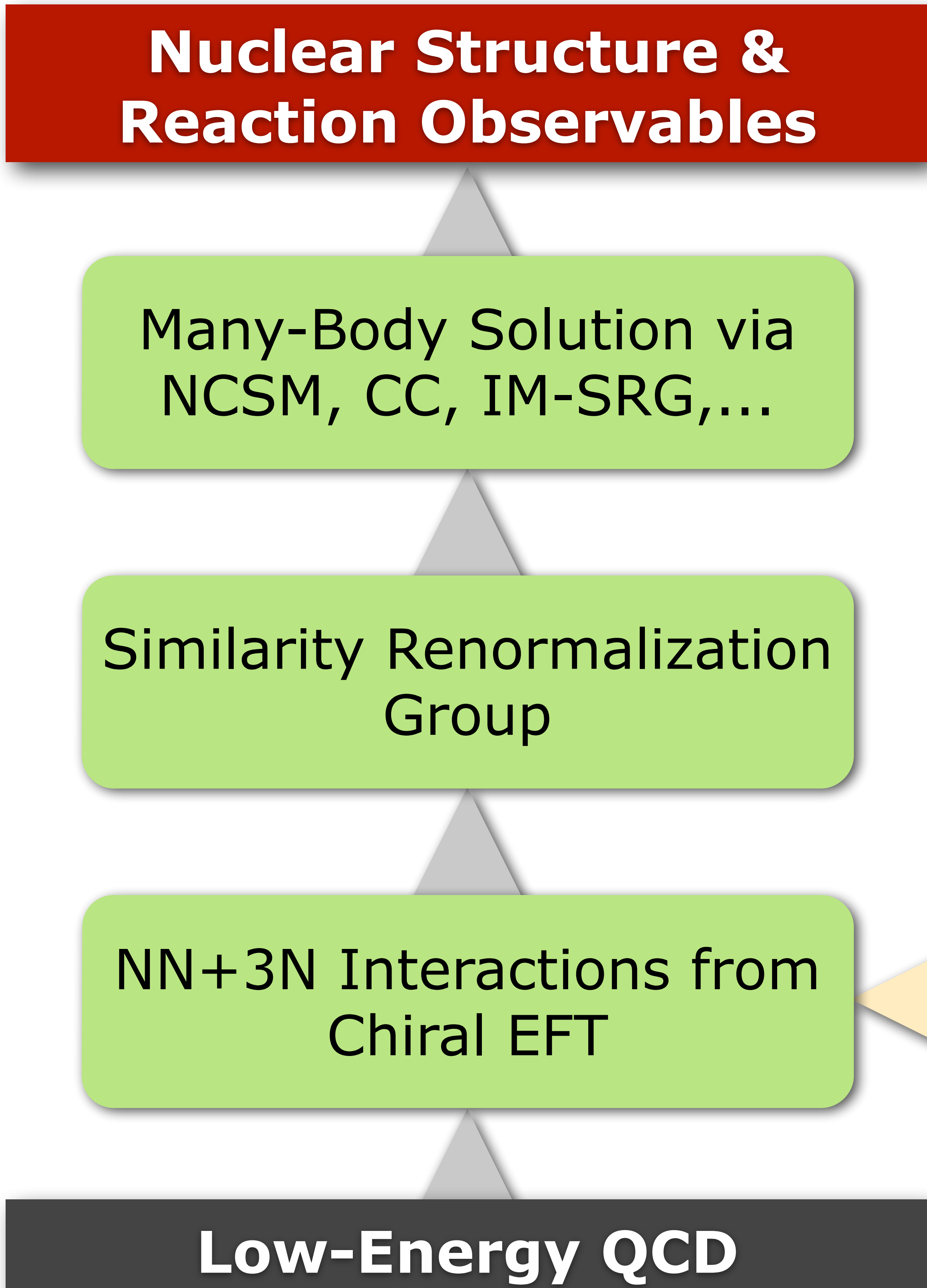
News from Ab Initio Theory

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Workflow



- chiral EFT offers systematics, improvability and uncertainty estimation
- typically one "chiral interaction" is used in nuclear structure
- improved chiral EFT interactions offer opportunity to quantify uncertainties systematically

Ab Initio Workflow

Nuclear Structure & Reaction Observables

↑

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

↑

Similarity Renormalization Group

↑

NN+3N Interactions from Chiral EFT

↑

Low-Energy QCD

- drastically improves convergence but induces many-body forces
- induced beyond-3N interactions are a major limitation for many applications
- improvement: either include or suppress induced forces

Ab Initio Workflow

Nuclear Structure & Reaction Observables

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

Similarity Renormalization Group

NN+3N Interactions from Chiral EFT

Low-Energy QCD

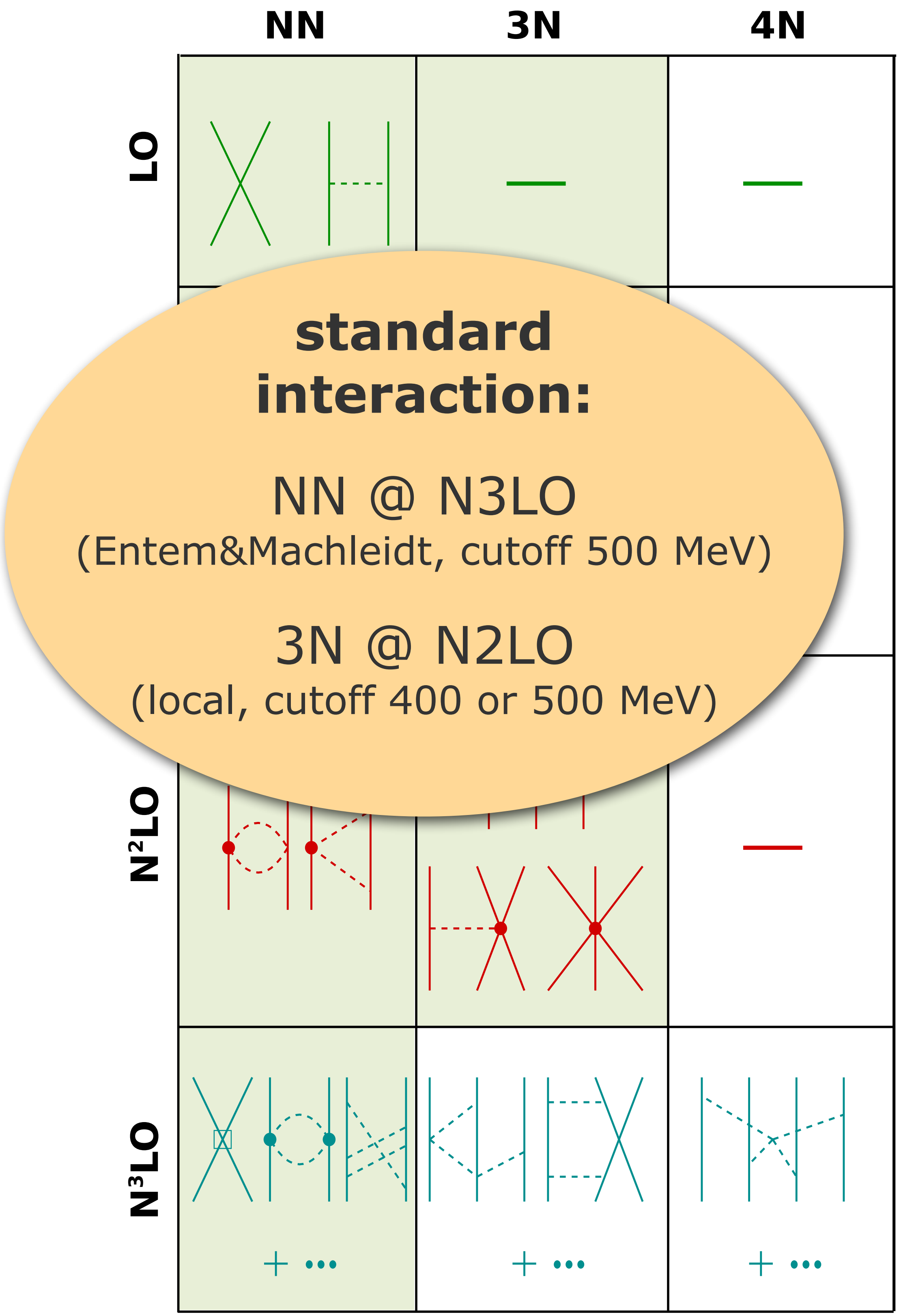
- different many-body methods for different observables and mass regimes
- hot topics: continuum & open-shell medium-mass nuclei

Interactions

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 current operators
- many **ongoing developments**
  - improved NN up to N4LO
  - 3N interaction up to N3LO
  - 4N interaction at N3LO
  - improved fits and error analysis



Similarity Renormalization Group

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

continuous unitary transformation driving Hamiltonian towards diagonal form

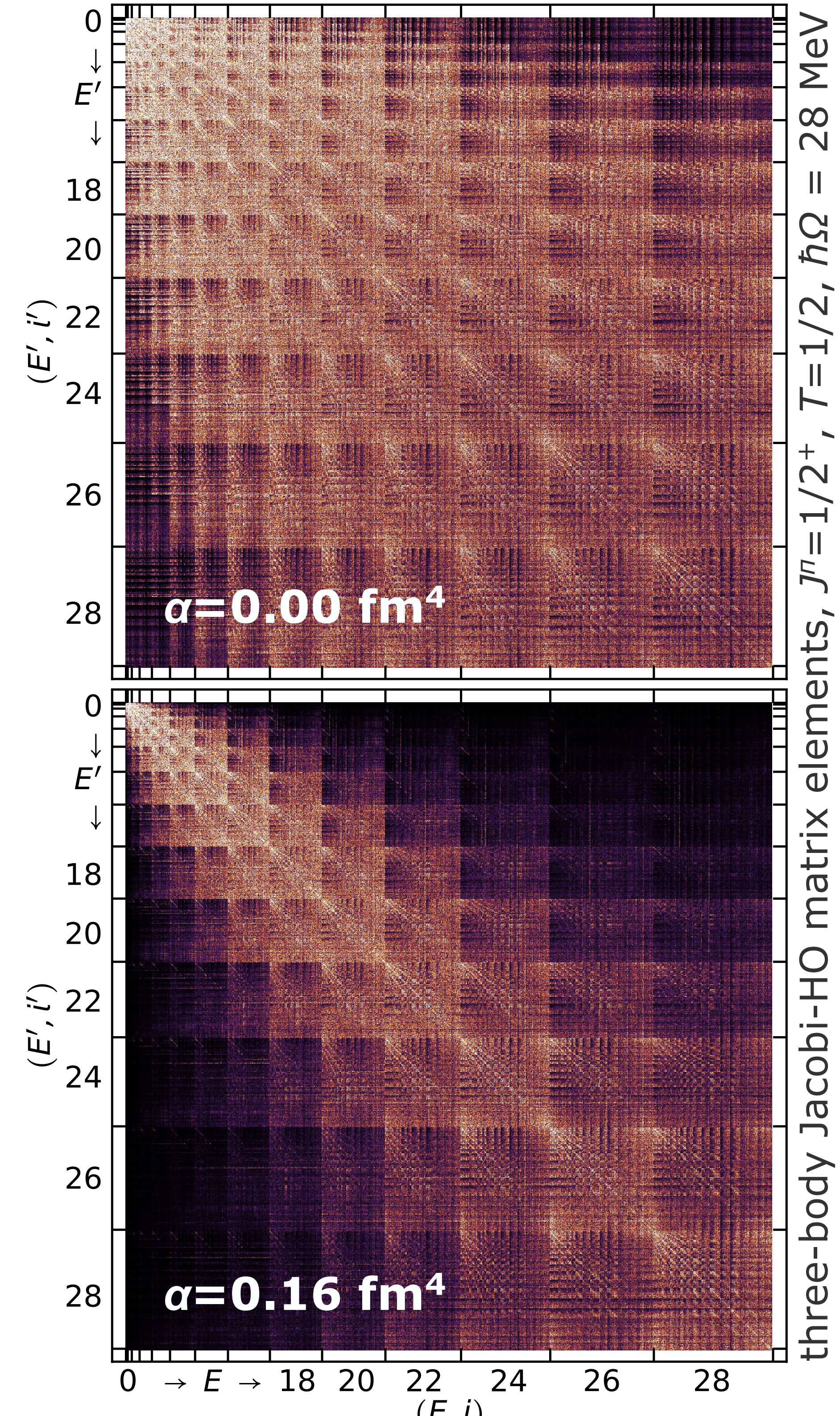
- unitary transformation via flow equation

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

- 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

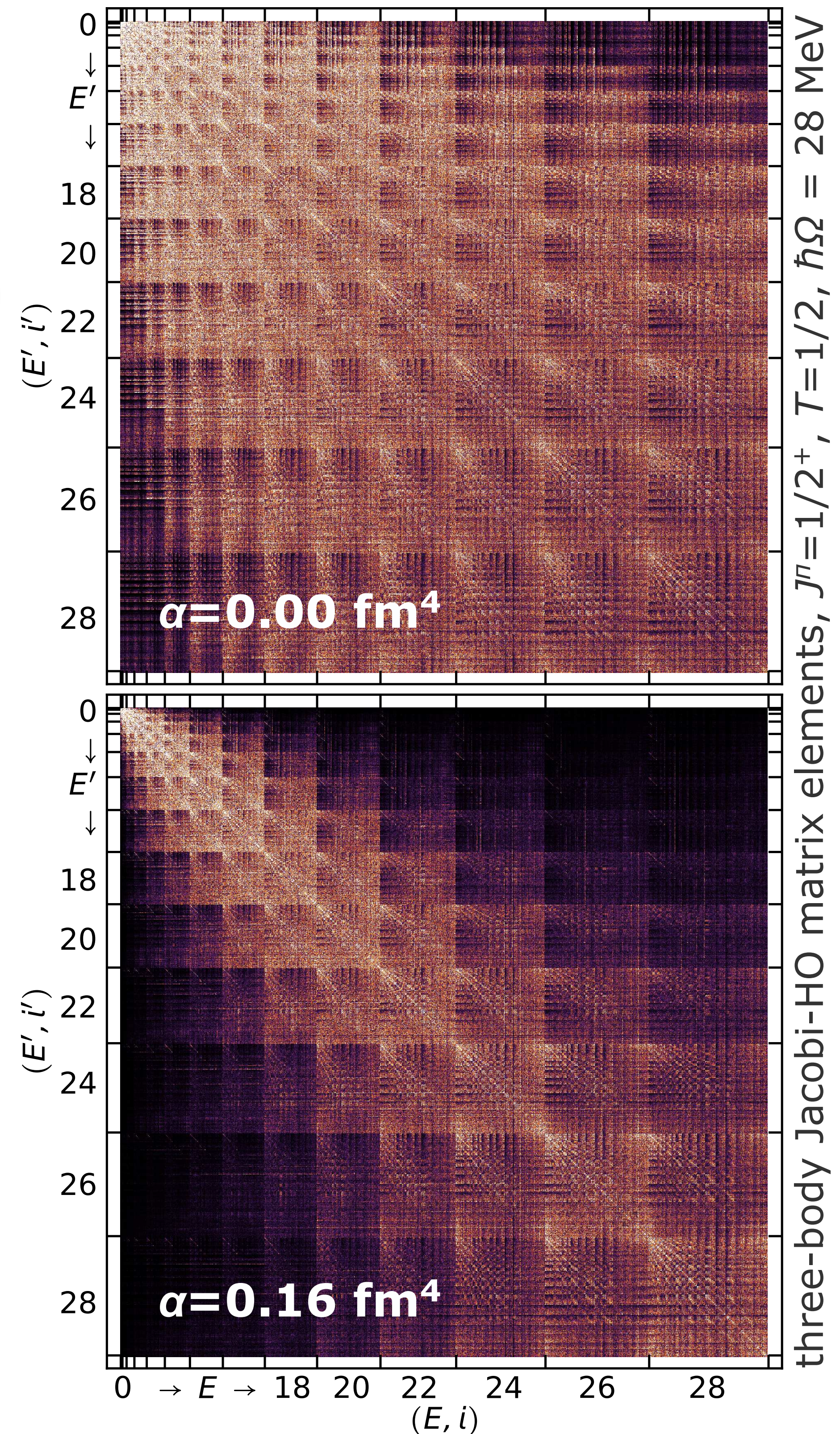
con:
induces many-body interactions

- 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$_{\text{ind}}$**
    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

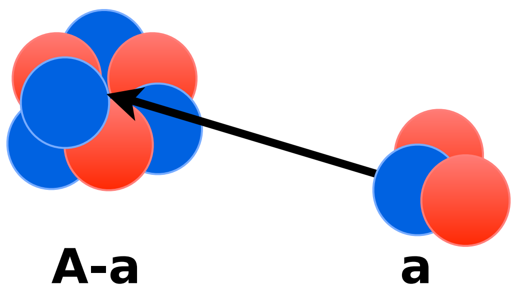
- **NCSM**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
  - convergence of observables w.r.t. $N_{\max}$ is the only limitation and source of uncertainty
- **Importance-Truncated NCSM**: reduce 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, ...

NCSM with Continuum

Baroni, Navrátil, Quaglioni, Phys. Rev. Lett. 110, 022505 (2013)

comprehensive ab initio description of light nuclei

bound states
& spectroscopy



resonances
& scattering states

(IT-)NCSM
ab initio description of nuclear clusters

NCSMC

RGM
describing relative motion of clusters

focus on NCSMC with 3N interactions
for p-shell spectroscopy

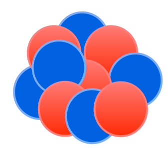
NCSMC with 3N Forces

Hupin, Langhammer, Navrátil, Quaglioni, Calci, Roth; Phys. Rev. C 88, 054622 (2013)

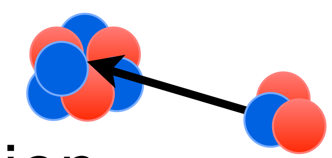
- representing $H|\psi^{J\pi T}\rangle = E|\psi^{J\pi T}\rangle$ using the **over-complete basis**

$$|\Psi^{J\pi T}\rangle = \sum_{\lambda} c_\lambda |\Psi_A E_\lambda J^\pi T\rangle + \sum_{\nu} \int \mathrm{d}r\, r^2 \frac{\chi_\nu(r)}{r} |\xi^{J\pi T}_{\nu r}\rangle$$

expansion in A-body (IT-)NCSM eigenstates



identical to the NCSM/RGM expansion



leads to the **NCSMC equations**

$$\begin{pmatrix} H_{\text{NCSM}} & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} =$$

access targets beyond ^{4}He using uncoupled densities and on-the-fly algorithm

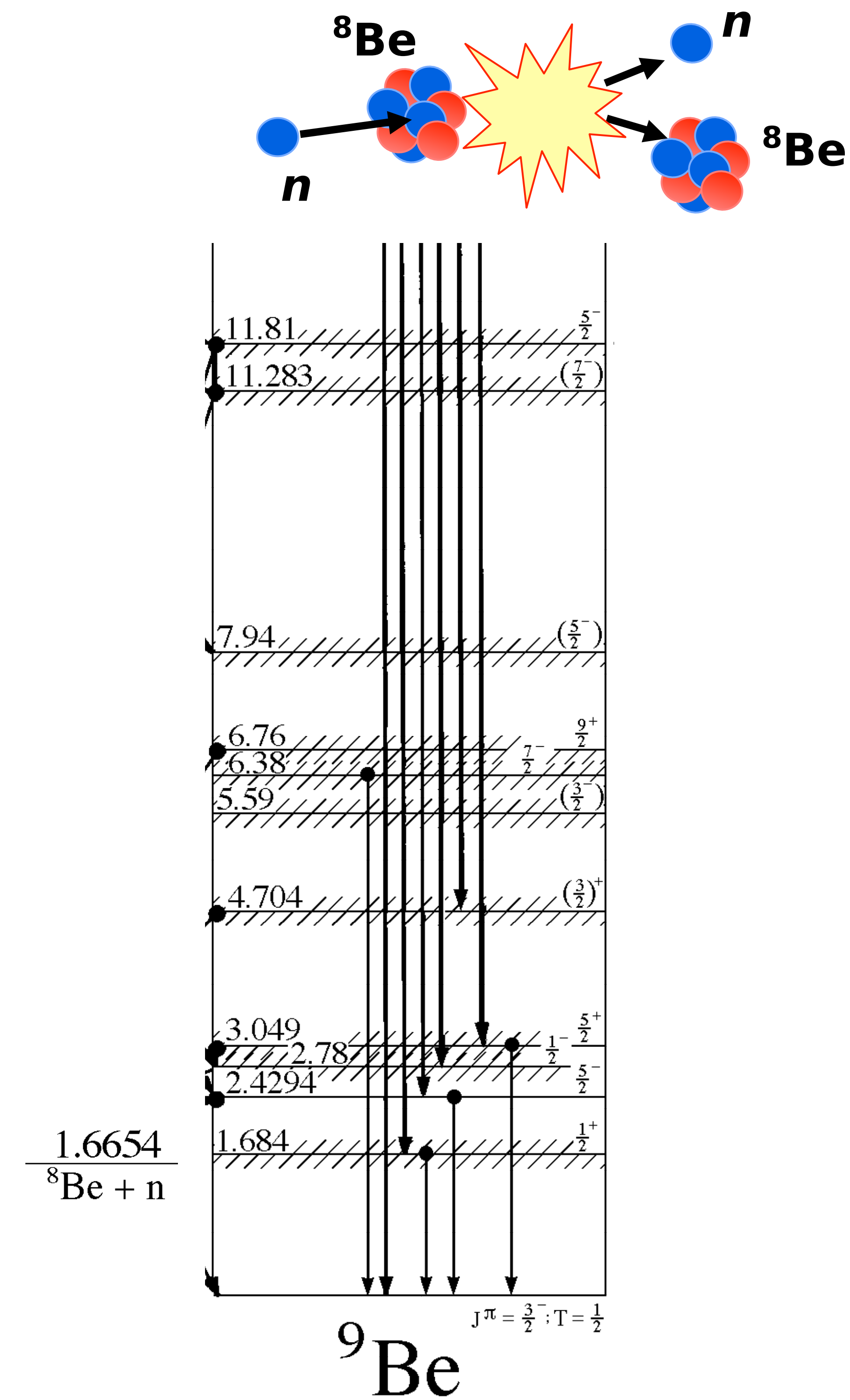
with 3N contributions in

H_{NCSM}	h	$\mathcal{H}$
covered by (IT-)NCSM	given by $\langle \Psi_A E_{\lambda'} J^\pi T | \hat{H} | \xi^{J\pi T}_{\nu r}\rangle$	contains NCSM/RGM Hamiltonian kernel

Spectrum of ^{9}Be

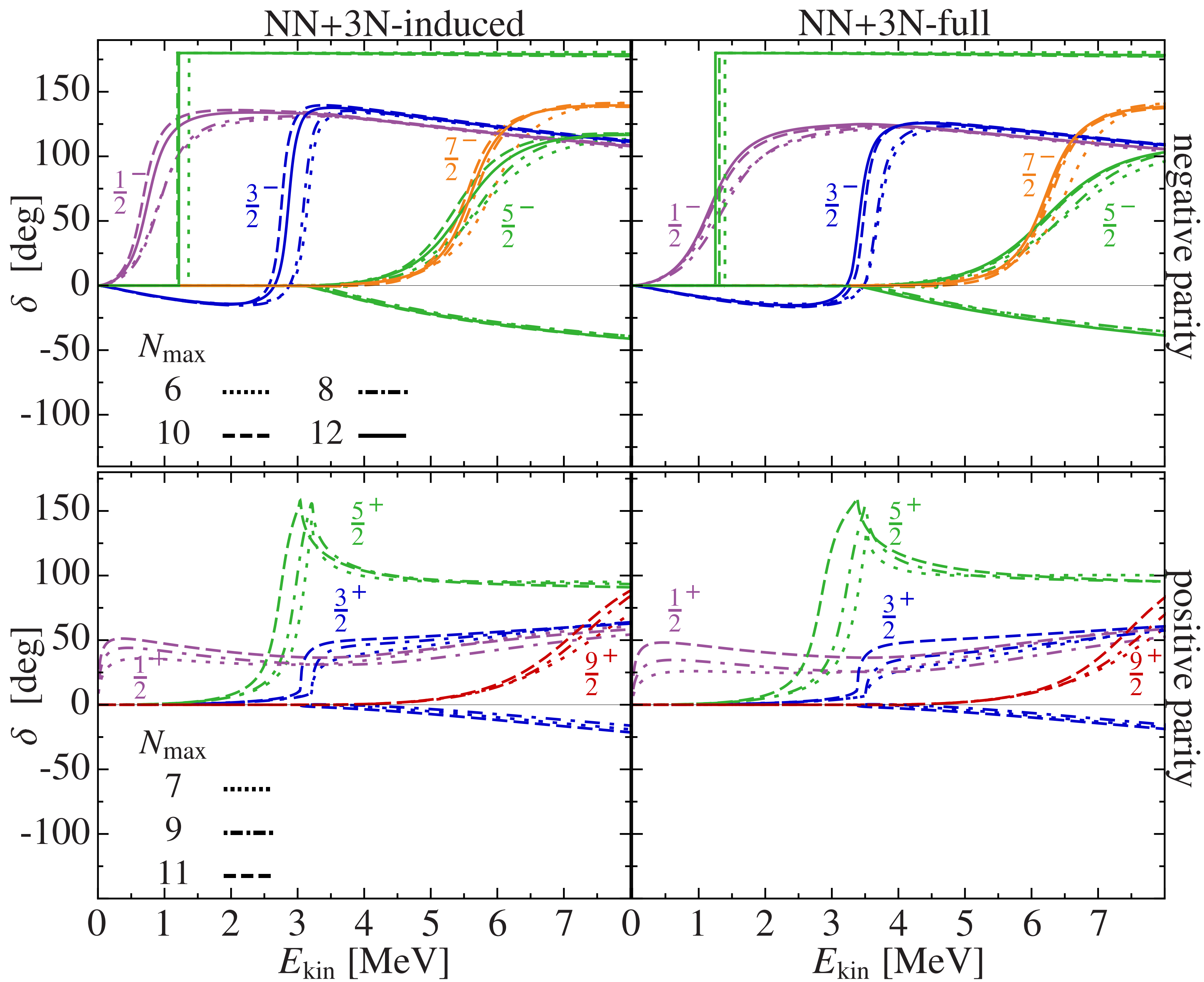
Langhammer et al.; PRC 91, 021301(R) (2015)

- ^{9}Be is excellent candidate to study continuum effects on spectra
- all excited states are resonances
- previous NCSM studies with NN interactions show clear discrepancies in spectrum: 3N or continuum effects?
- include n-^{8}Be continuum in NCSMC
  - use 0^+,2^+ NCSM states of ^{8}Be for n-^{8}Be dynamics
  - include 6 neg. and 4 pos. parity NCSM states of ^{9}Be
- use standard NN+3N Hamiltonian
  - NN @ N3LO, Entem & Machleidt, cutoff 500 MeV
  - 3N @ N2LO, local, cutoff 500 MeV



Phase Shifts for n-^{8}Be Scattering

Langhammer et al.; PRC 91, 021301(R) (2015)

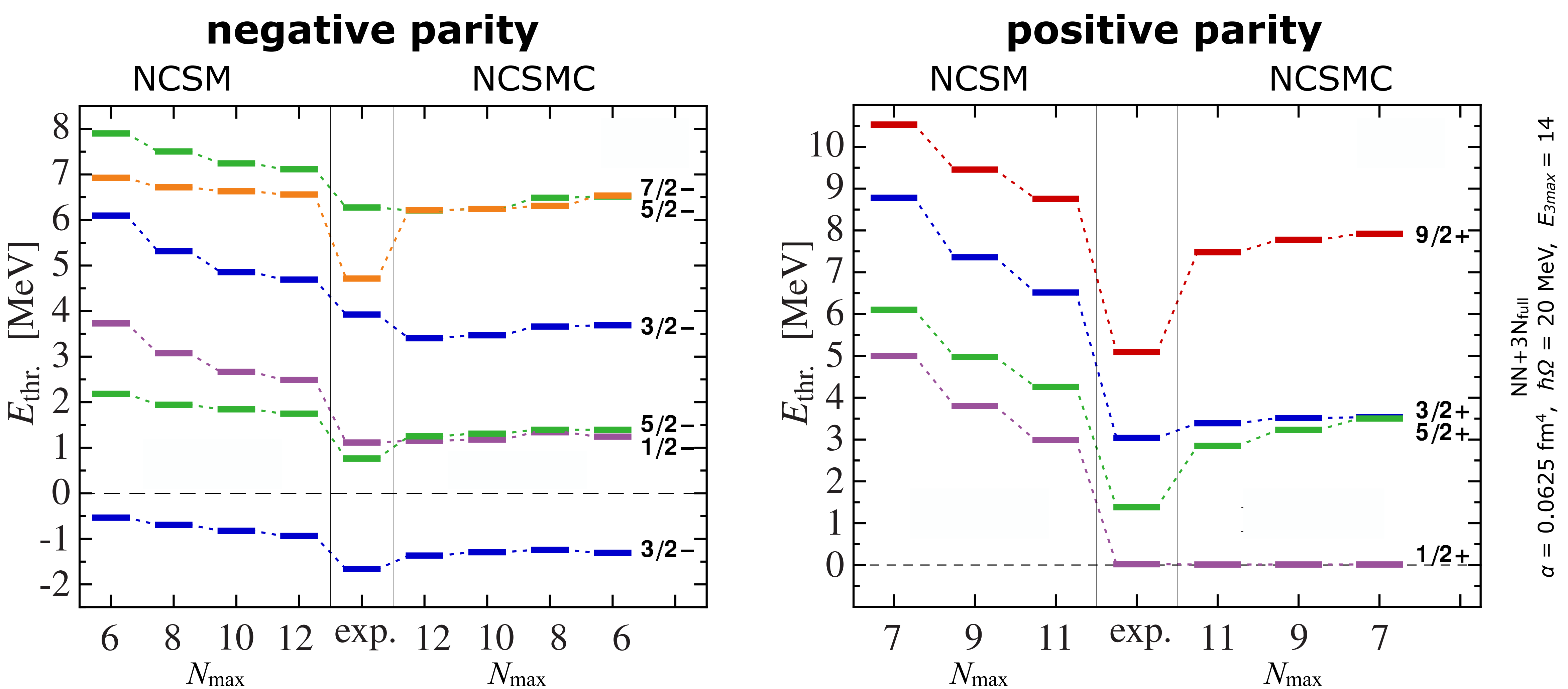


- negative parity phase-shifts are well converged, positive parity more difficult
- extract resonance parameters from inflection point and derivative

$\alpha = 0.0625\ \text{fm}^4$, $\hbar\Omega = 20$ MeV, $E_{3max} = 14$

^{9}Be: NCSM vs. NCSMC

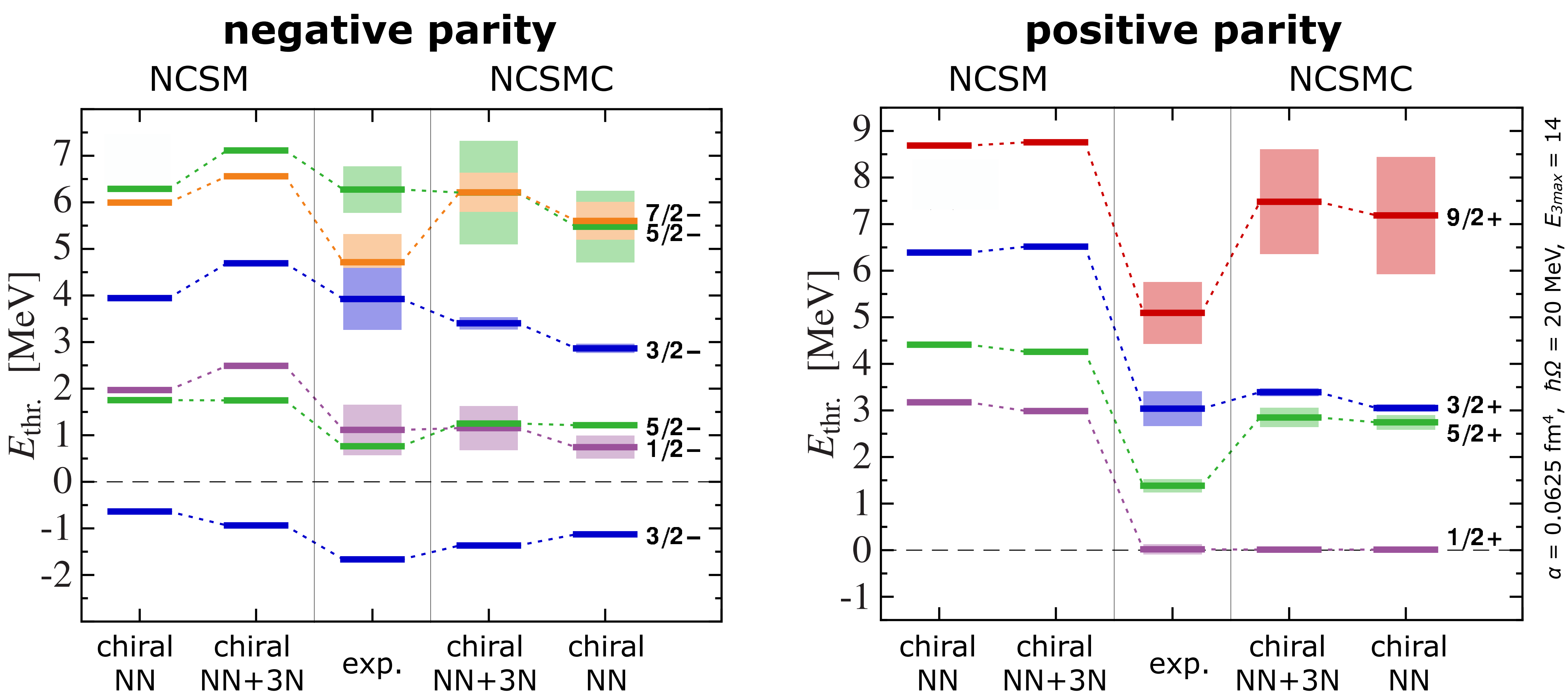
Langhammer et al.; PRC 91, 021301(R) (2015)



- NCSMC shows much better N_{max} convergence
- NCSM tries to capture continuum effects via large N_{max}
- drastic difference for the $1/2^+$ state right at threshold

^{9}Be: Spectrum

Langhammer et al.; PRC 91, 021301(R) (2015)



- continuum plays more important role than chiral 3N interaction
- NCSMC predictions for widths are in fair agreement with experiment

Bridge to Medium-Mass Nuclei

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)

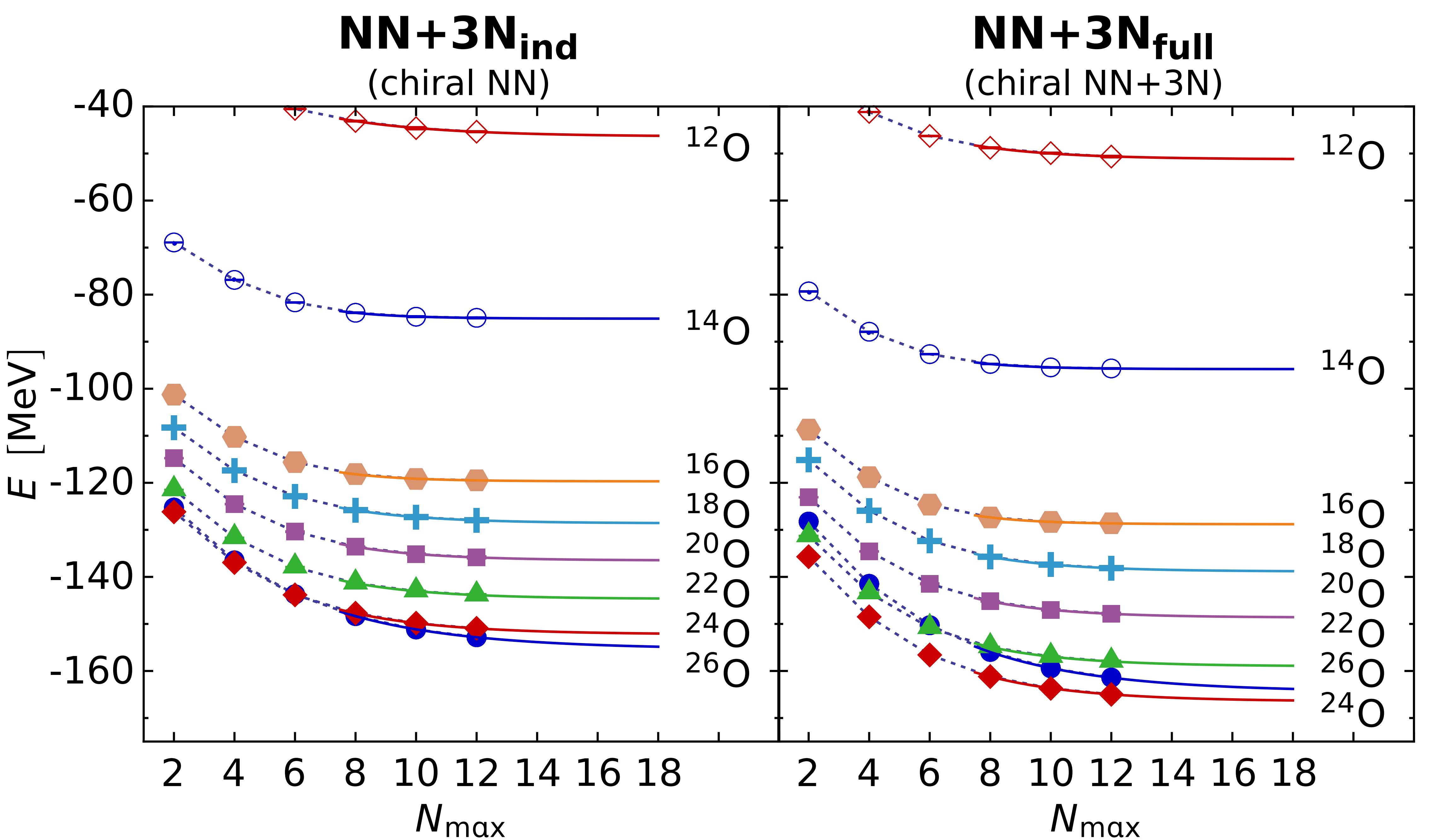
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

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

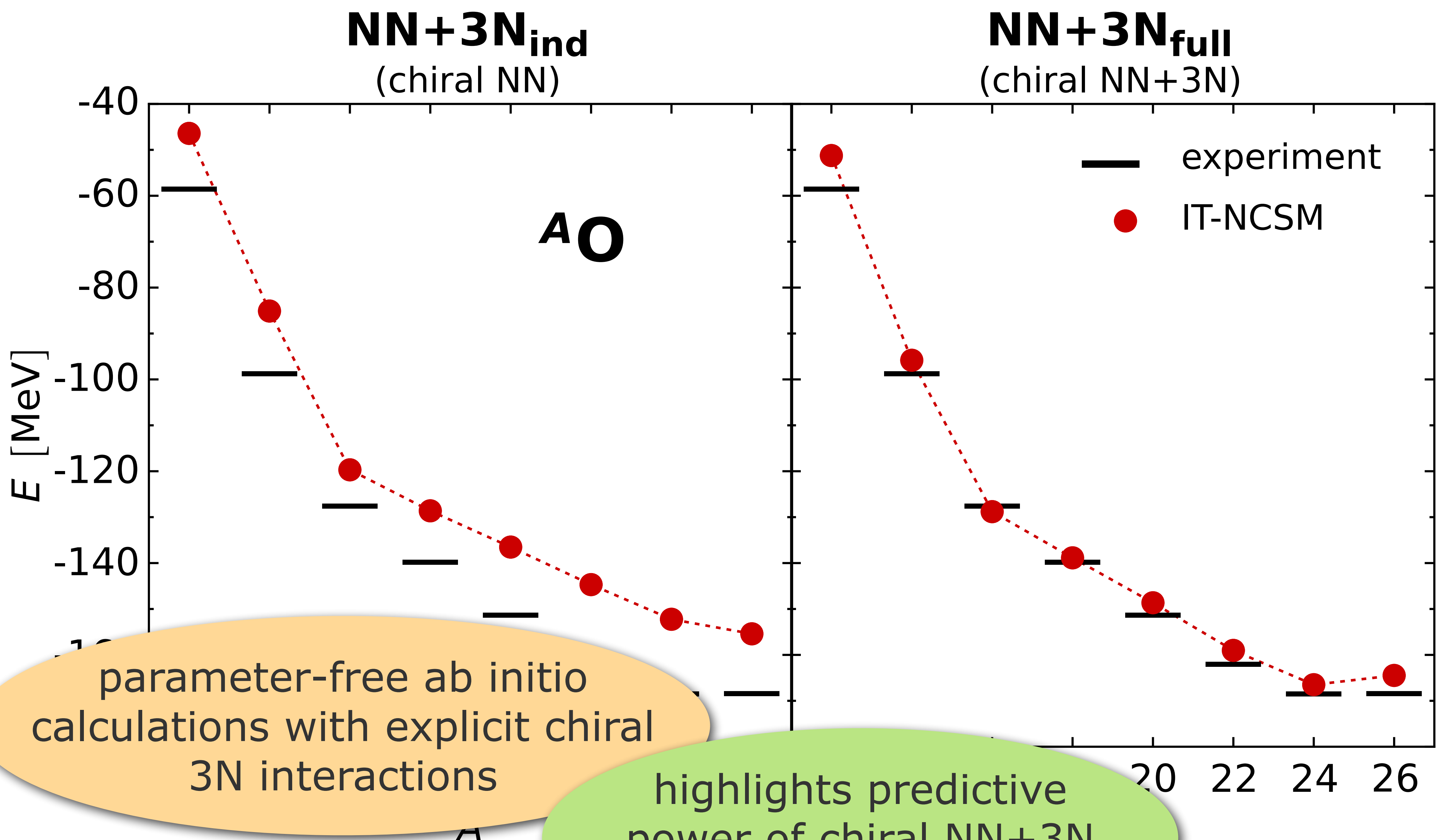
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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)



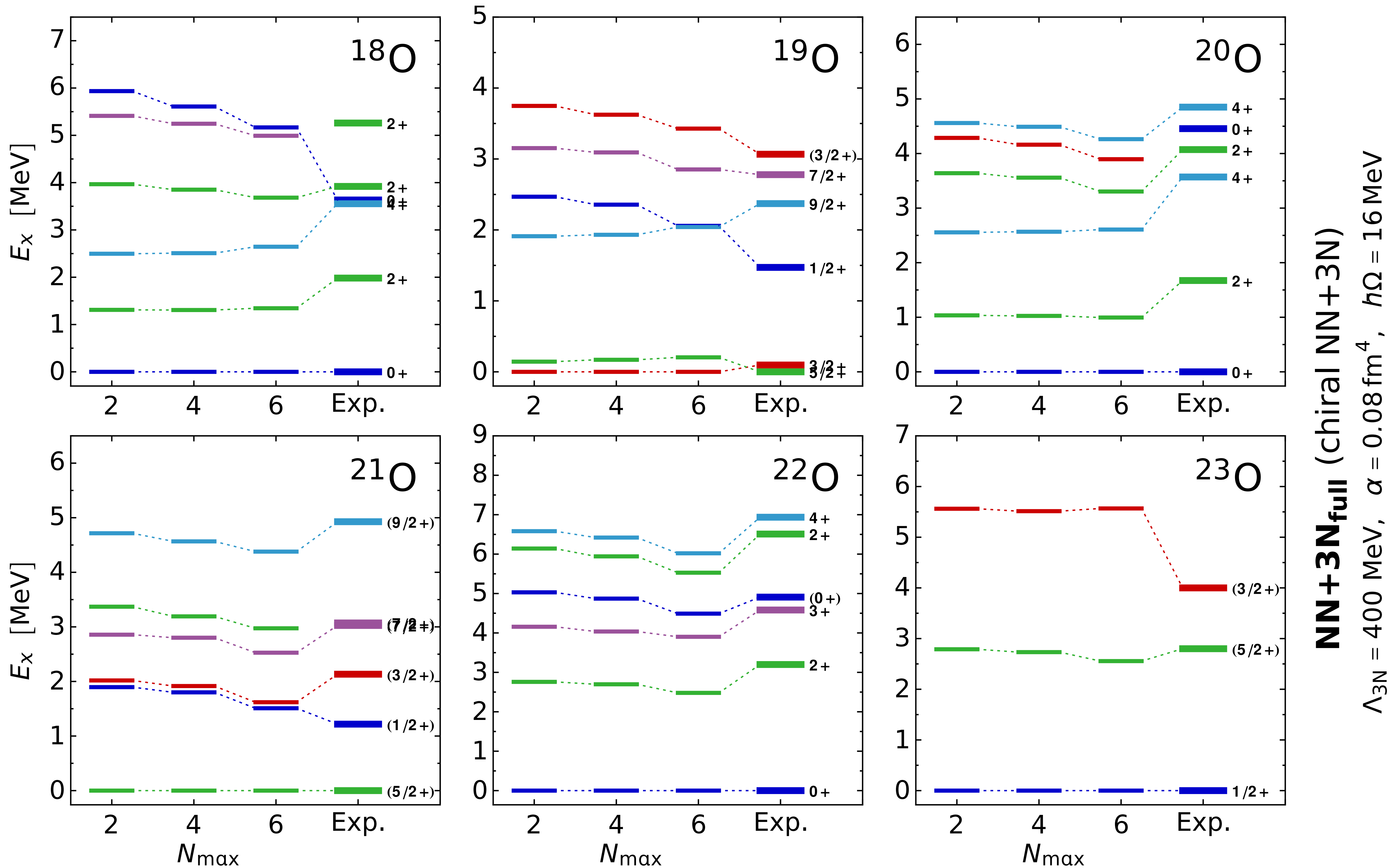
parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

Λ_{3N} = 400 MeV, α = 0... ...ptimal $\hbar\Omega$

Spectra of Oxygen Isotopes

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



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

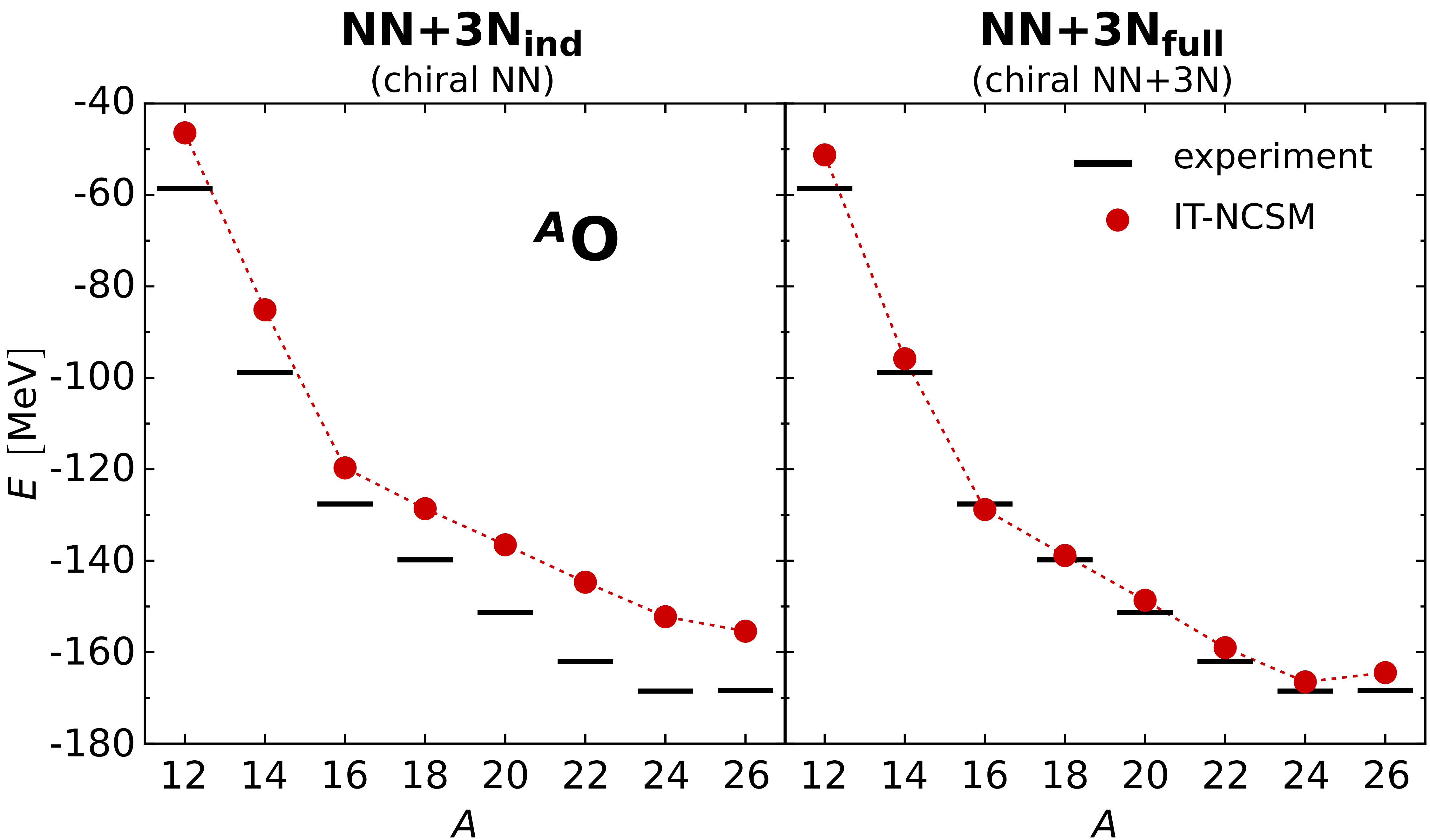
Barbieri, Soma, Duguet,...

- 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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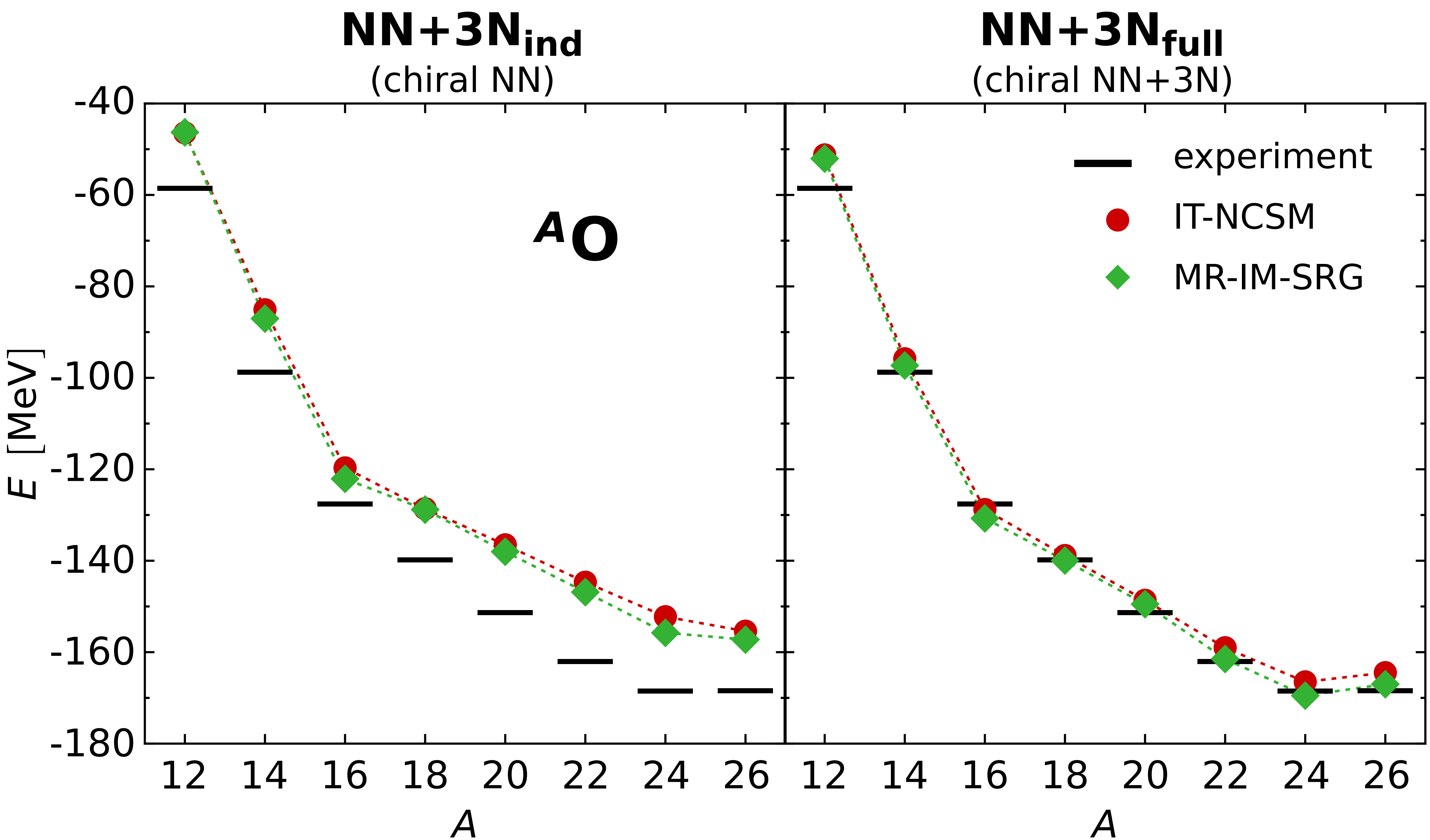
Ground States of Oxygen Isotopes

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



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Ground States of Oxygen Isotopes

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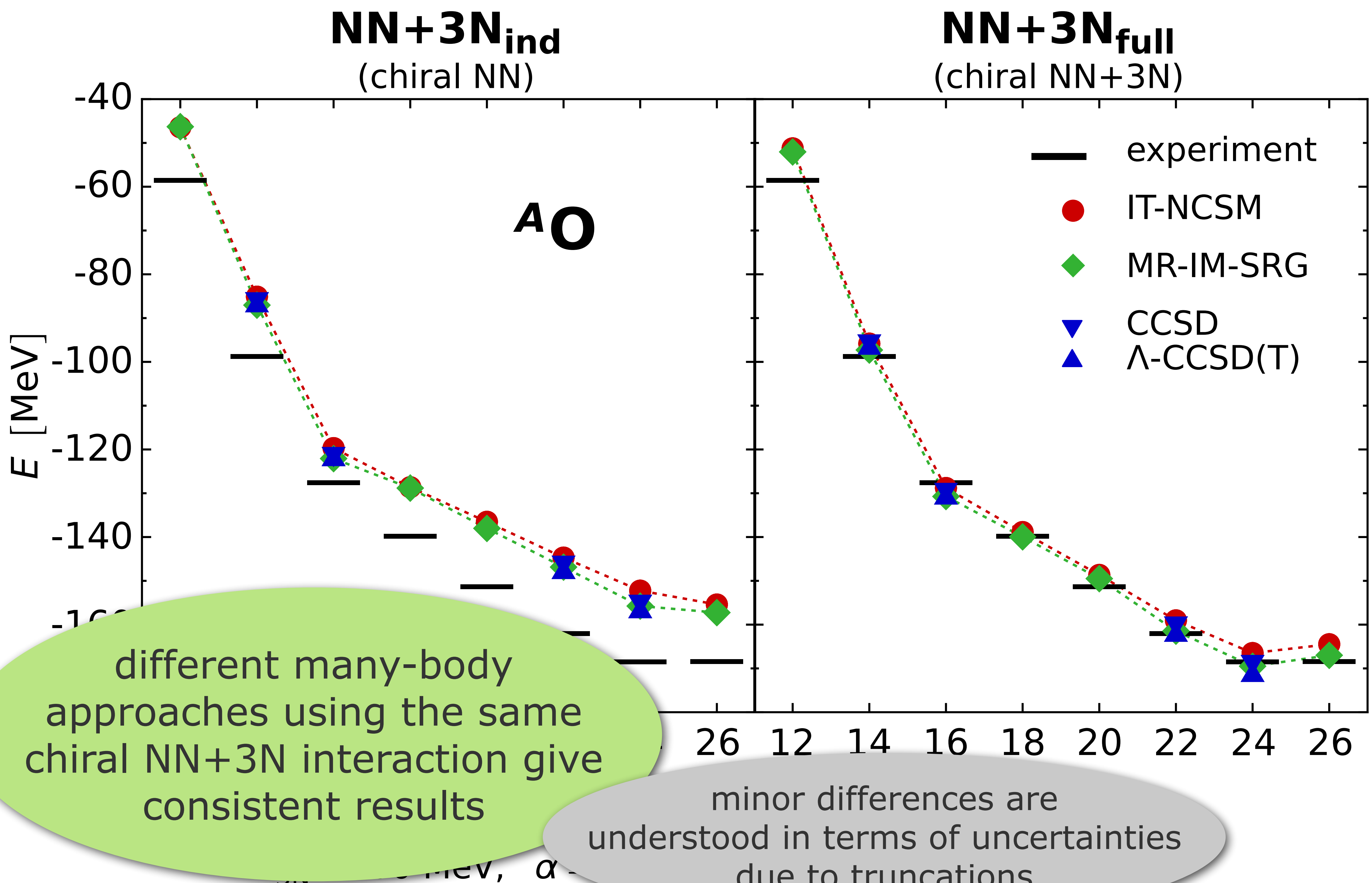
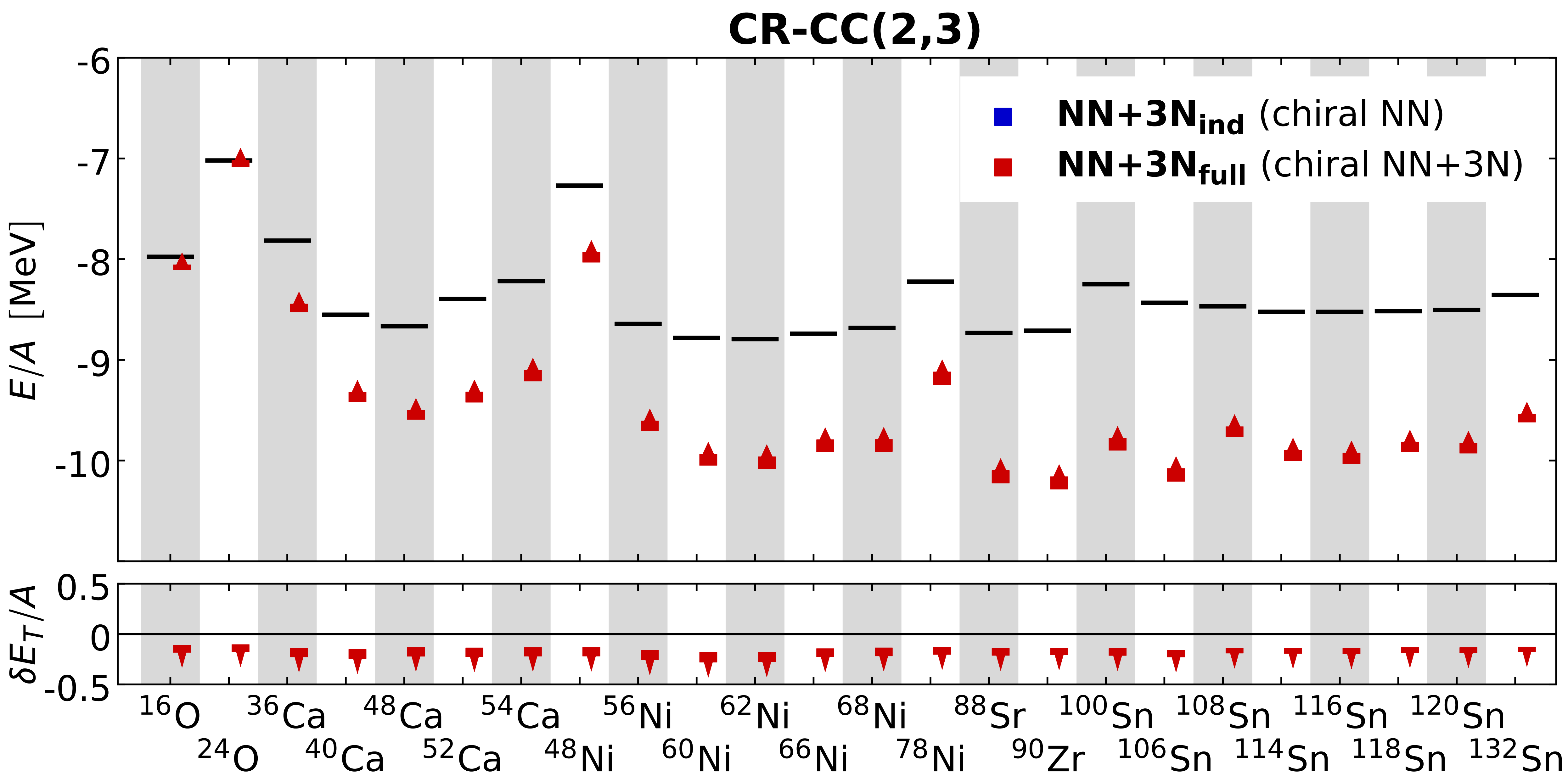


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Towards Heavy Nuclei - Ab Initio

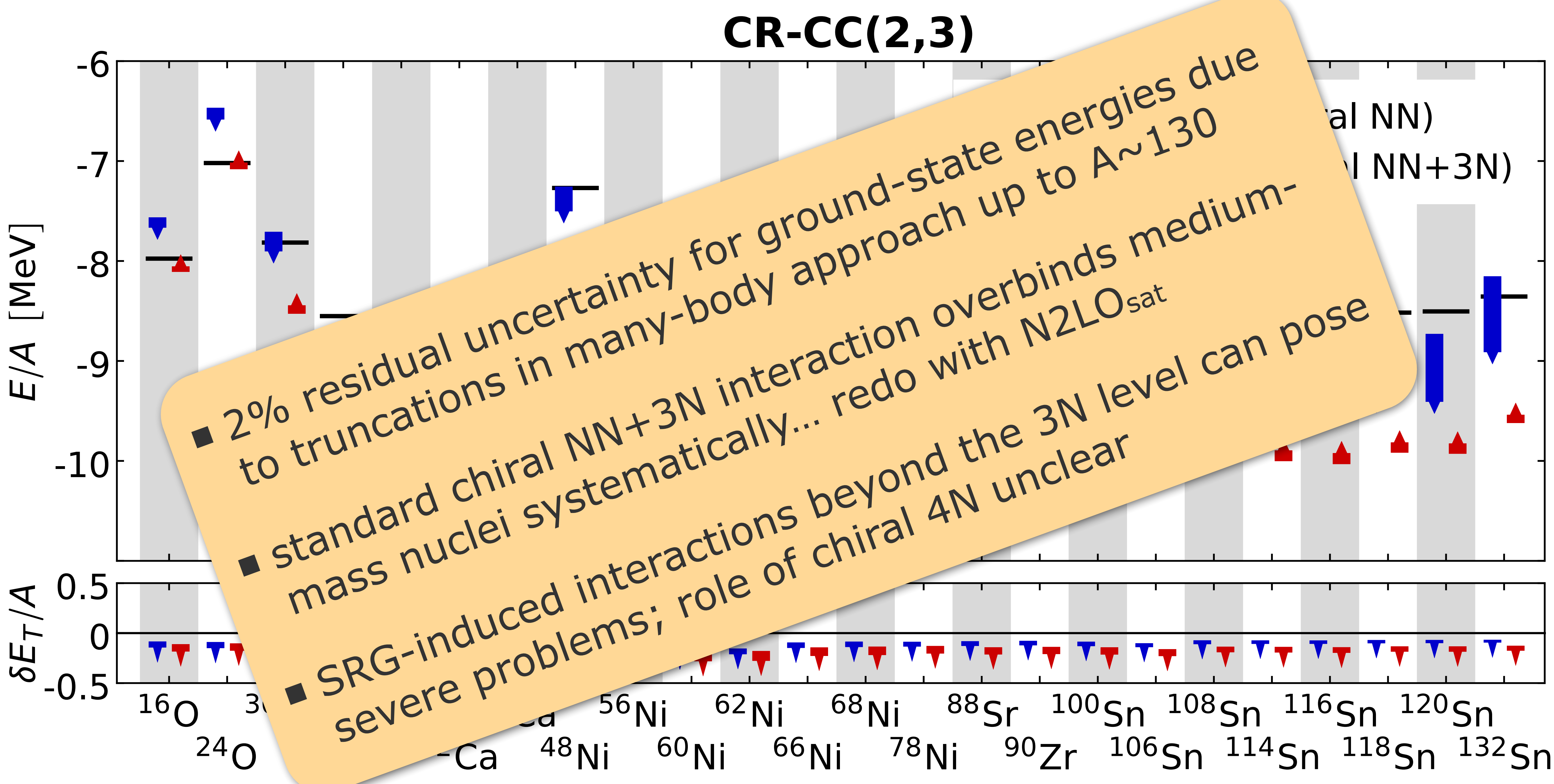
Binder et al., PLB 736, 119 (2014)



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

Towards Heavy Nuclei - Ab Initio

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

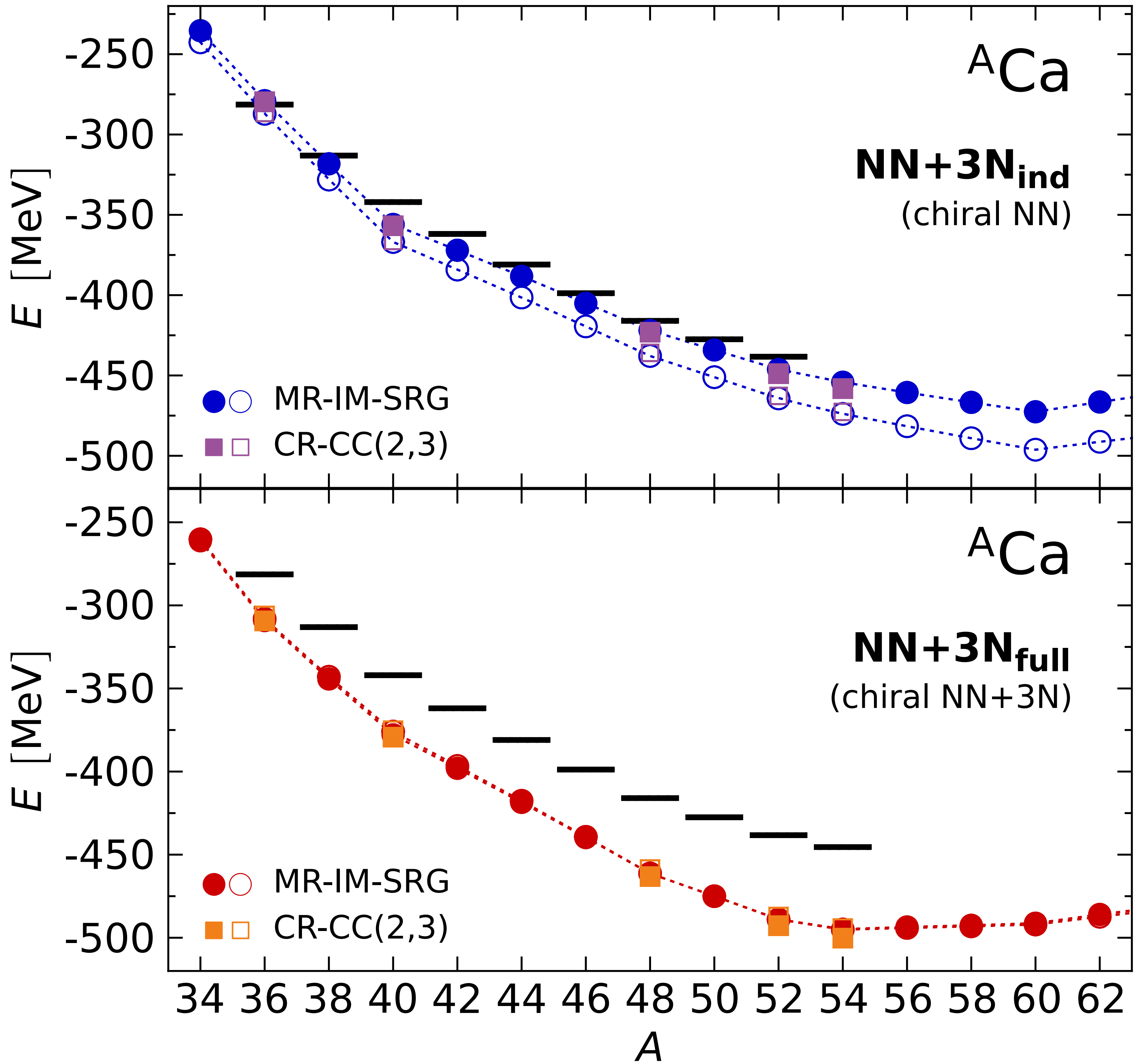


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically… redo with N2LO$_{sat}$
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

$\Lambda_{3N} = 400$ 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)

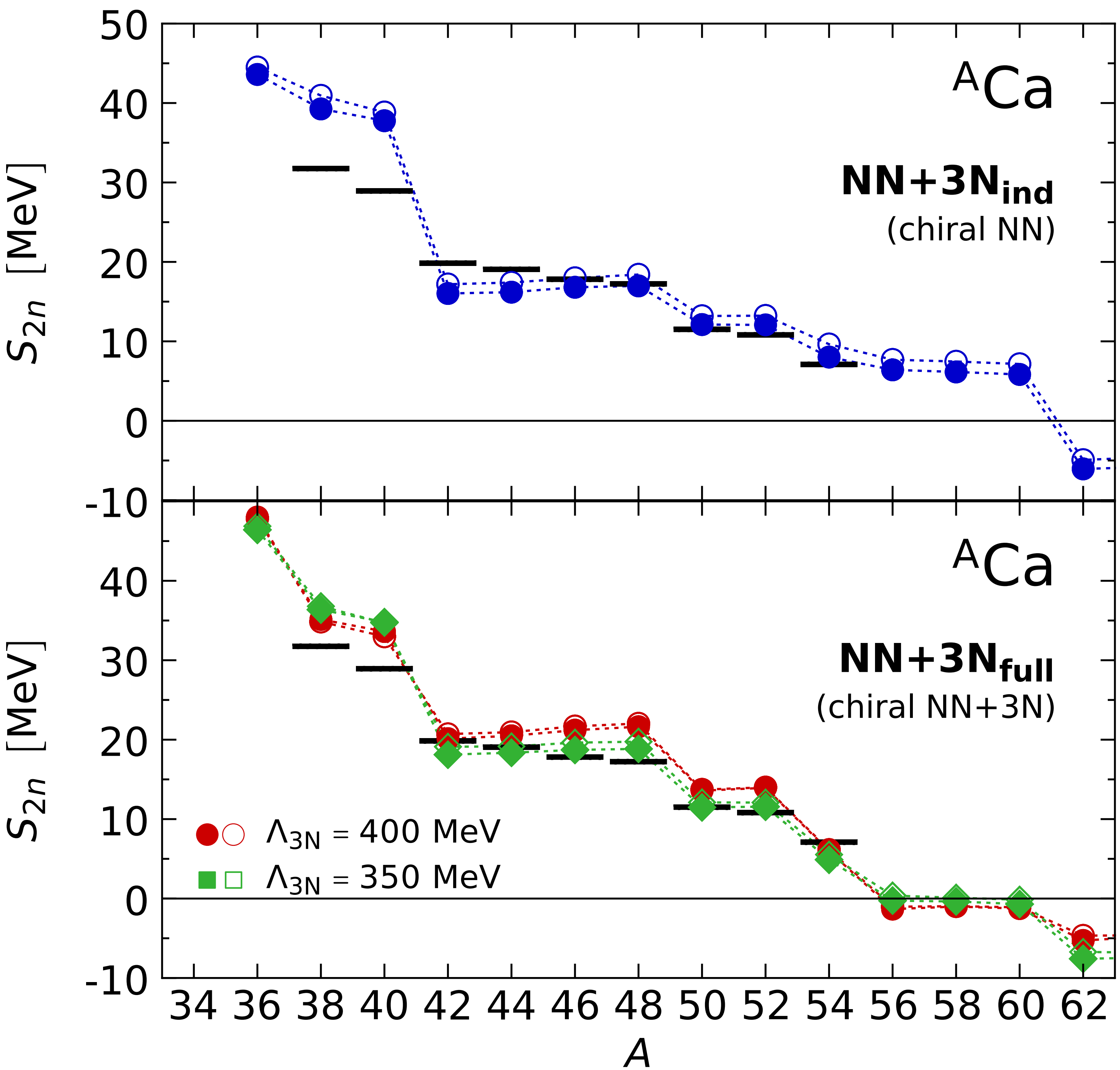


- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

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

News:

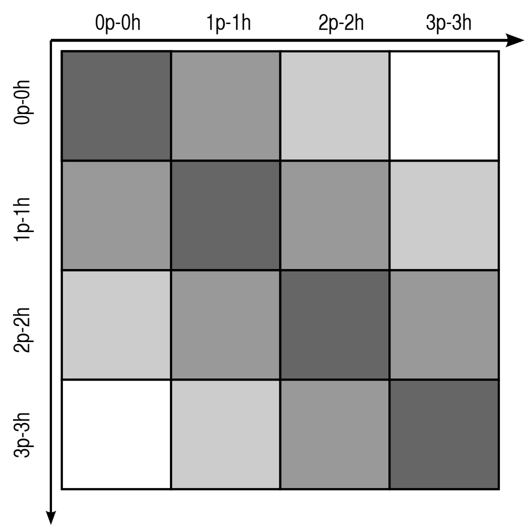
Merging NCSM and IM-SRG

with

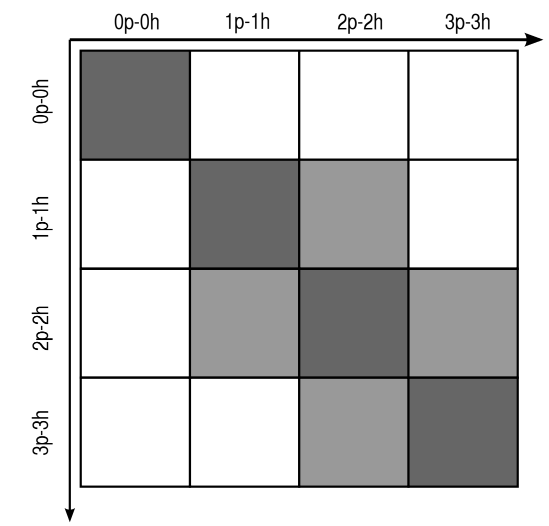
Eskendr Gebrerufael, Heiko Hergert, Klaus Vobig

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

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

IM-SRG Generators

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

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

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

$$\eta_2^1 = (\Delta_2^1)^{-1}\, n_1 \bar{n}_2\, f_2^1 - [1 \longleftrightarrow 2]$$

$$\eta_{34}^{12} = (\Delta_{34}^{12})^{-1}\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma_{34}^{12} - [12 \longleftrightarrow 34]$$

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

$$\eta_2^1 = \mathrm{sgn}(\Delta_2^1)\, n_1 \bar{n}_2\, f_2^1 - [1 \longleftrightarrow 2]$$

$$\eta_{34}^{12} = \mathrm{sgn}(\Delta_{34}^{12})\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma_{34}^{12} - [12 \longleftrightarrow 34]$$

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

$$\eta_2^1 = \left\langle \Phi \right| [\tilde{A}_2^1, H] \left| \Phi \right\rangle$$

$$\eta_{34}^{12} = \left\langle \Phi \right| [\tilde{A}_{34}^{12}, H] \left| \Phi \right\rangle$$

Interfaces with NCSM

NCSM before IM-SRG

- use 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

NCSM after IM-SRG

- use normal-ordered Hamiltonian $H(s)$ at some value of the flow parameter for a subsequent NCSM or CI calculation
- access to excited states and full spectroscopy, additional diagnostics for the ground state
- can use the in-medium evolved Hamiltonian also in other approaches, e.g., equations-of-motion methods, RPA, Second-RPA
- this is different from IM-SRG for generating shell-model interactions

NCSM-MR-IM-SRG-NCSM Workflow

- pick interaction and nucleus
- solve NCSM problem in small N_{max}
- ground state defines reference state

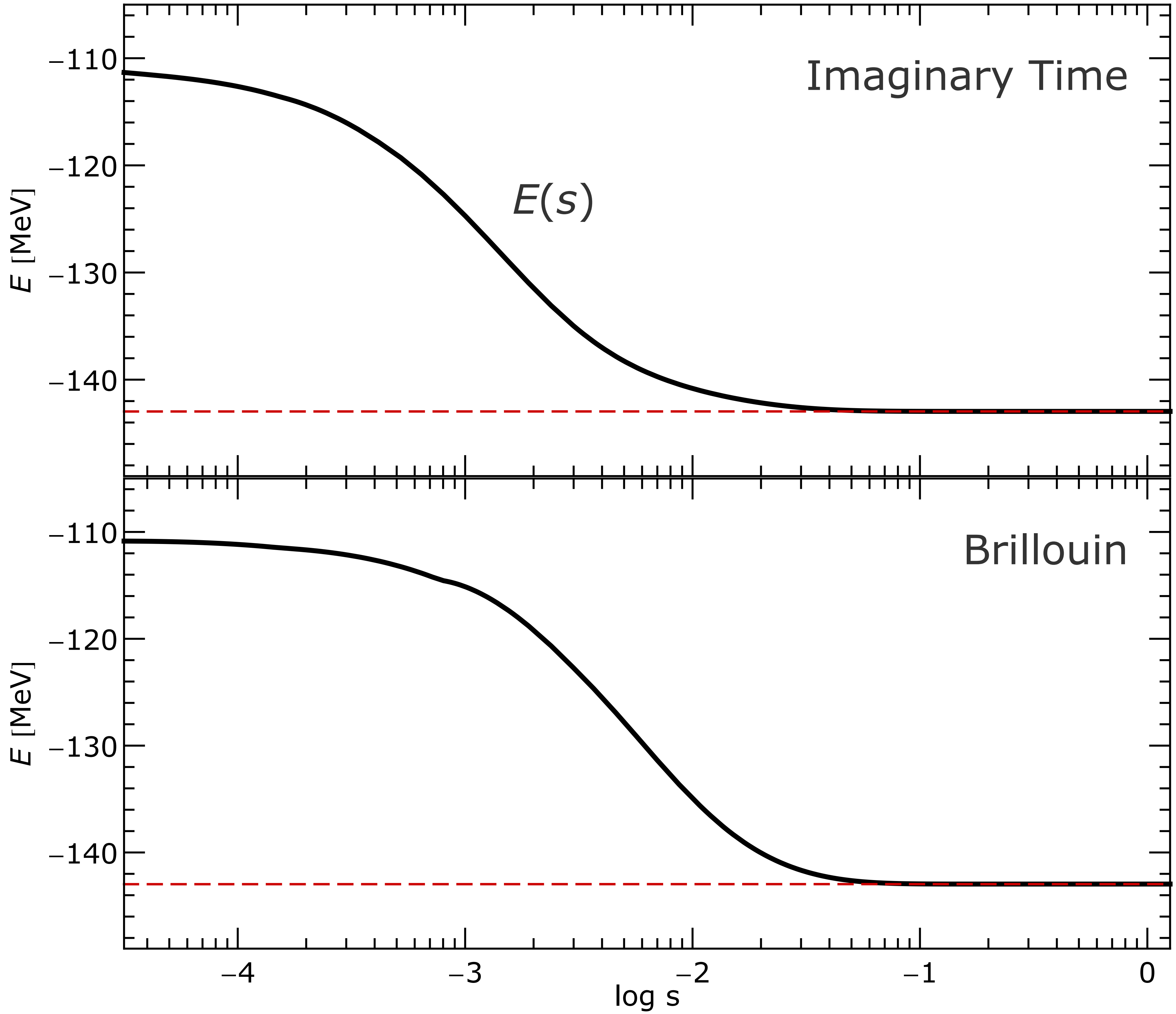
compute density matrices and multi-ref. normal-ordered Hamiltonian

- solve MR-IM-SRG flow equations
- spherical formulation limited to scalar densities for now

extract evolved Hamiltonian in vacuum representation

- NCSM or CI calculation for ground and excited states
- …

^{16}O: Flowing Energy



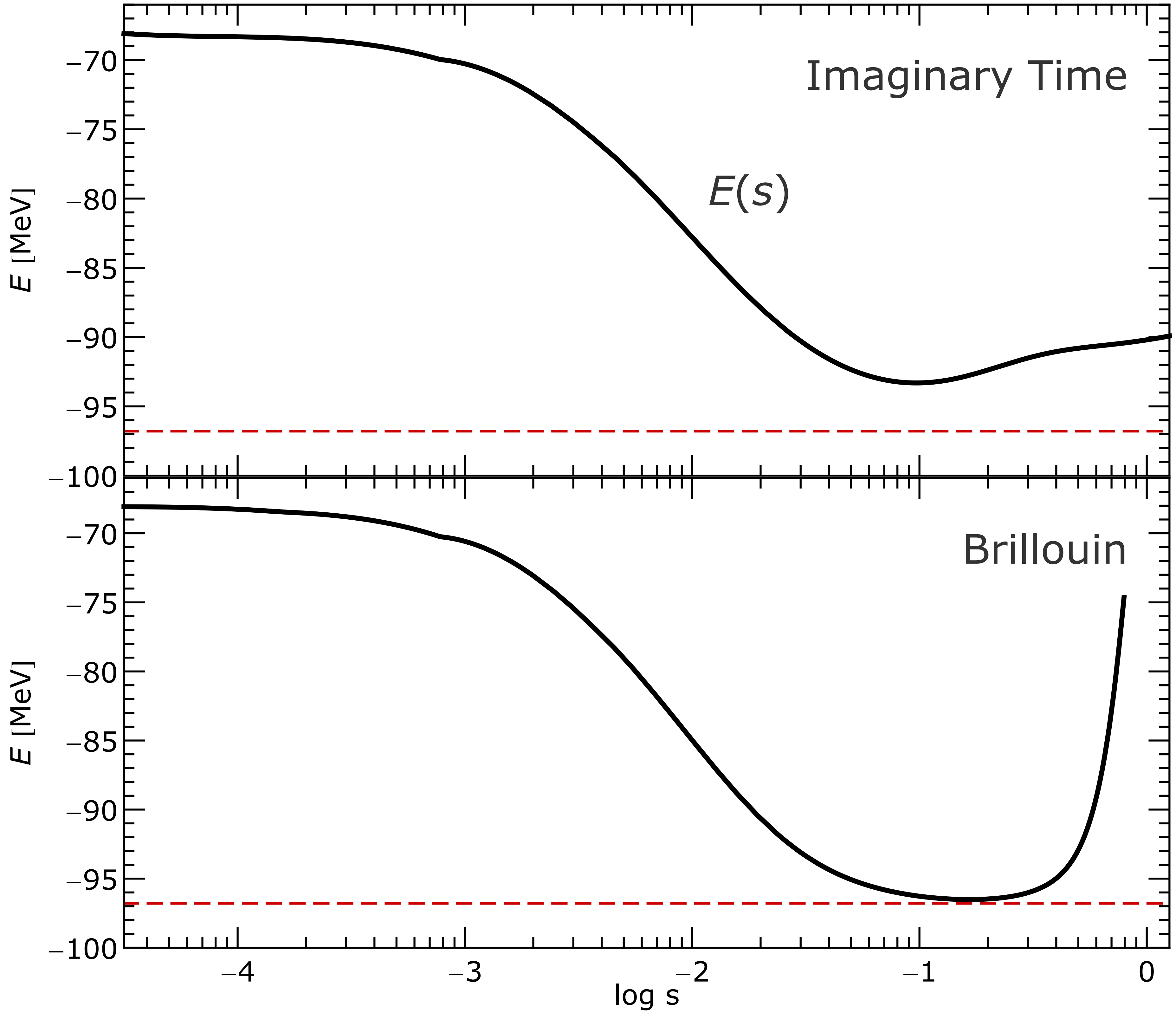
^{16}O

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

N_{max}=0
reference state

e_{max}=4

^{12}C: Flowing Energy



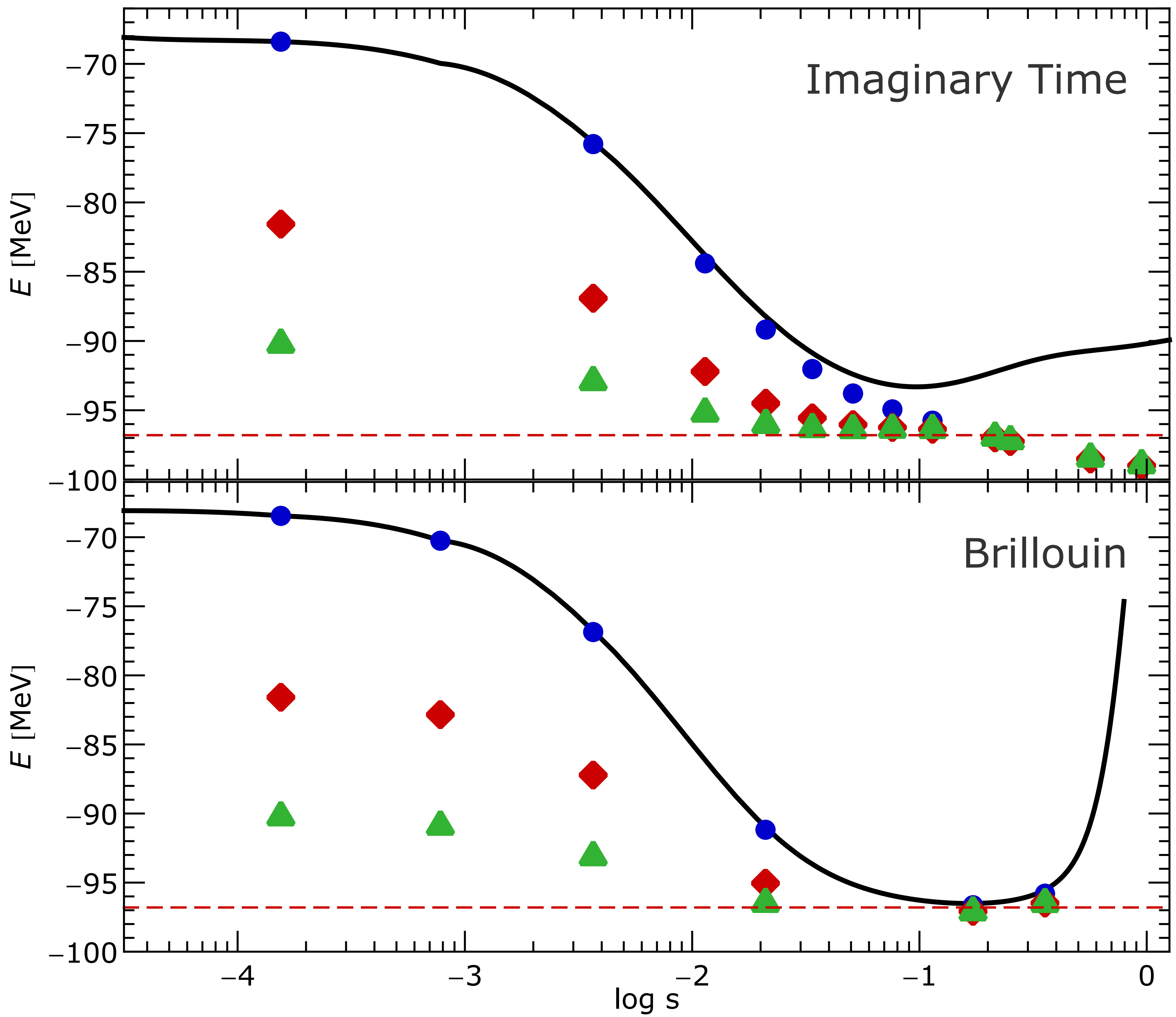
^{12}C

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

N_{max}=0
reference state

e_{max}=4

^{12}C: Flowing Energy



^{12}C

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

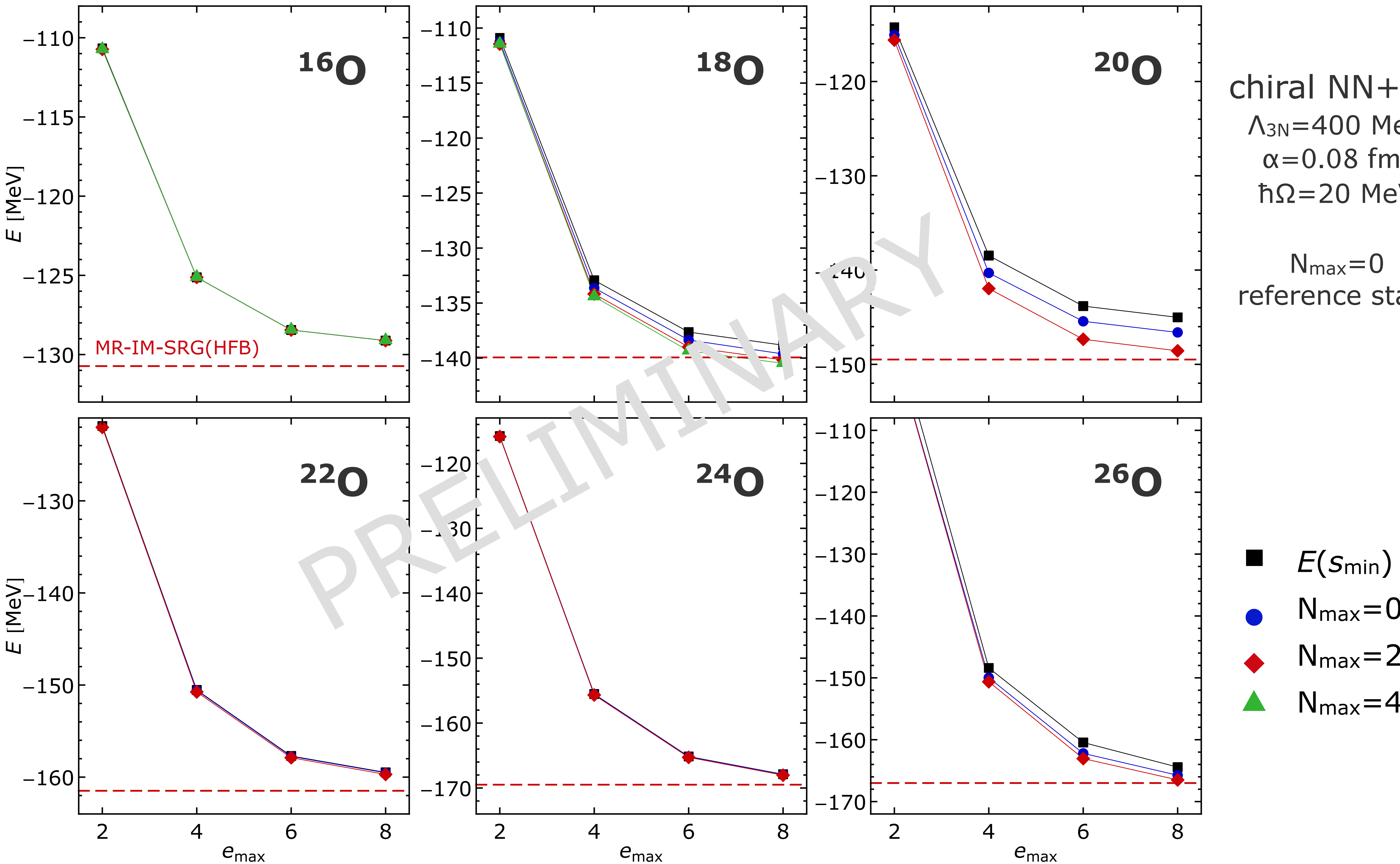
N_{max}=0
reference state

e_{max}=4

NCSM with flowing Hamiltonian

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

Oxygen Isotopes



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

N_{max}=0
reference state

News:

Importance Truncated Shell Model

with Christina Stumpf

Importance Truncation

PRC 79, 064324 (2009), PRL 99, 092501 (2007)

adaptive and physics-driven truncation criterion based on a perturbative estimate for the amplitude of individual basis states

- **importance measure** for basis state $|\Phi_\nu\rangle$ for the description of target state represented by $|\Psi_{\text{ref}}\rangle$

$$\kappa_\nu = -\frac{\langle\Phi_\nu| H |\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- reduce model space to important basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$ for a given **importance threshold** κ_{min}

- solve eigenvalue problem for a set of importance thresholds and extrapolate a posteriori to full space

Importance Truncated SM

- valence-space shell model also **limited by model-space dimension**, specifically for pf-shell and beyond or multi-shell valence spaces

- apply **importance truncation** for a sequence of T_{max}-truncated model spaces, analogously to N_{max} sequence in NCSM

- **sequential IT-SM** algorithm:

  (1) do full SM calculation up to convenient T_{max}

  (2) use components of eigenstates with $|C_\nu| \geq C_{\text{min}}$ to define reference states

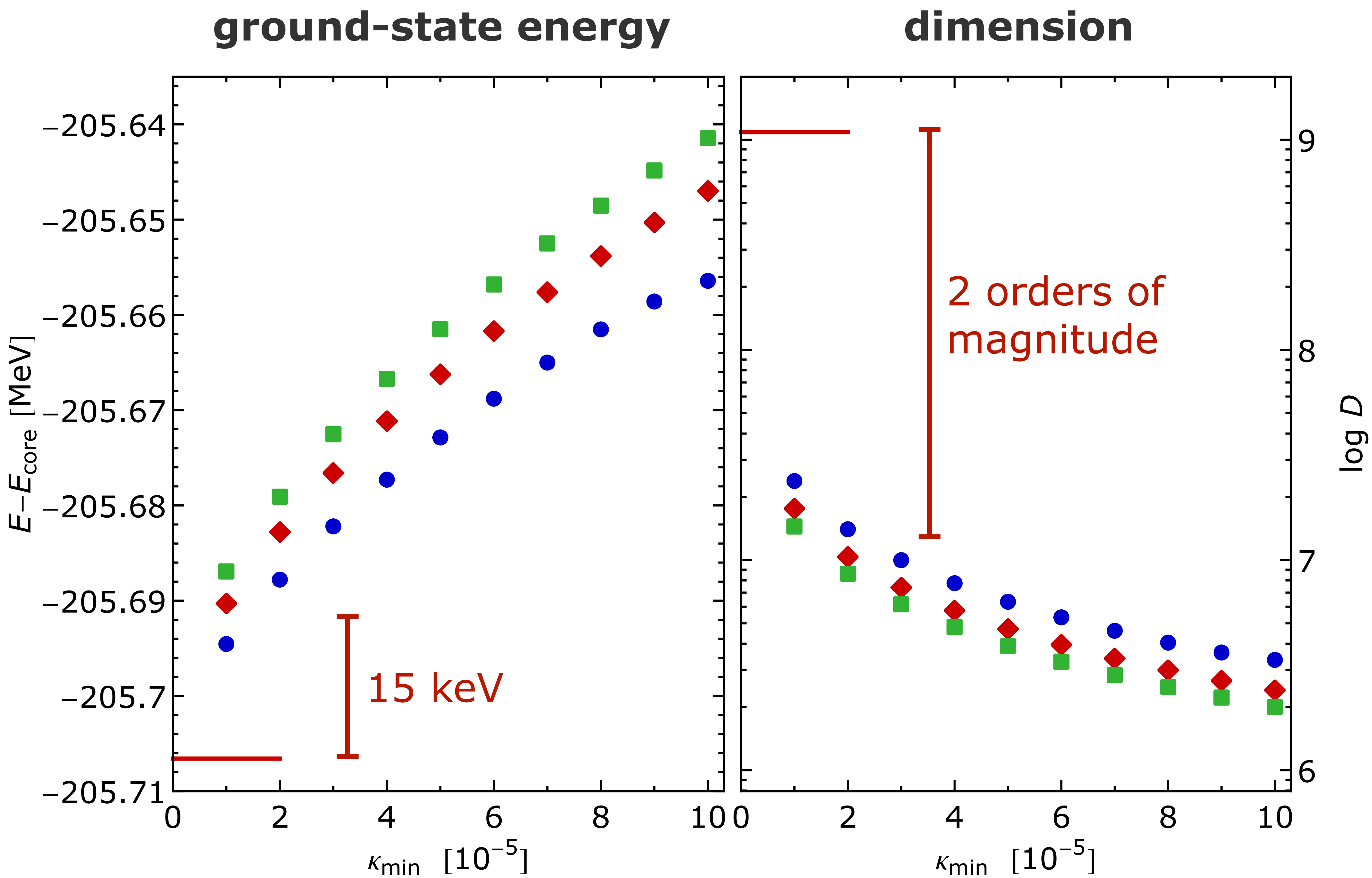
  (3) consider all basis states from $T_{\text{max}} = T_{\text{max}}+2$ space and add those with $|\kappa_\nu| \geq \kappa_{\text{min}}$ to importance truncated space

  (4) solve eigenvalue problem in importance truncated space (for set of κ_{min})

  (5) goto (2)

- in the limit $\kappa_{\text{min}}, C_{\text{min}} \to 0$ the full T_{max}-truncated model space is recovered

^{56}Ni: Threshold Dependence



^{56}Ni

GXPF1A

full pf space
(T_{max}=16)

C_{min}

- 1×10^{-4}
- 2×10^{-4}
- 3×10^{-4}

full SM; Horoi, Brown et al; PRC 73, 061305(R) (2006)

Energy Variance

energy variance provides a model-independent measure for the “distance” of an approximate state (truncated space) from a true eigenstate (full space)

$$\Delta E^2 = \langle \Psi | H^2 | \Psi \rangle - \langle \Psi | H | \Psi \rangle^2$$

- energy shows predominantly linear dependence on ΔE^2, use quadratic term as sub-leading correction

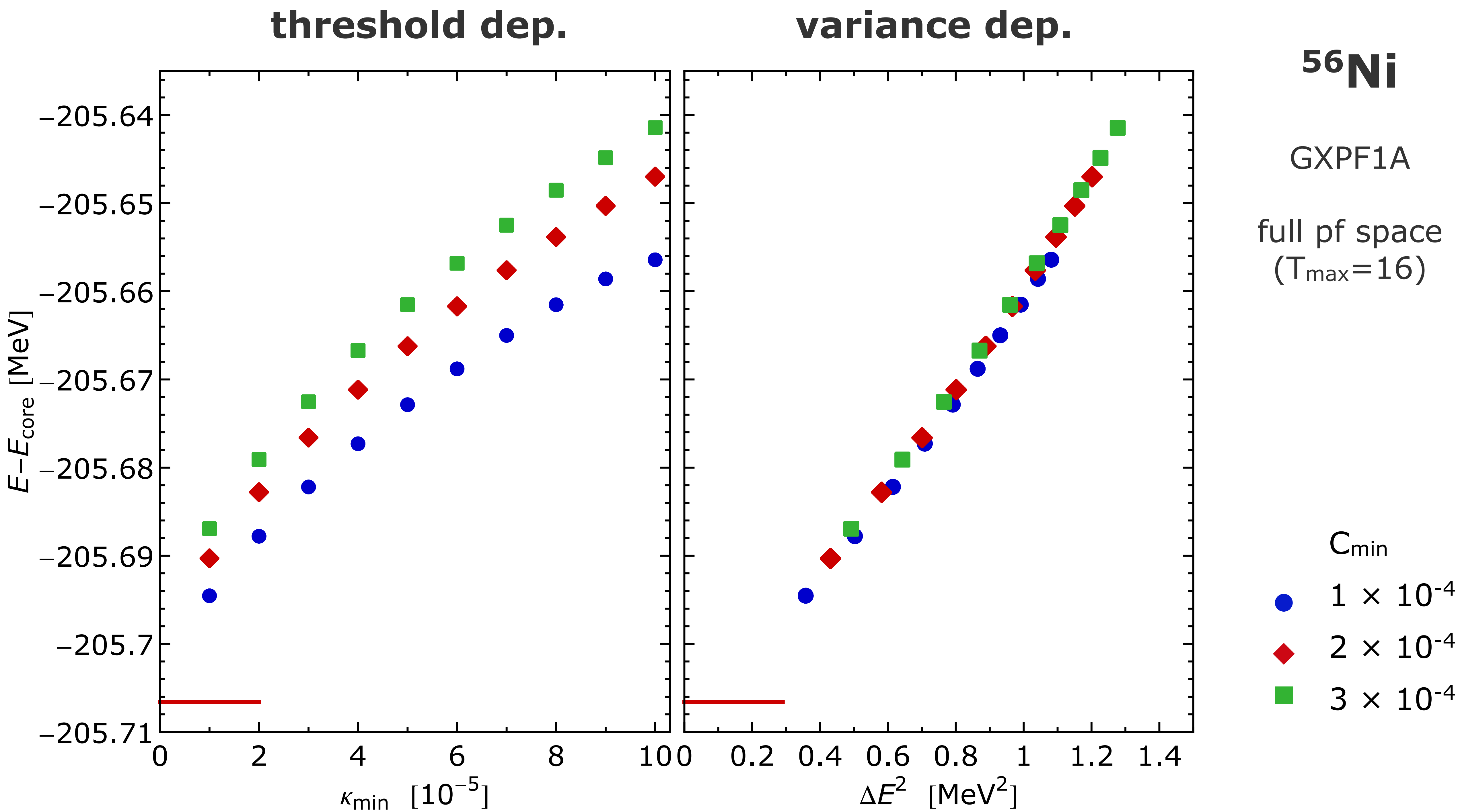
Mizusaki, Imada, PRC 67, 041301 (2003)

- evaluation of expectation value of H^2 is expensive…
  - NCSM: insert completeness relation for full N_{max} space
  - SM: compute valence-space matrix elements of H^2 explicitly (up to 4B)

- was explored in NCSM and is applied routinely in MCSM calculations

Zhan, Nogga, et al., PRC 69, 034302 (2004)
Shimizu, Abe, et al., Prog. Theo. Exp. Physics 2012, 01A205 (2012)

^{56}Ni: Threshold vs. Variance

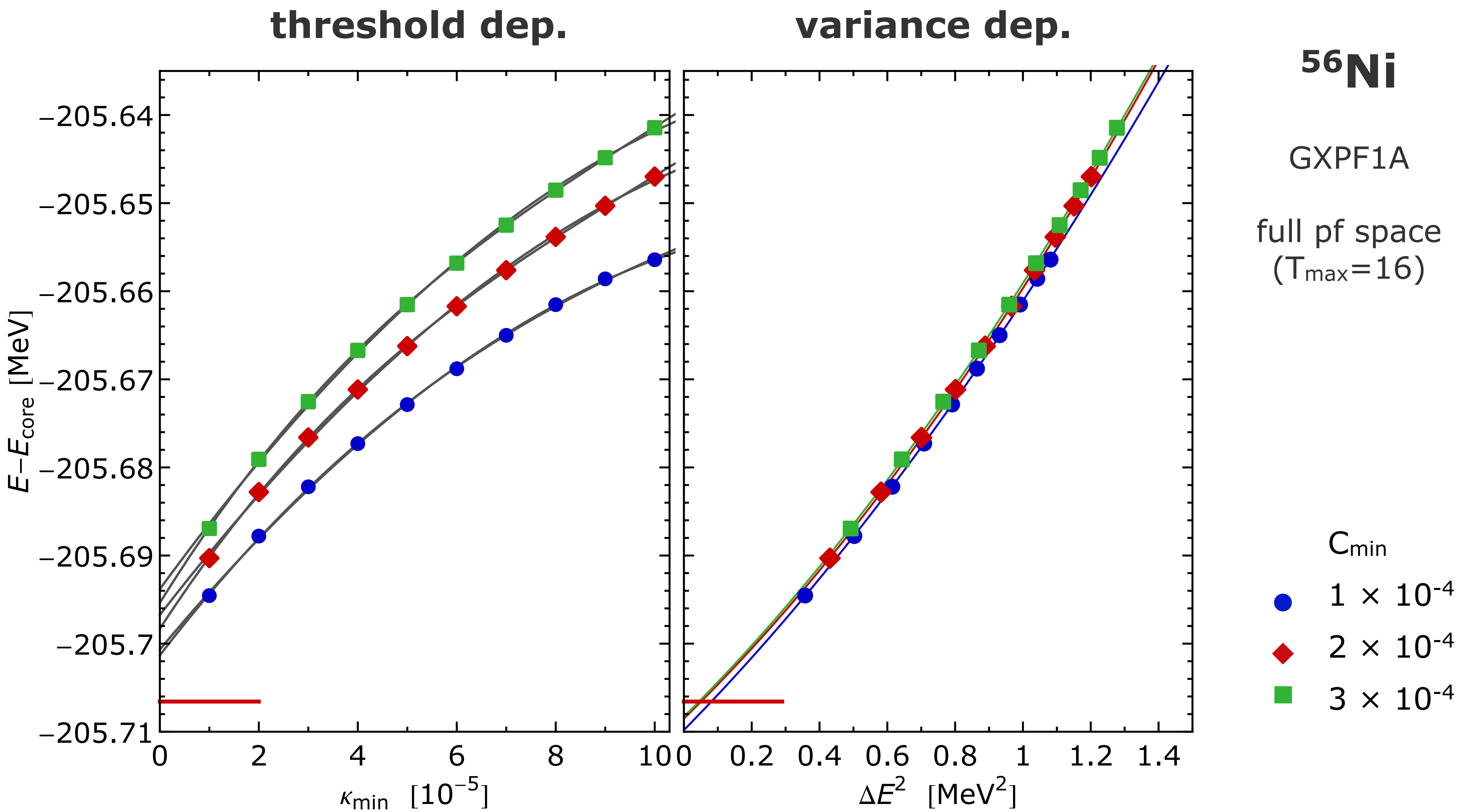


^{56}Ni

GXPF1A

full pf space (T_{max}=16)

^{56}Ni: Threshold vs. Variance

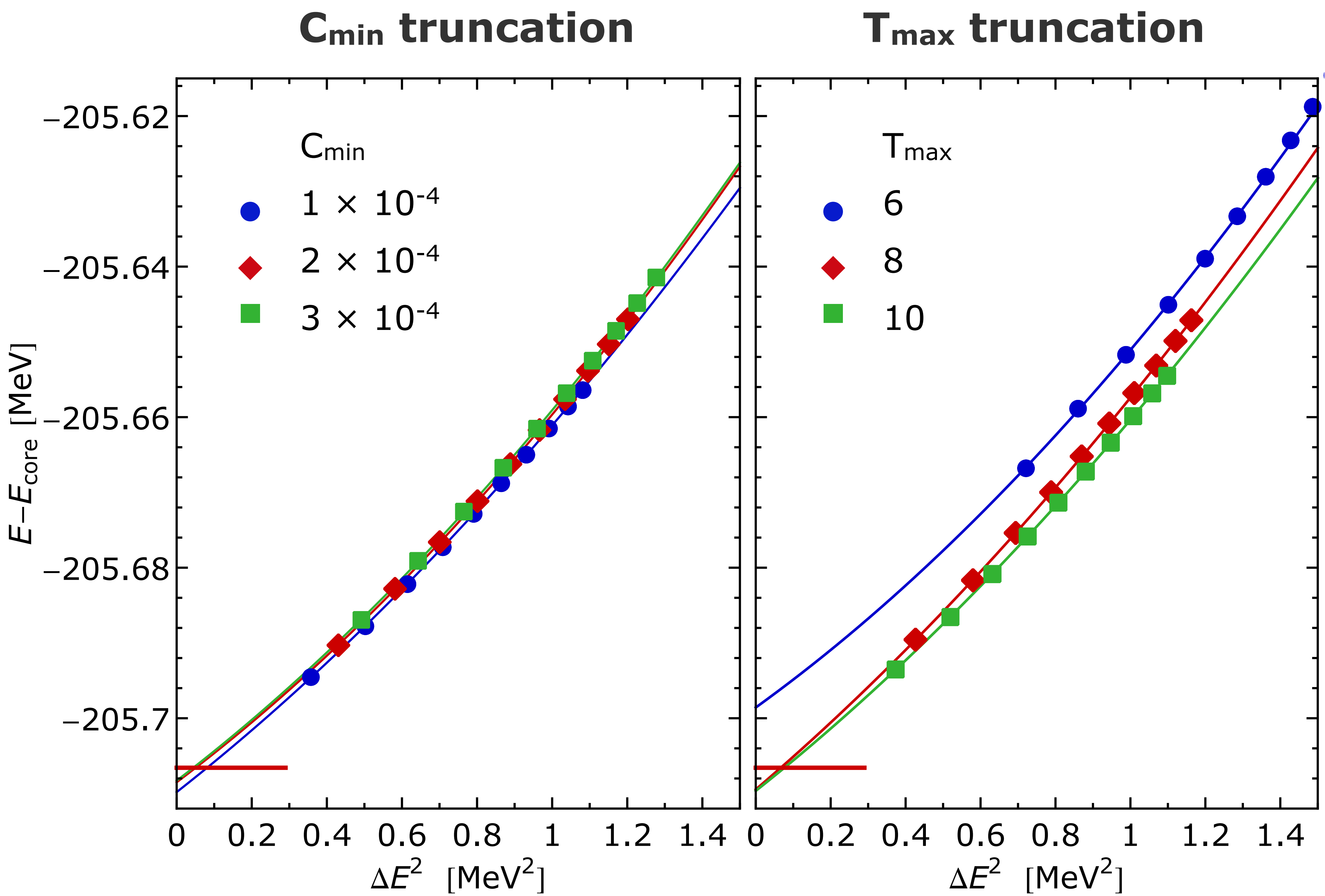


^{56}Ni

GXPF1A

full pf space
(T_{max}=16)

^{56}Ni: Variance with T_{max} Truncation

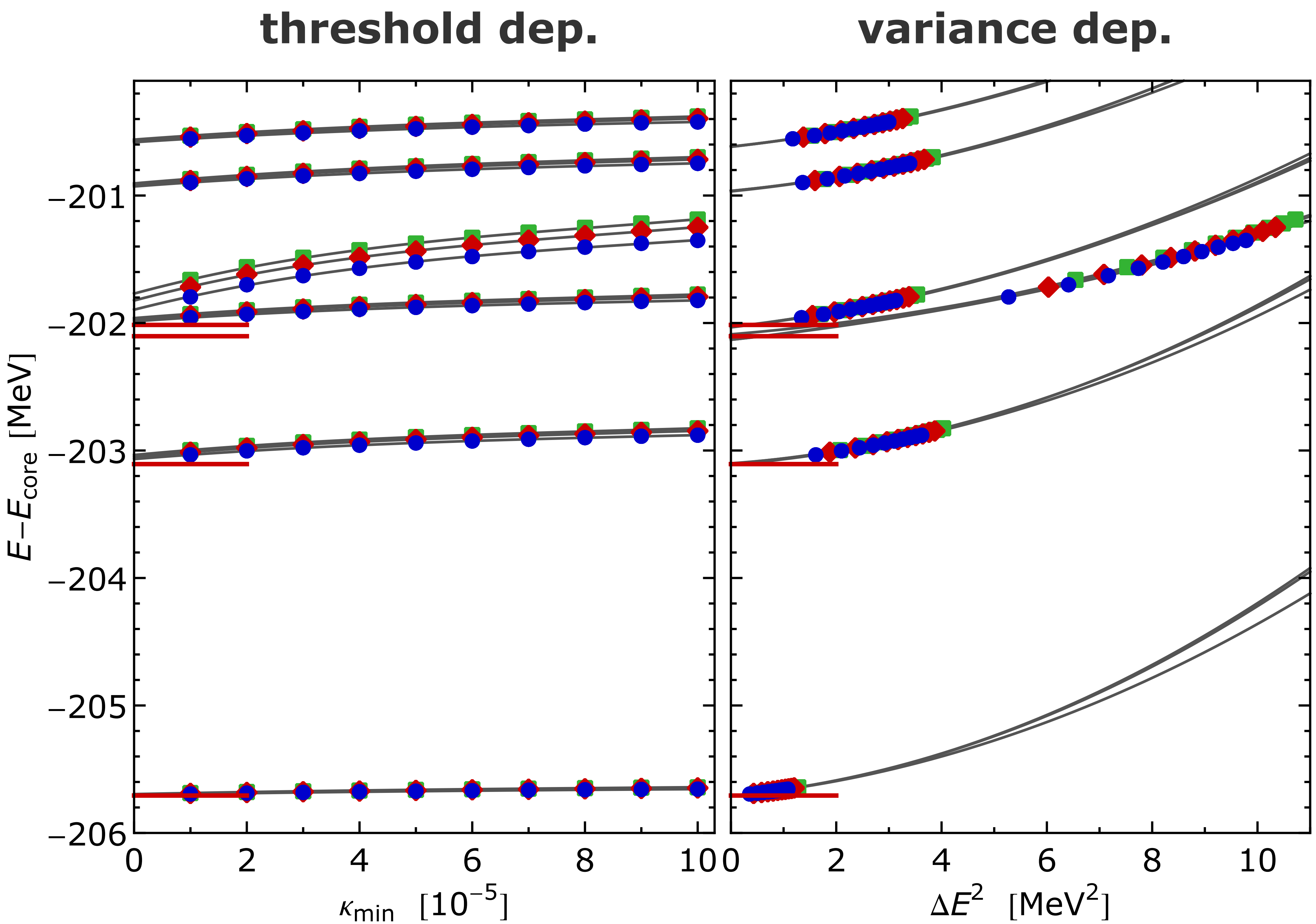


^{56}Ni

GXPF1A

pf space

^{56}Ni: Excitation Spectrum



^{56}Ni

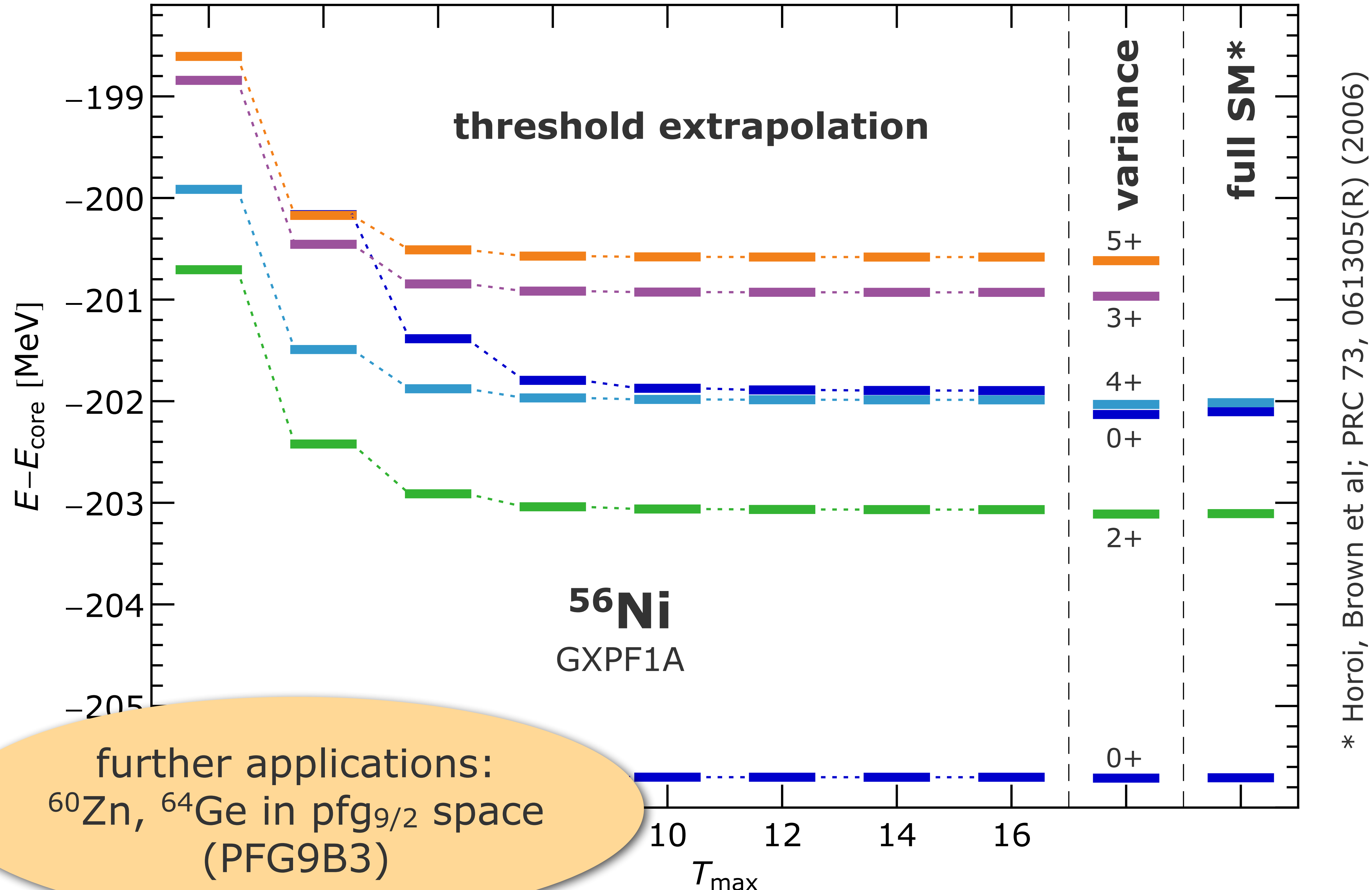
GXPF1A

full pf space (T_{max}=16)

C_{min}

- 1×10^{-4}
- 2×10^{-4}
- 3×10^{-4}

^{56}Ni: Excitation Spectrum



further applications:
^{60}Zn, ^{64}Ge in pfg$_{9/2}$ space
(PFG9B3)

Epilogue

- **thanks to my group and my collaborators**
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