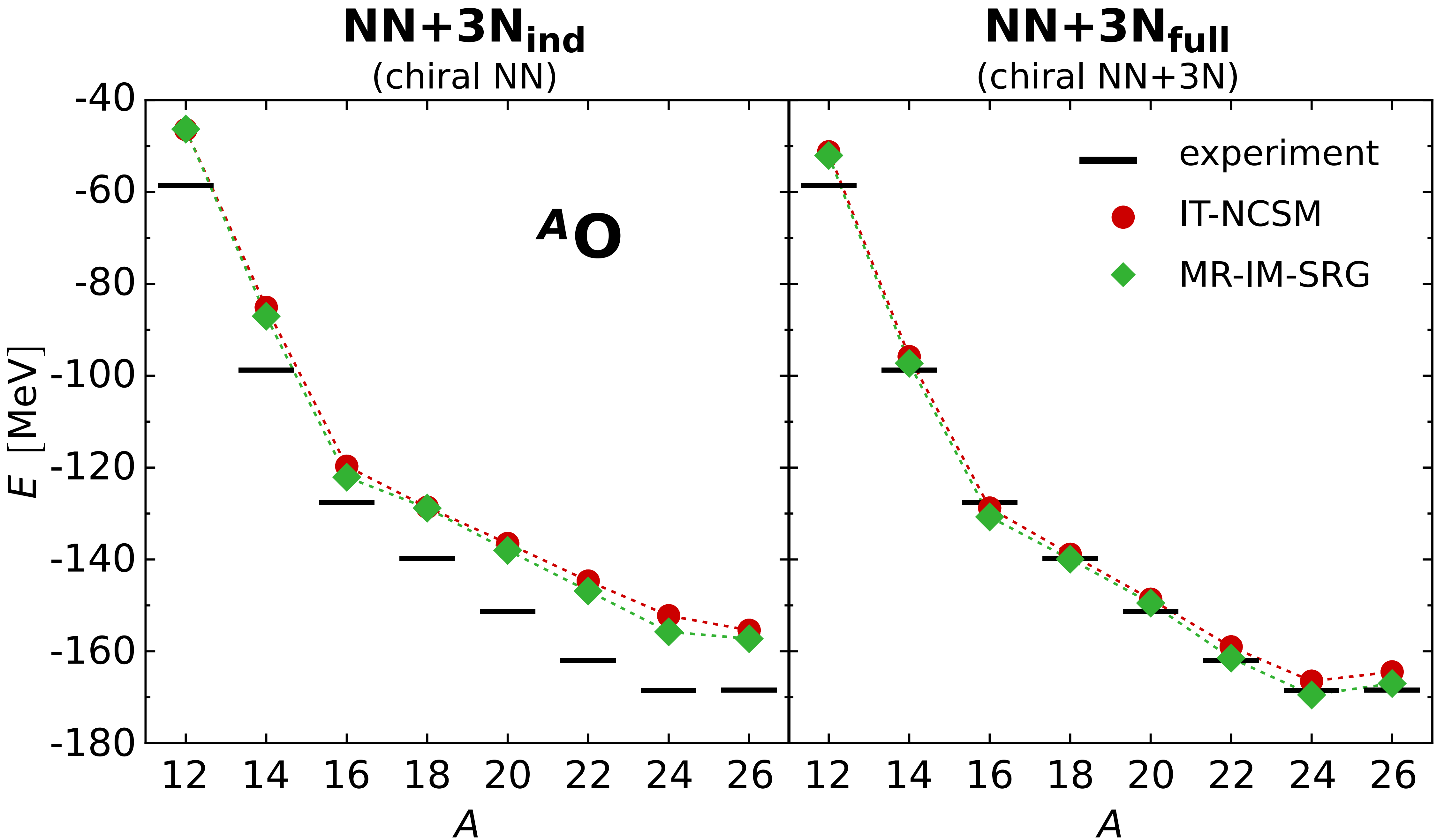
Ground States of Oxygen Isotopes

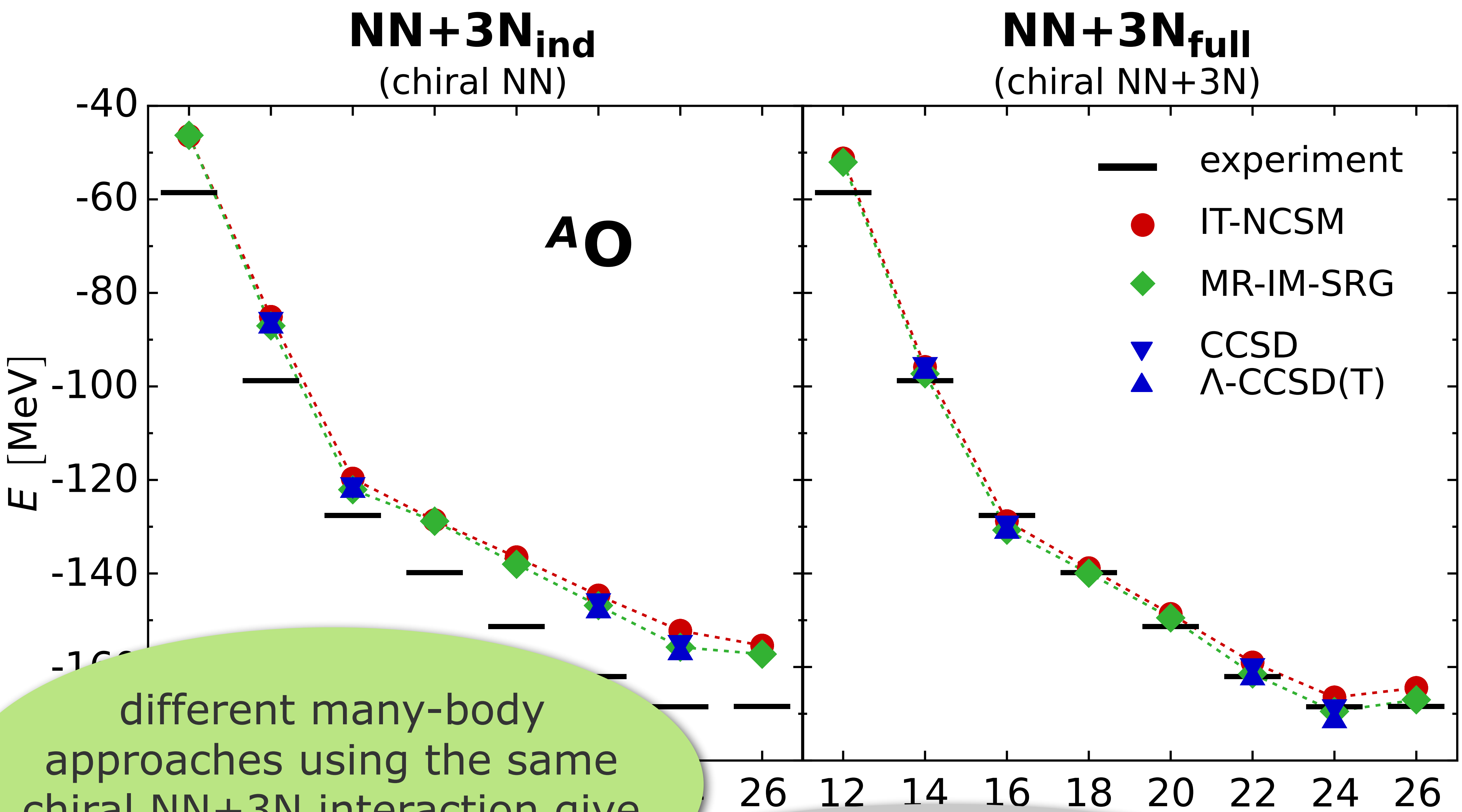
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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

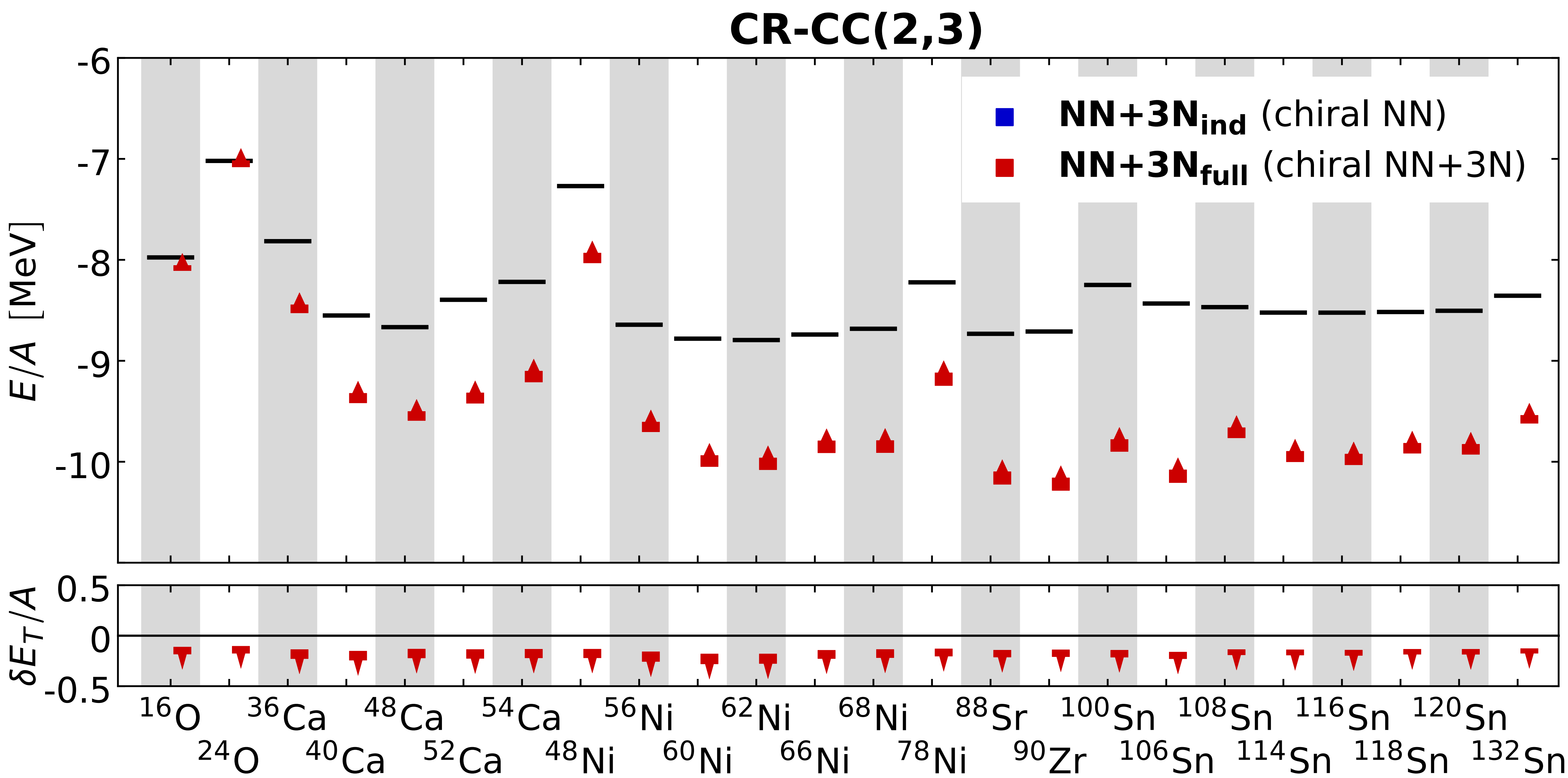


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Towards Heavy Nuclei - Ab Initio

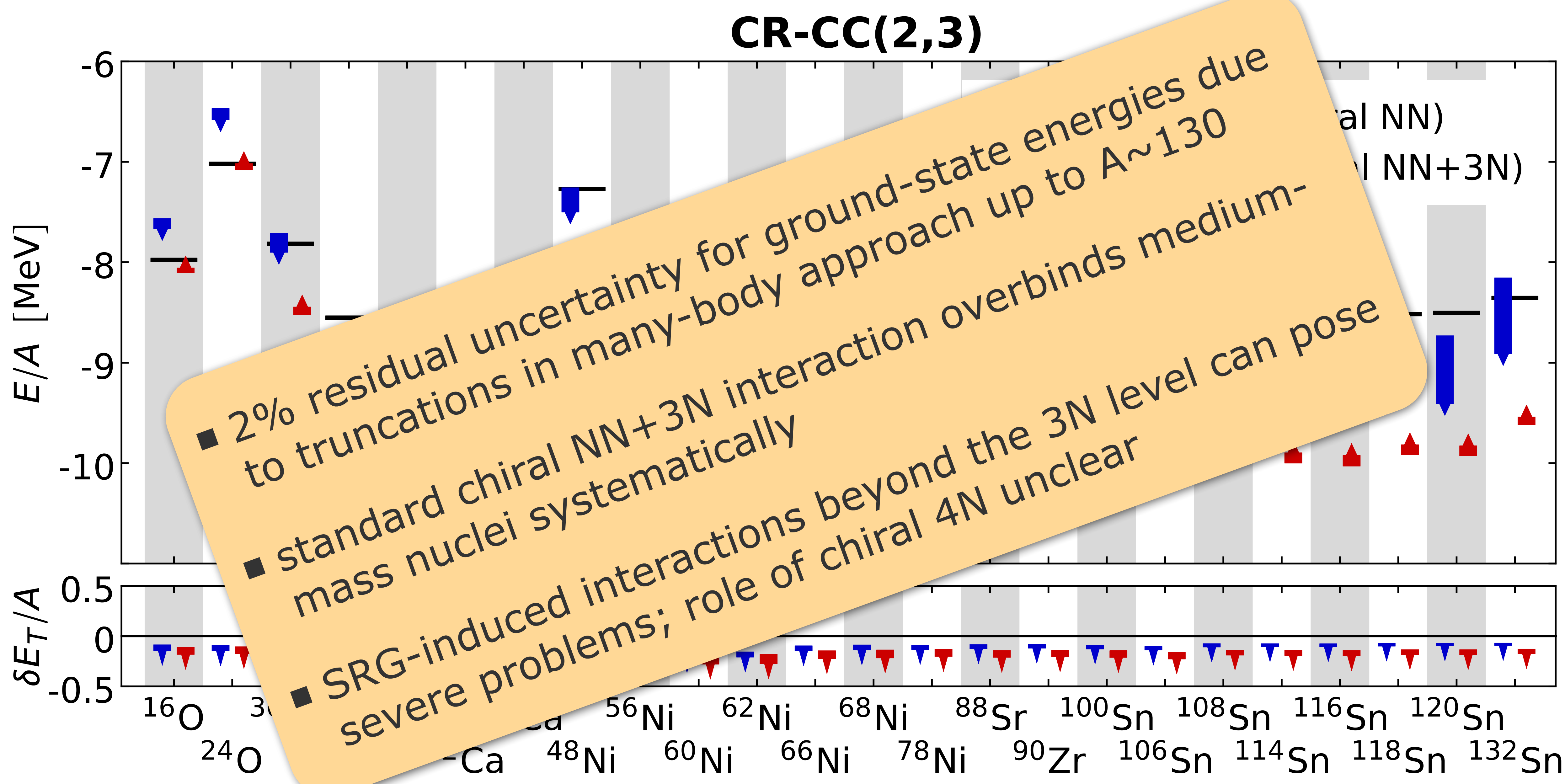
Binder et al., PLB 736, 119 (2014)



$\Lambda_{3N} = 400$ 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)

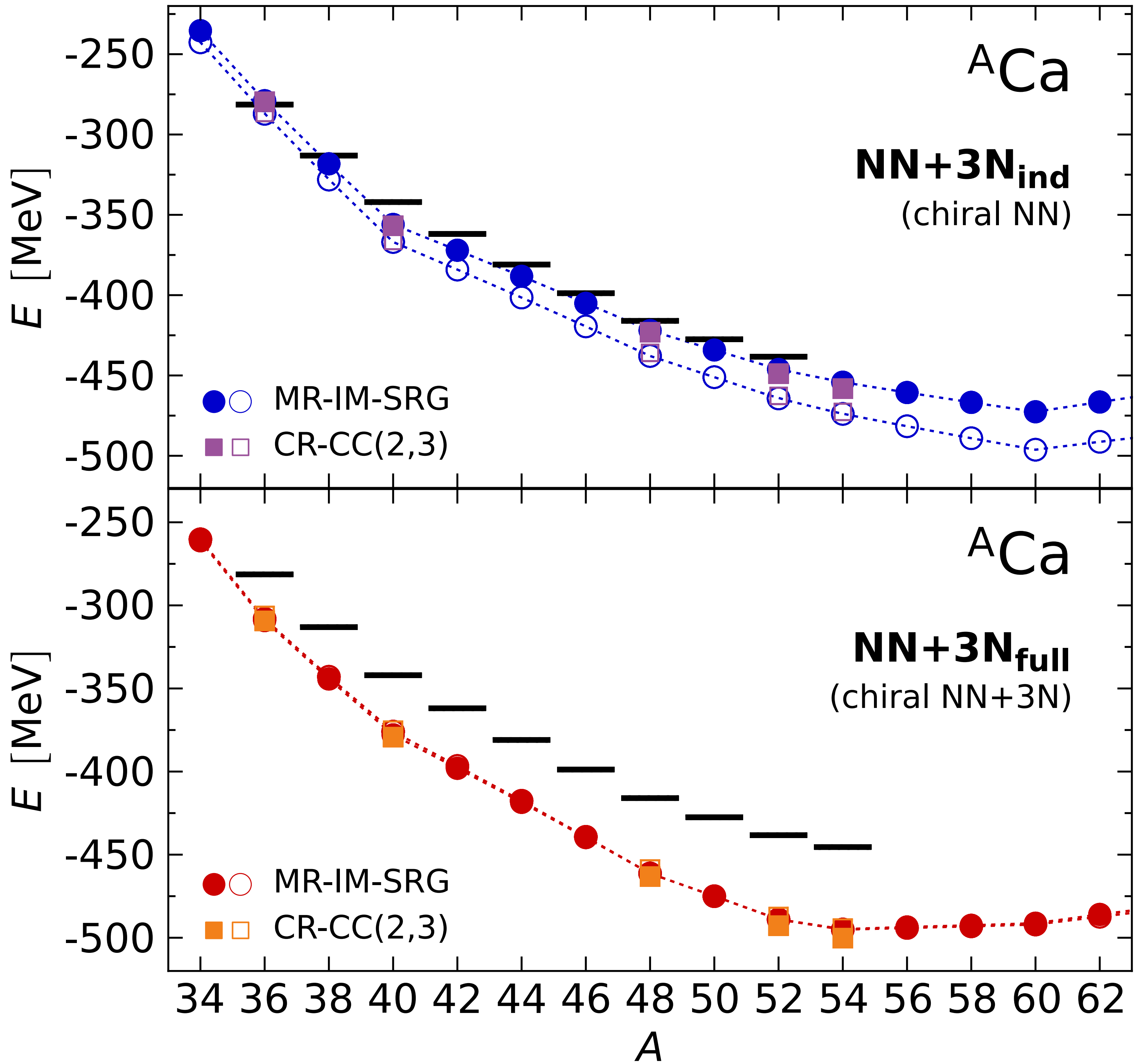


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

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

Open-Shell Medium-Mass Nuclei

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

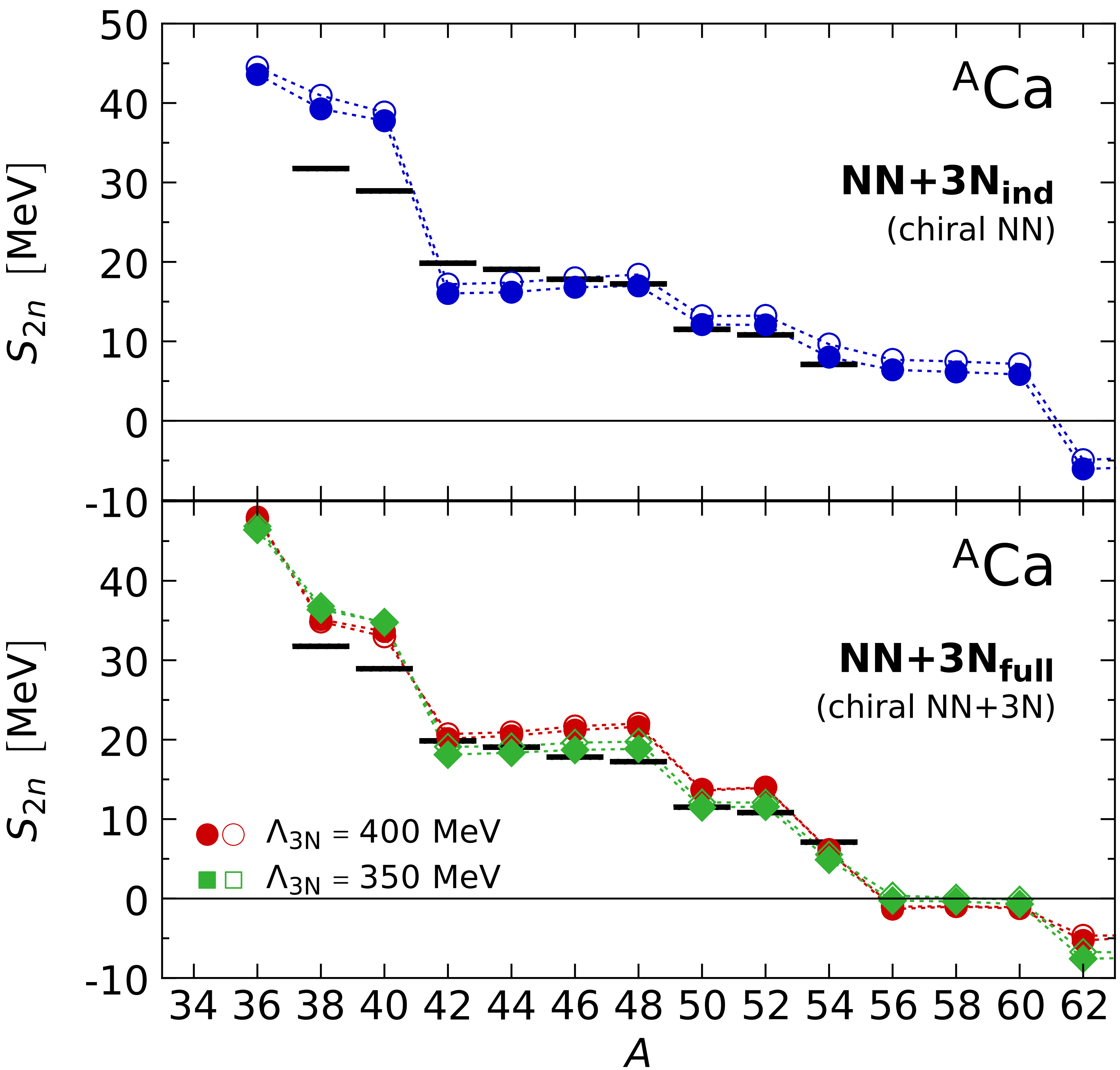


- systematic multi-reference IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

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_{3max} = 14, 16

Next Step:

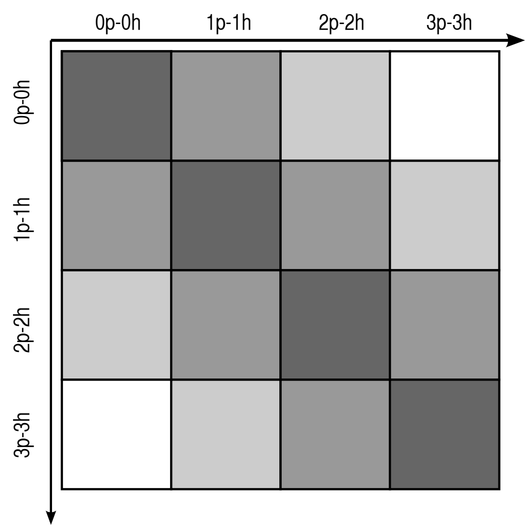
Merging NCSM and IM-SRG

with

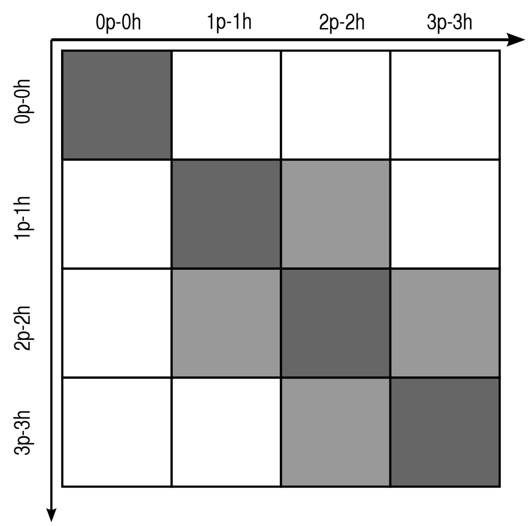
Eskendr Gebrerufael, Heiko Hergert, Klaus Vobig

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,...



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



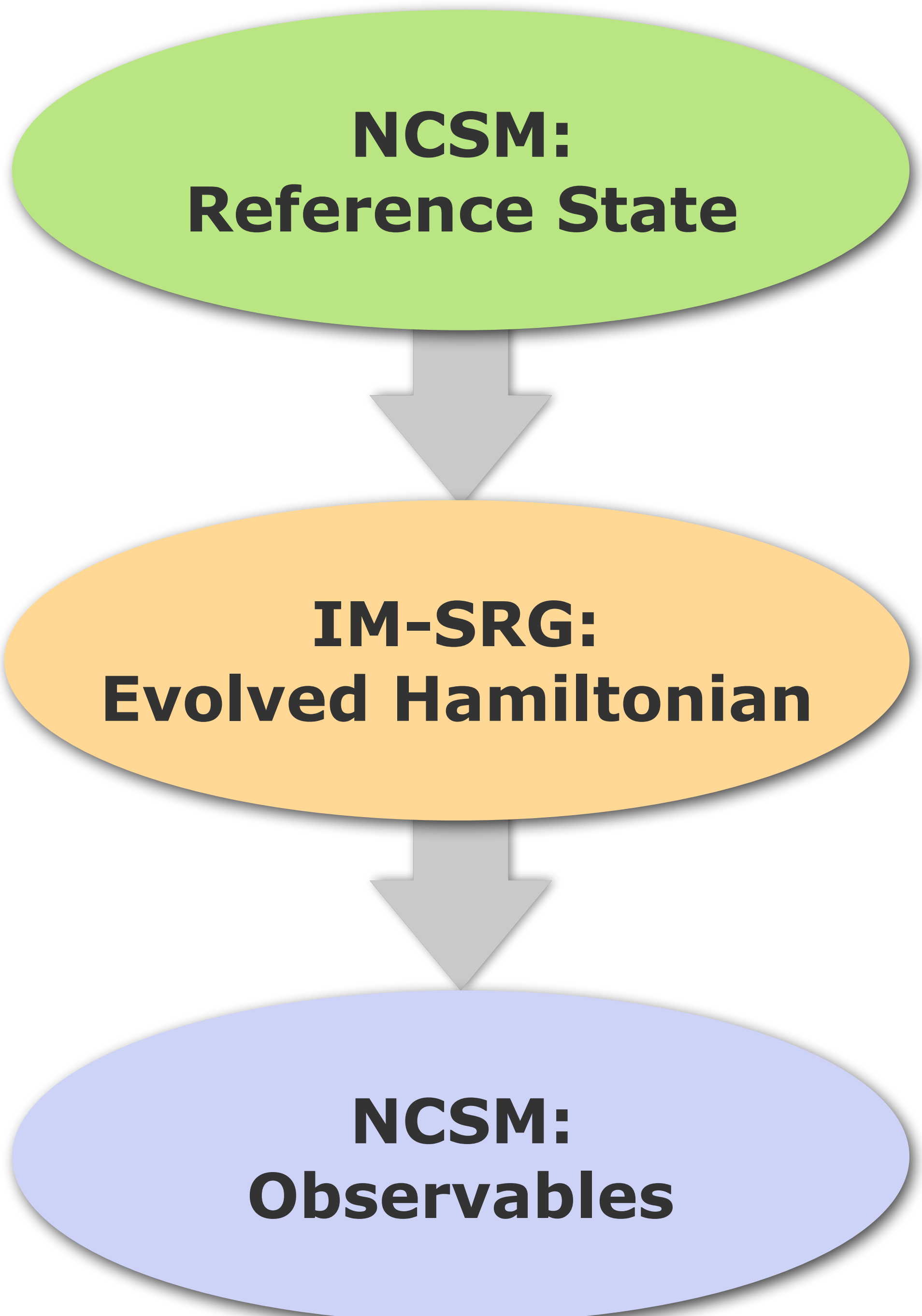
- flow equation for Hamiltonian

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

- 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

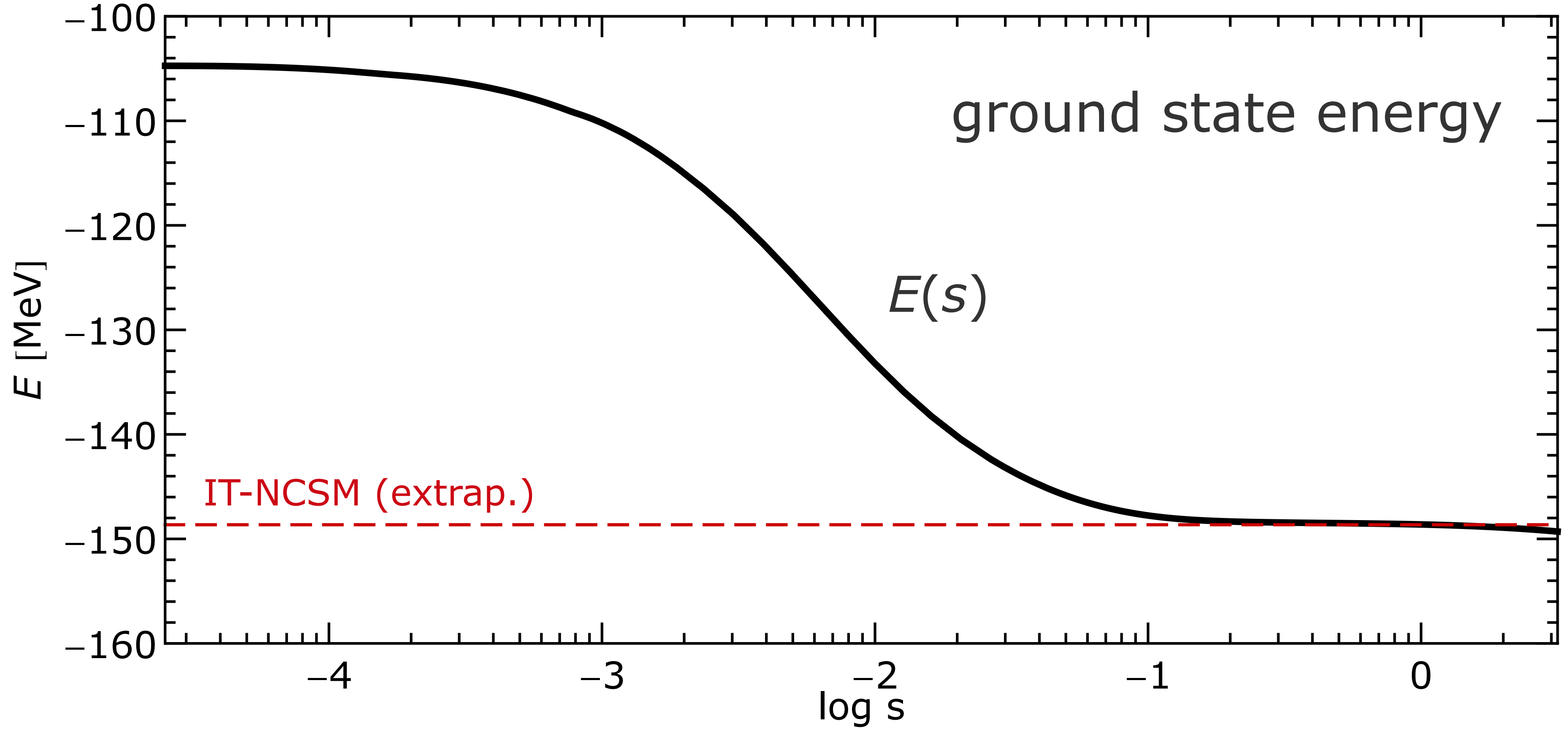


- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- not limited to subsets of open-shell nuclei and systematically improvable

- 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

- 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

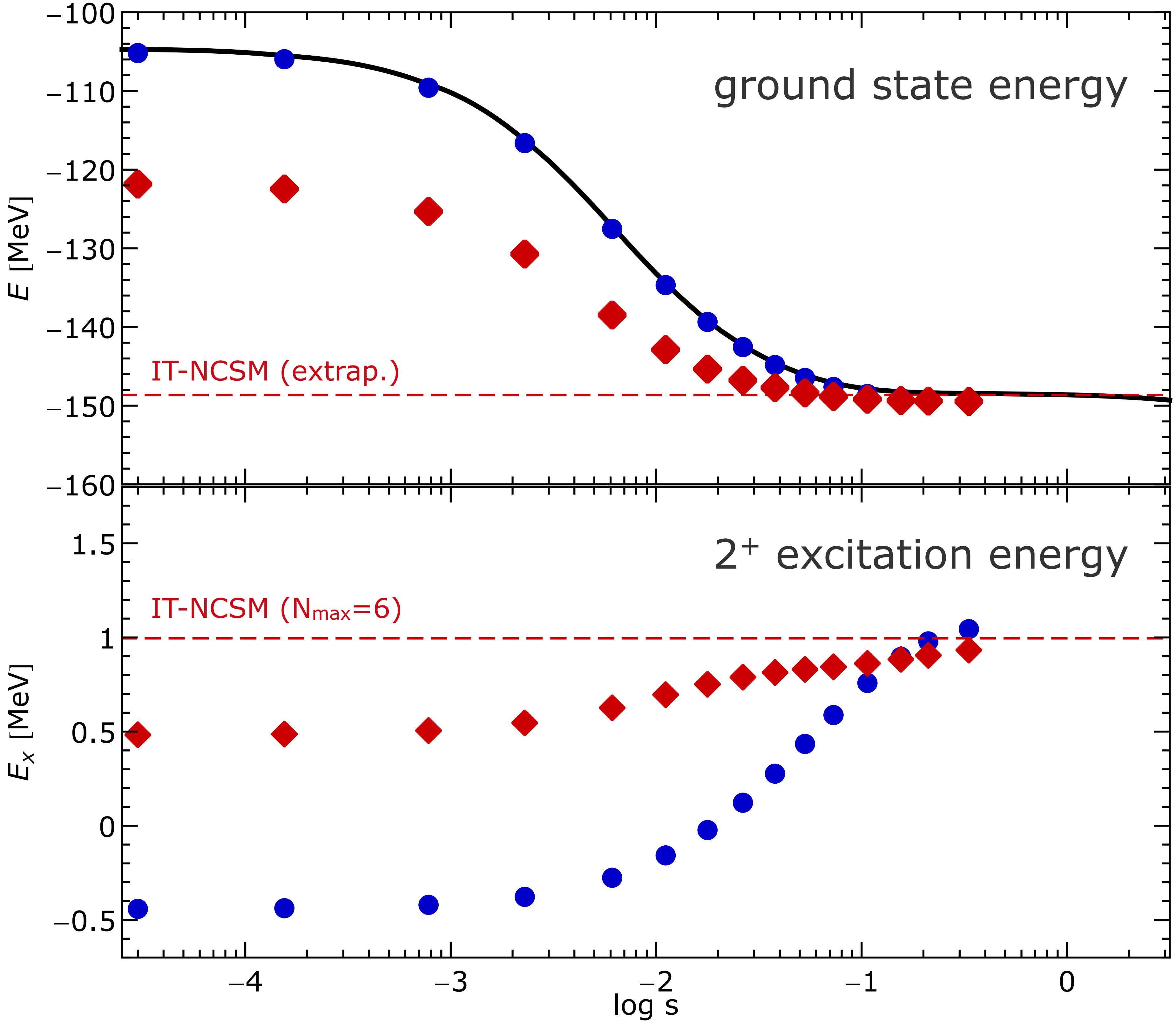
α=0.08 fm^4

ħΩ=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

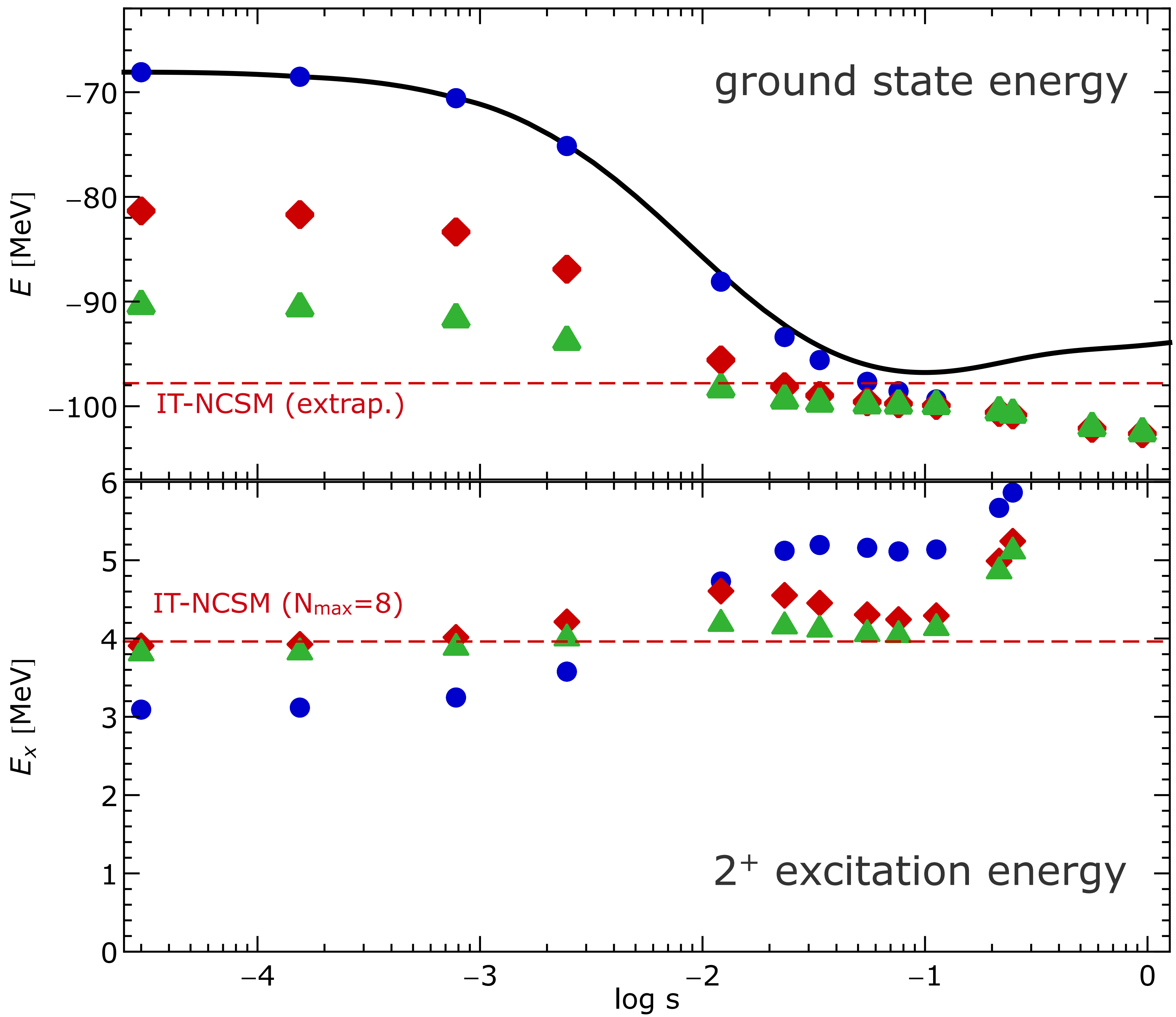
e_{max}=10

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

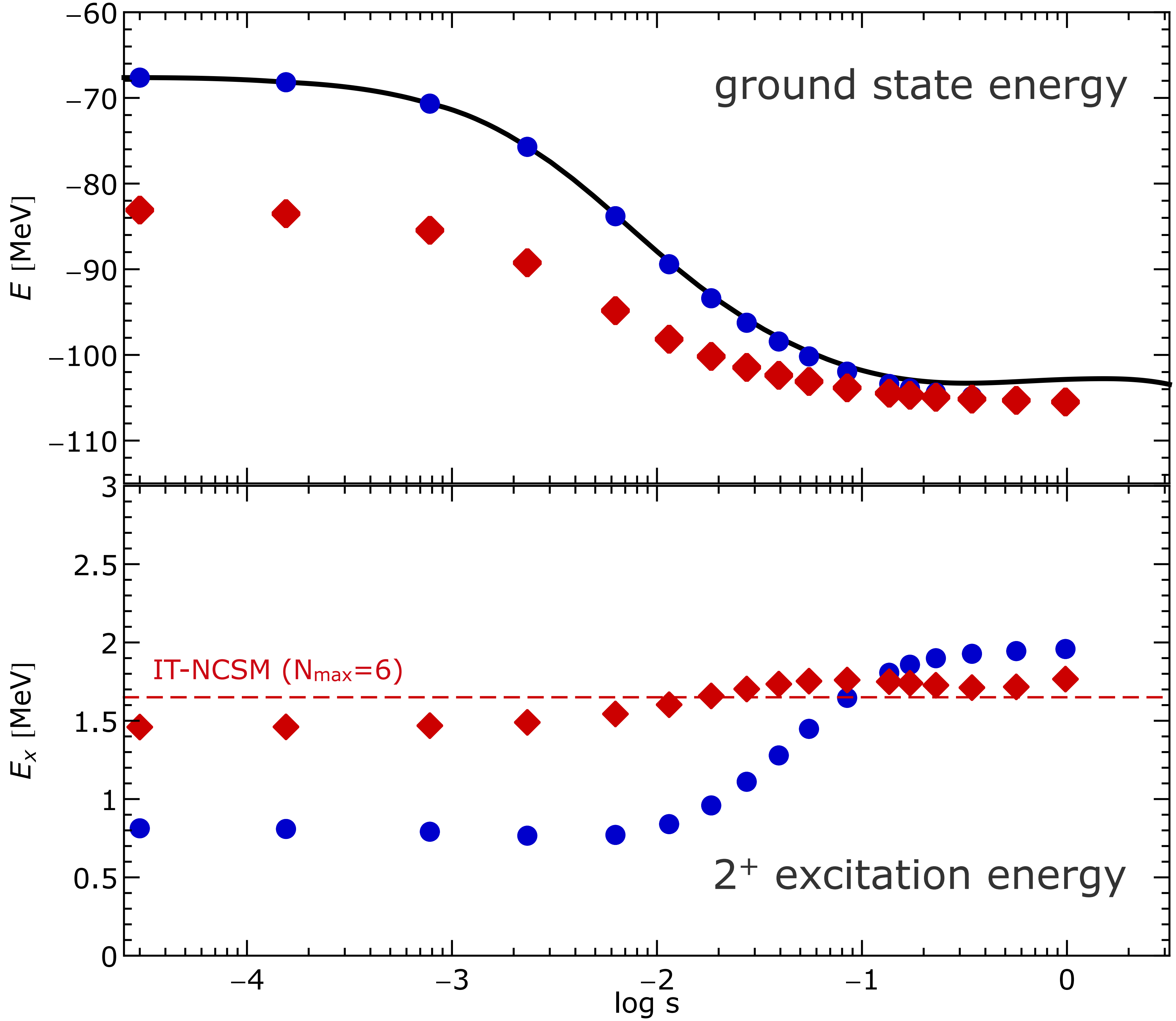
N_{max}=0
reference state

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

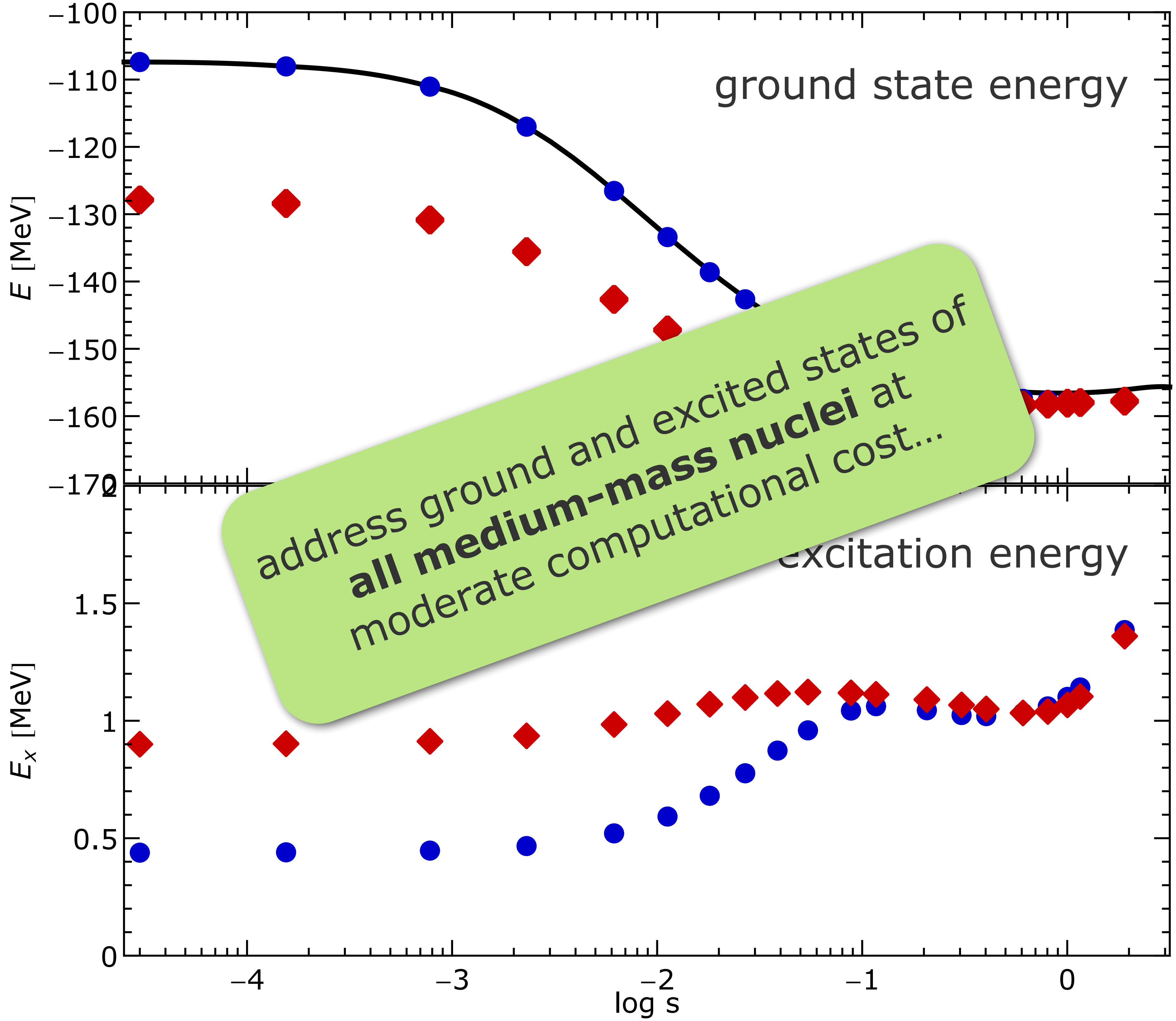
e_{max}=10

NCSM with flowing Hamiltonian

● N_{max}=0

◆ N_{max}=2

^{20}Ne: Flowing Energy



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

COMPUTING TIME

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Deutsche Forschungsgemeinschaft
DFG

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