Advances in Ab Initio Nuclear Structure Theory

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Ab Initio Nuclear Structure Theory

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

Interactions

- chiral effective field theory for nuclear interactions (NN+3N+...) and electroweak operators
- physics-conserving unitary transformation to adapt Hamiltonian to finite low-energy model spaces

Many-Body Method

- solve many-body Schrödinger equation numerically using only controlled truncations
- range of powerful methods for different mass ranges employing the same interaction

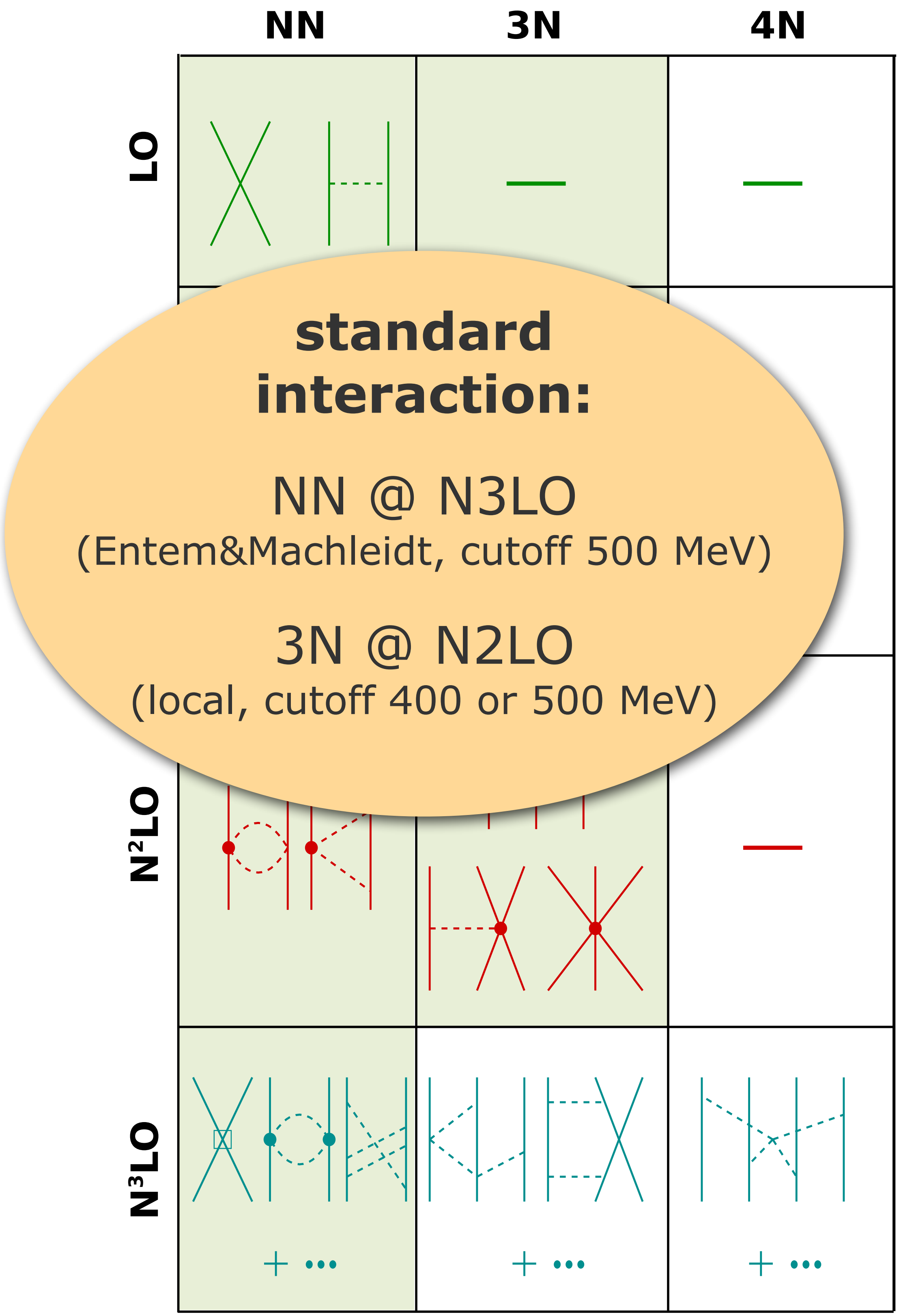
Quantification of Theory Uncertainties

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

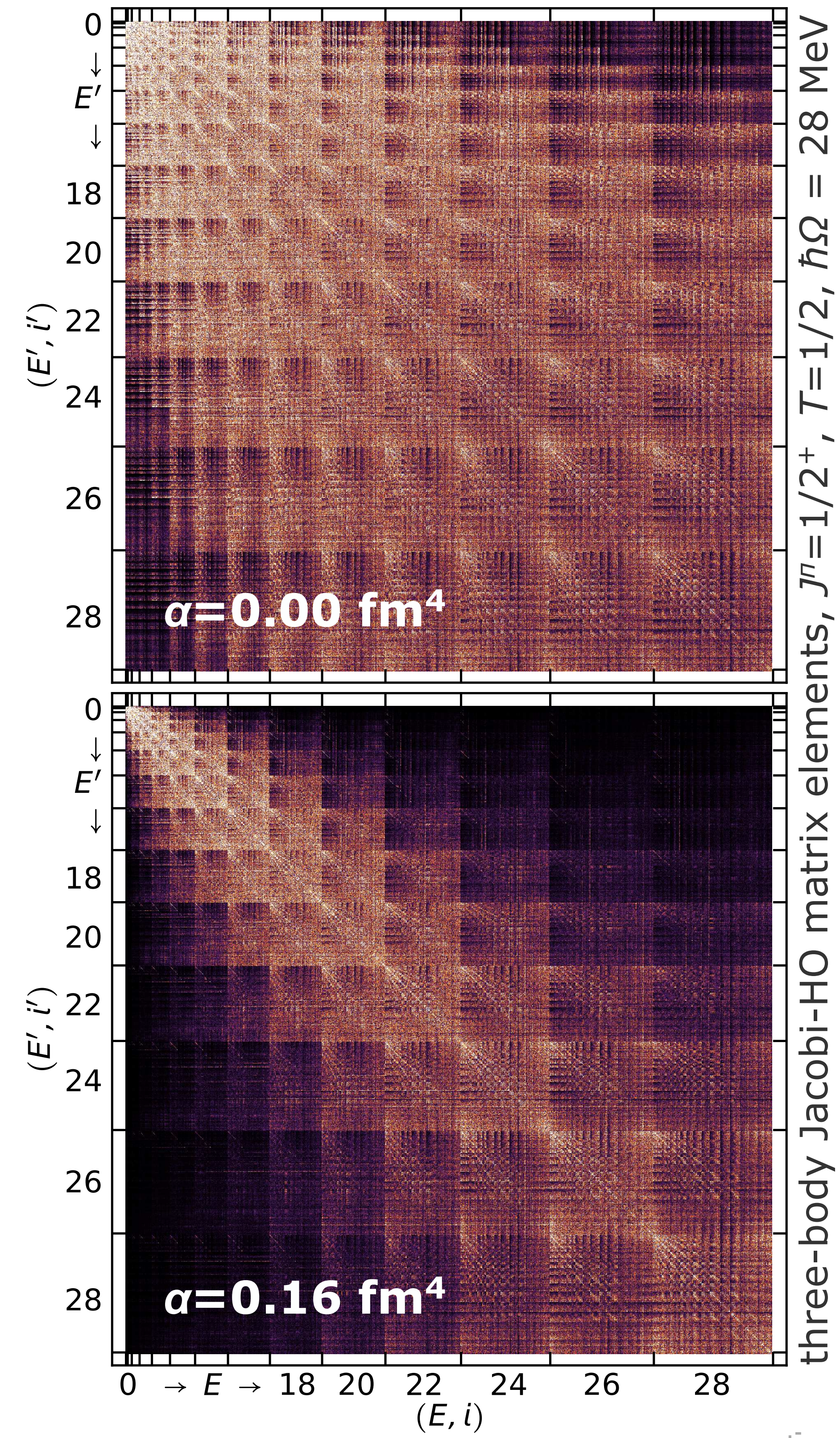
- unitary transformation via flow equation

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

- 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

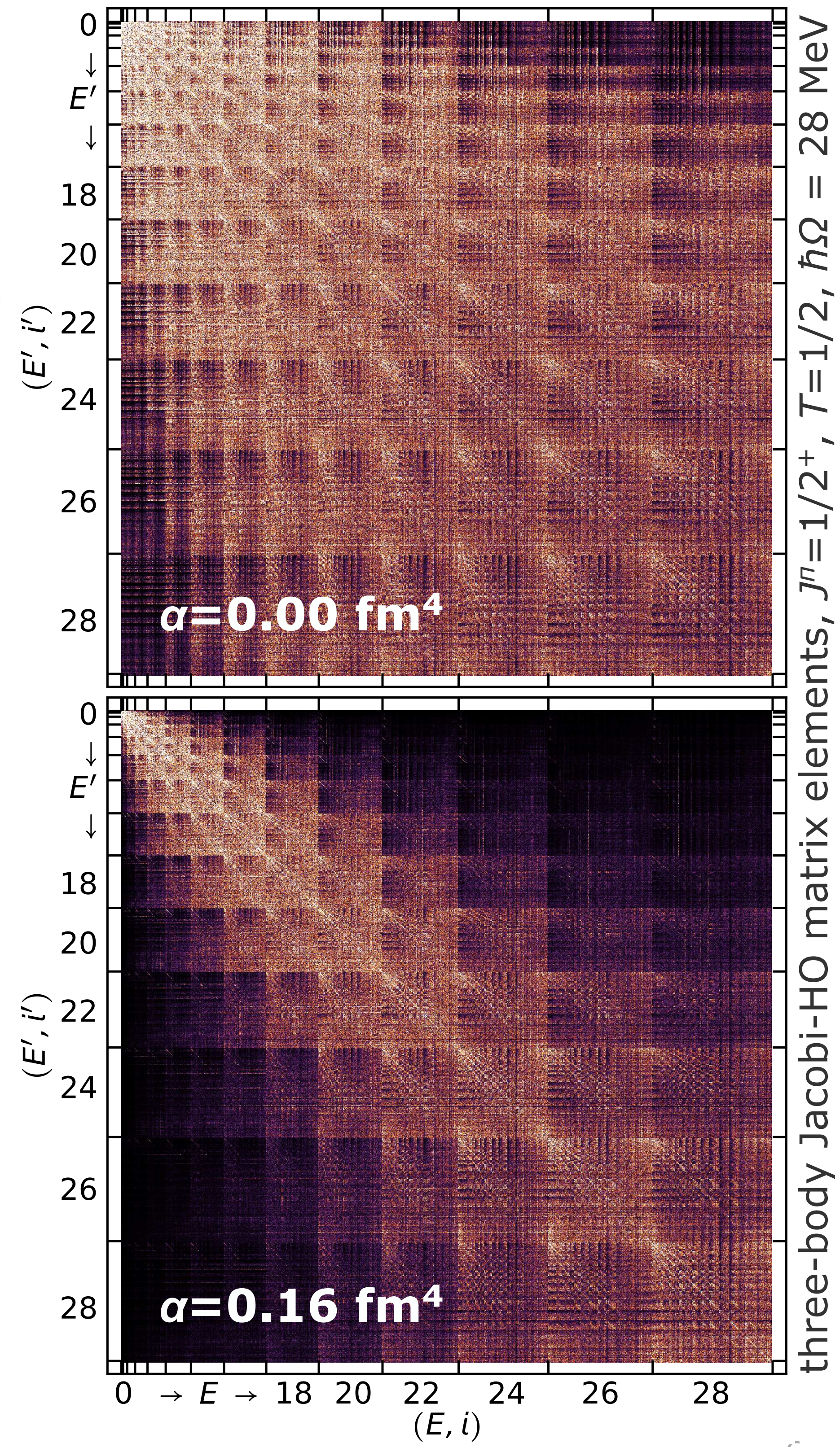
con:
induces many-body interactions

- 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**$_{\textbf{ind}}$
    use initial NN, keep evolved NN+3N
  - **NN+3N**$_{\textbf{full}}$
    use initial NN+3N, keep evolved NN+3N



Many-Body Methods I:

Light Nuclei

No-Core Shell Model & Friends

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

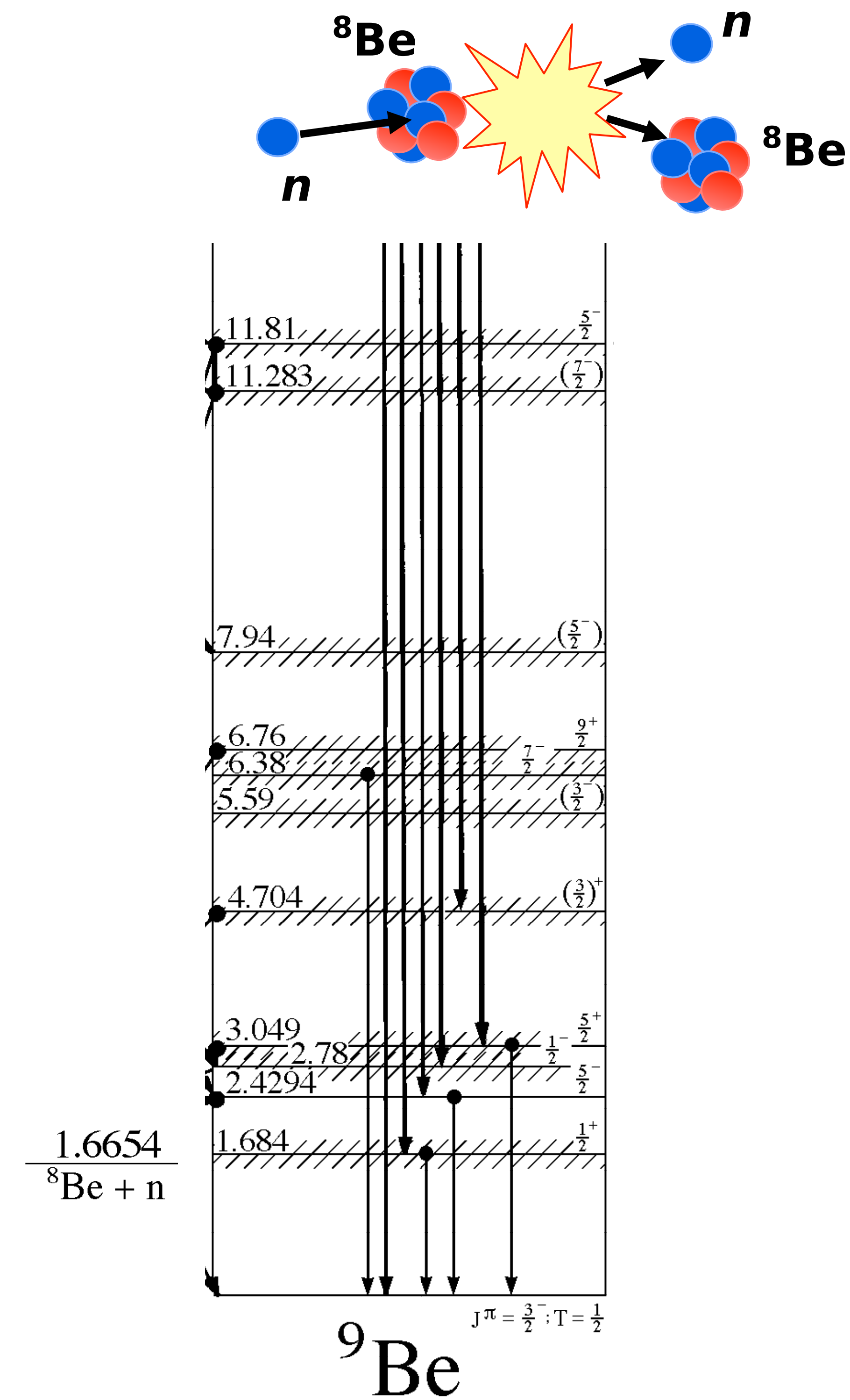
NCSM-type approaches are the
most powerful and universal ab initio methods for the
p- and lower sd-shell

- **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: Symplectic NCSM, Gamow NCSM,...

Spectrum of ^{9}Be

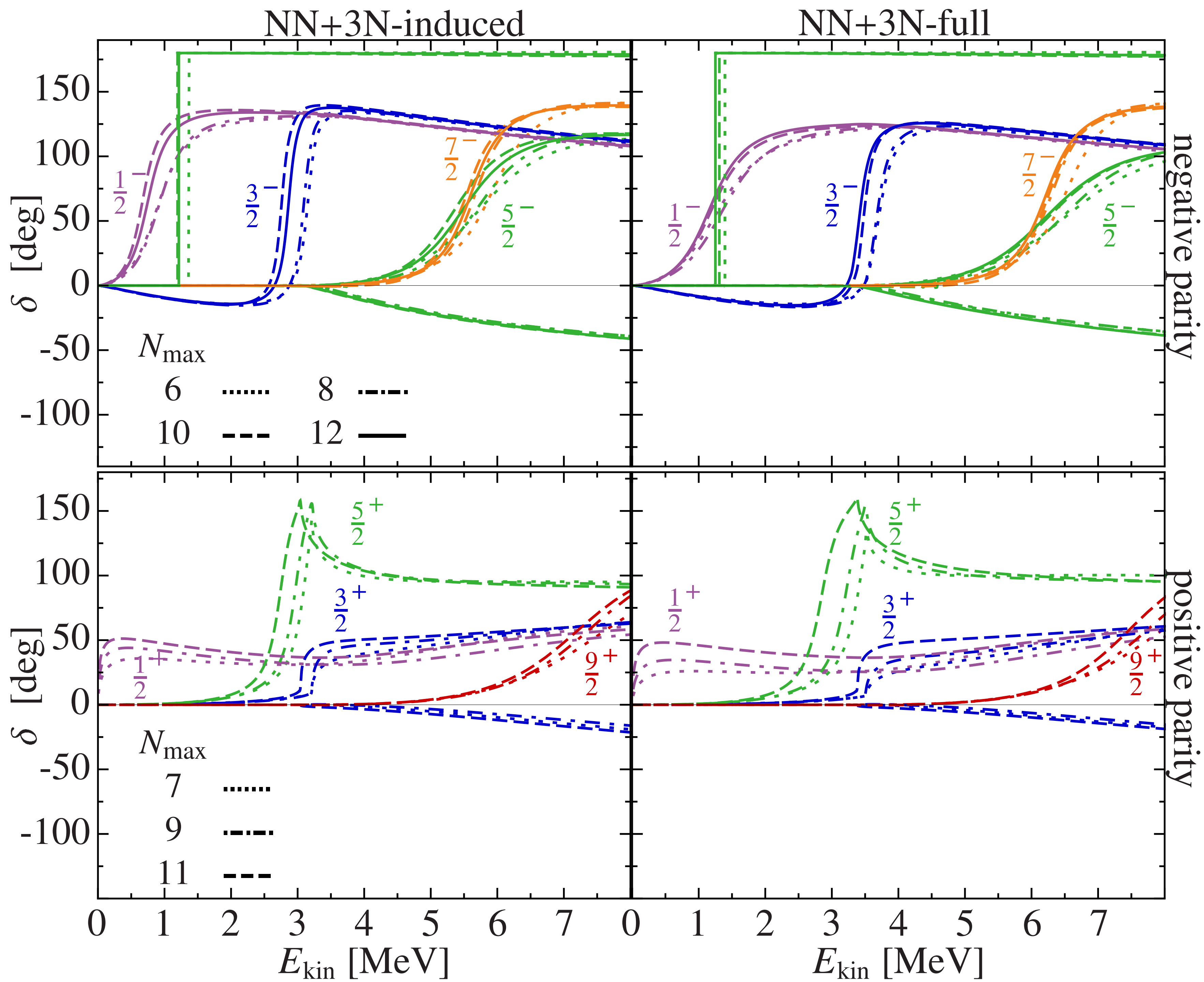
Langhammer et al.; PRC 91, 021301(R) (2015)

- ^{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)

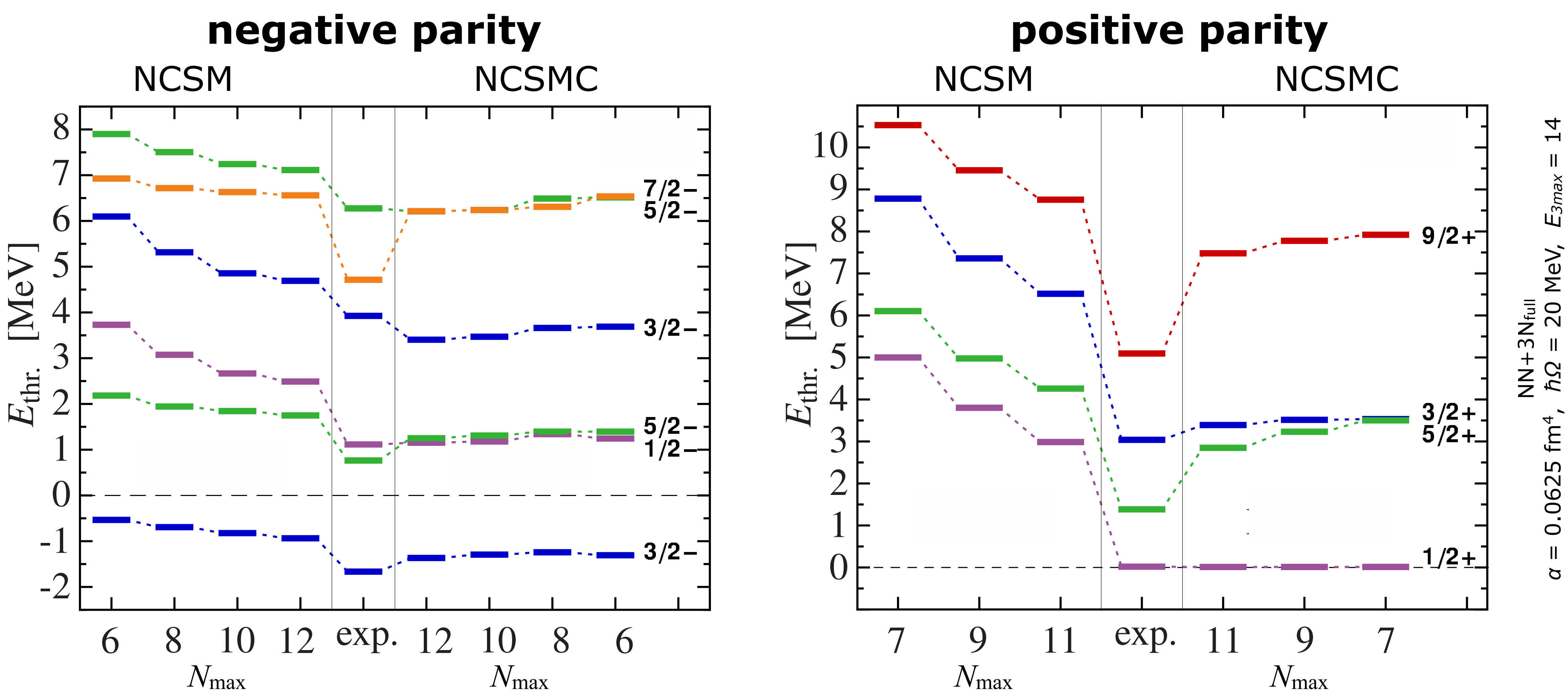


- negative parity phase-shifts are well converged, positive parity more difficult
- extract resonance parameters from inflection point and derivative

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

^{9}Be: NCSM vs. NCSMC

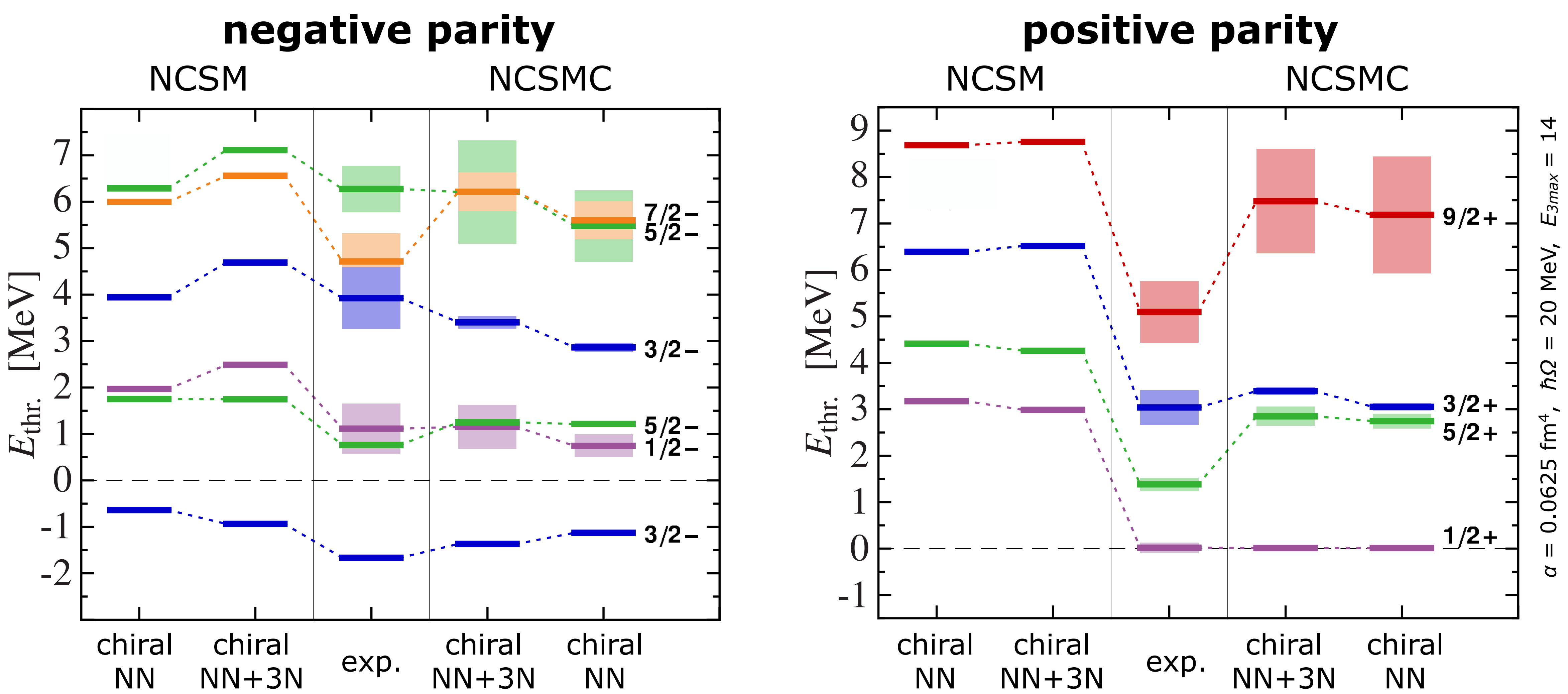
Langhammer et al.; PRC 91, 021301(R) (2015)



- 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

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)

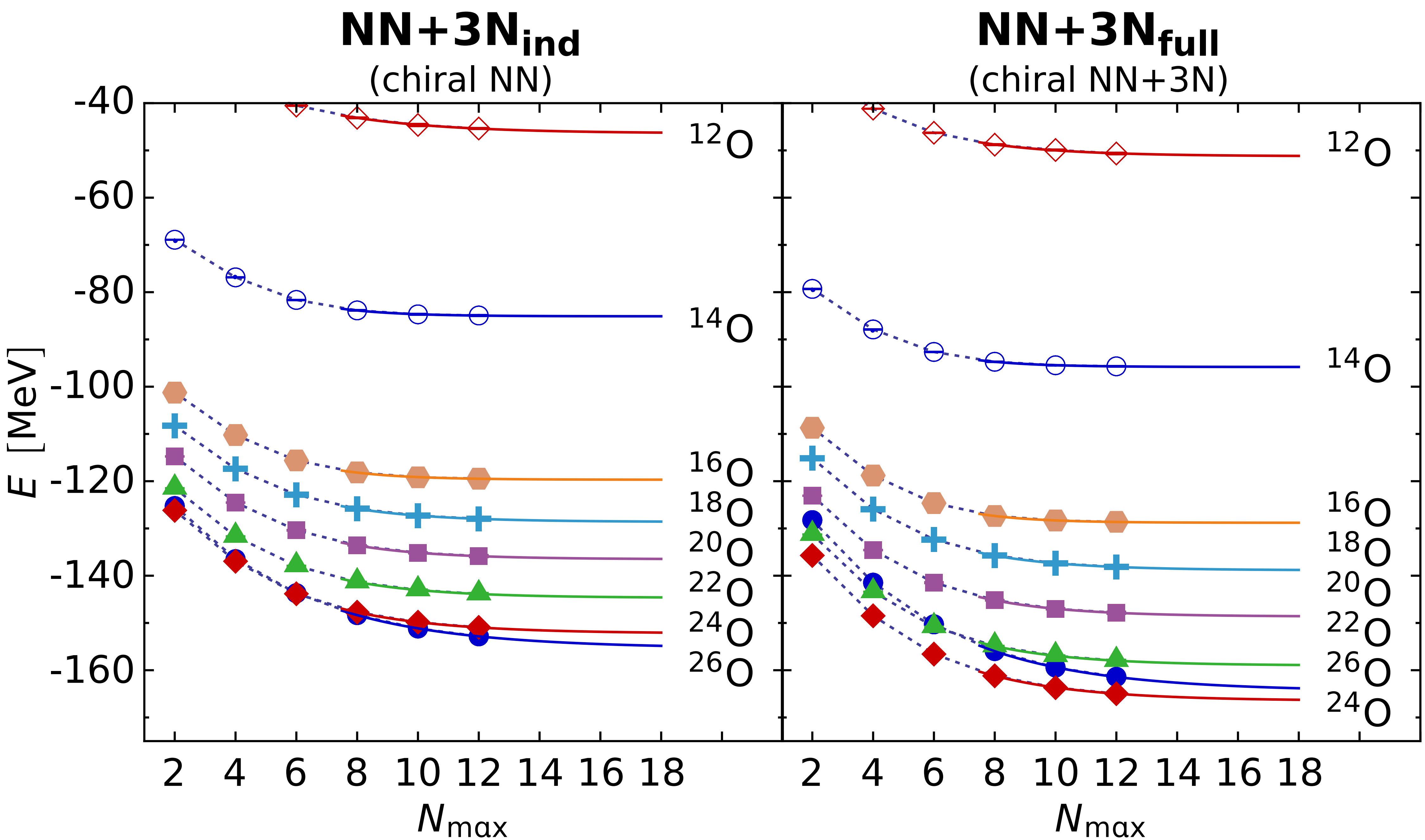
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

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

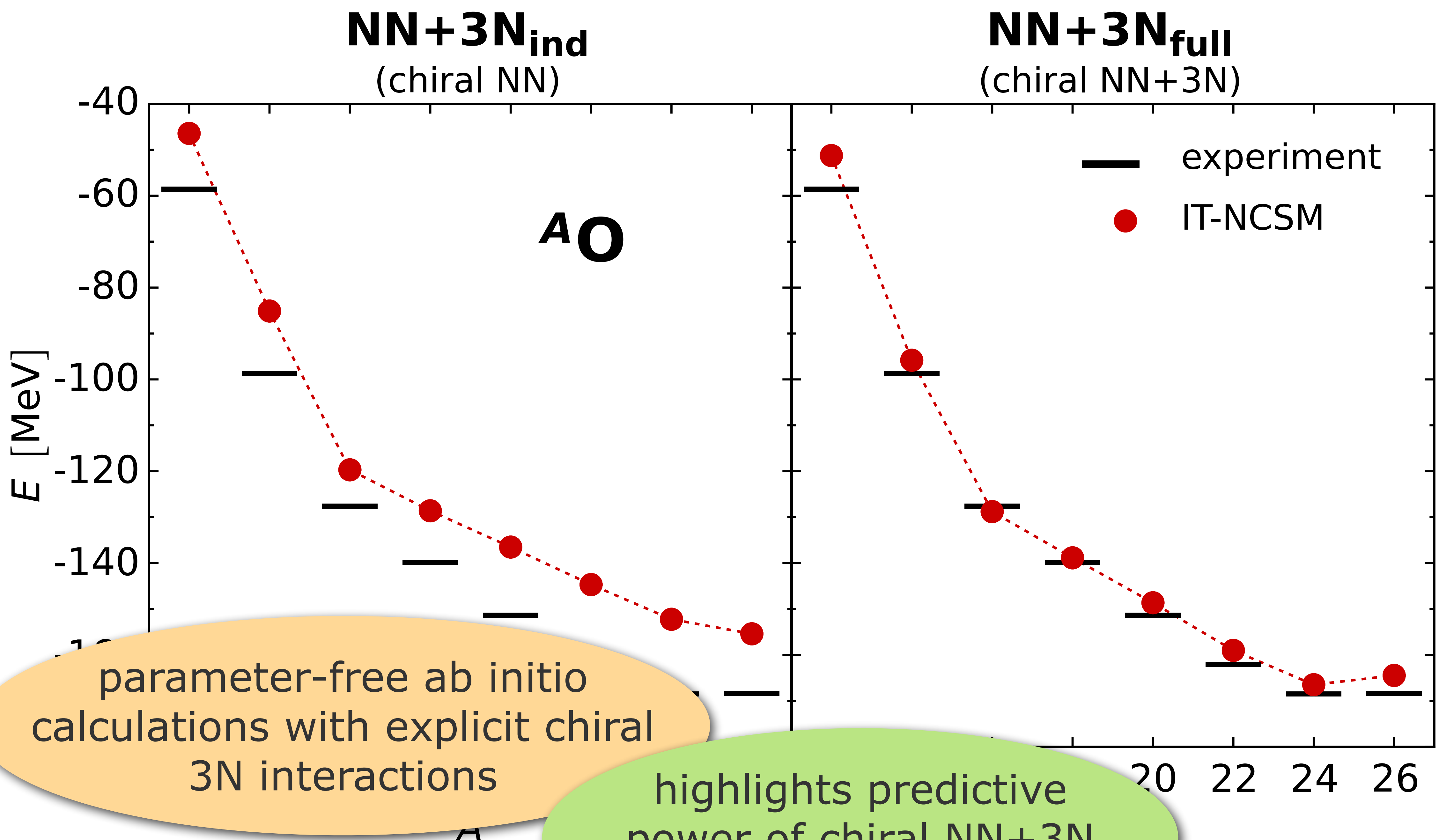
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



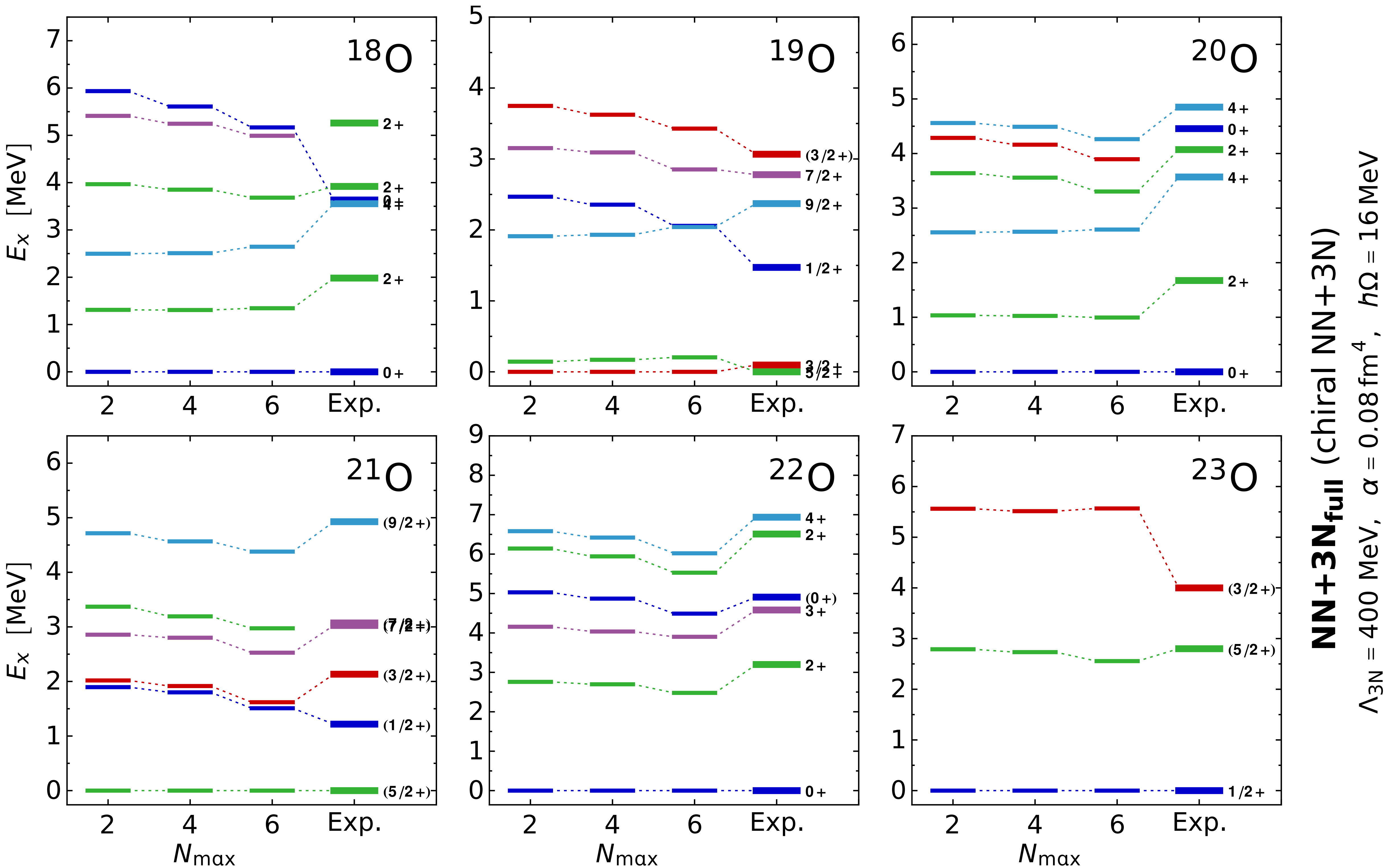
parameter-free ab initio calculations with explicit chiral 3N interactions

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.



Many-Body Methods II:

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 expone… 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
  - … …ground states; excitations via EOM or SM

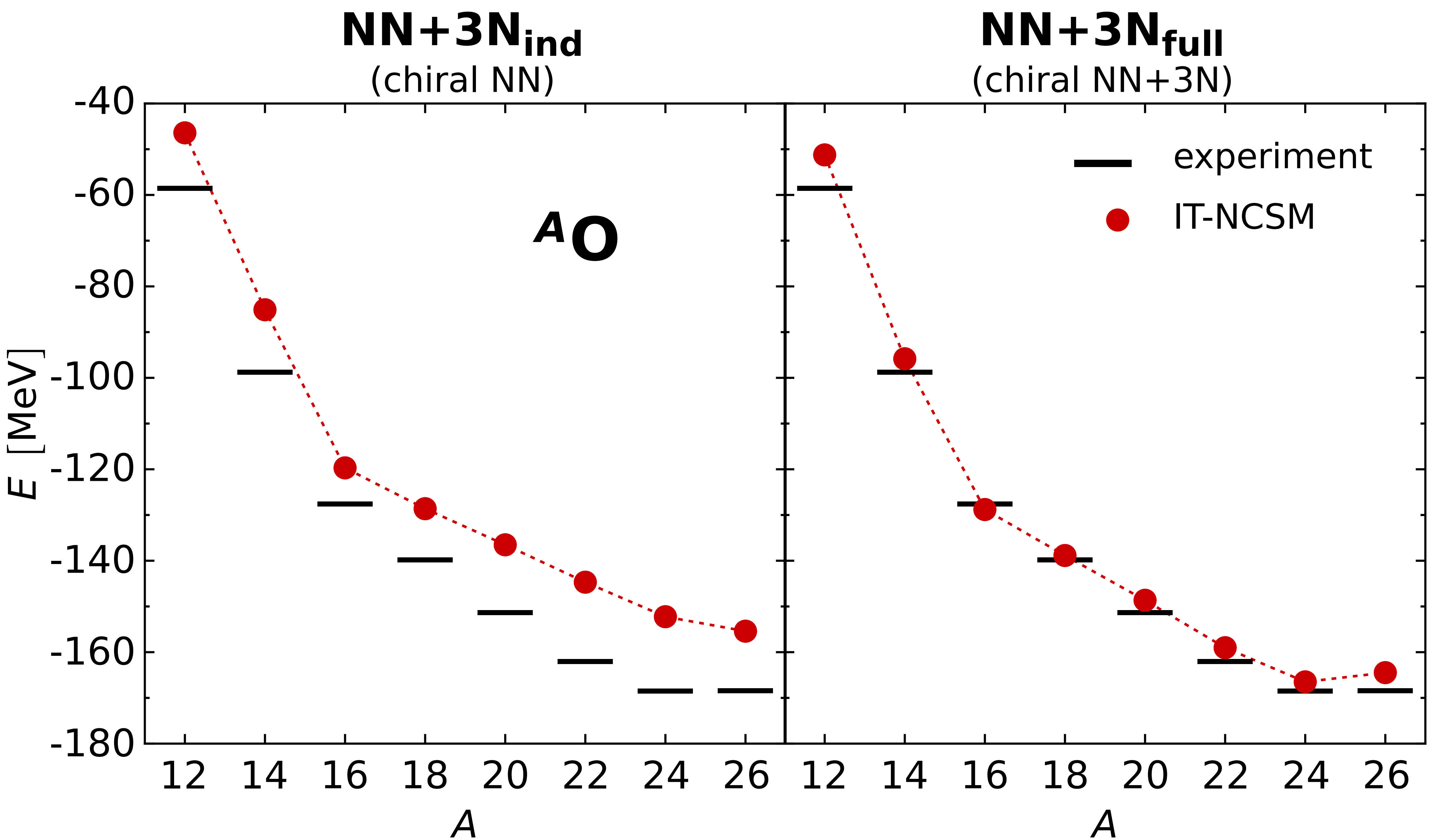
Barbieri, Soma, Duguet,...

- 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

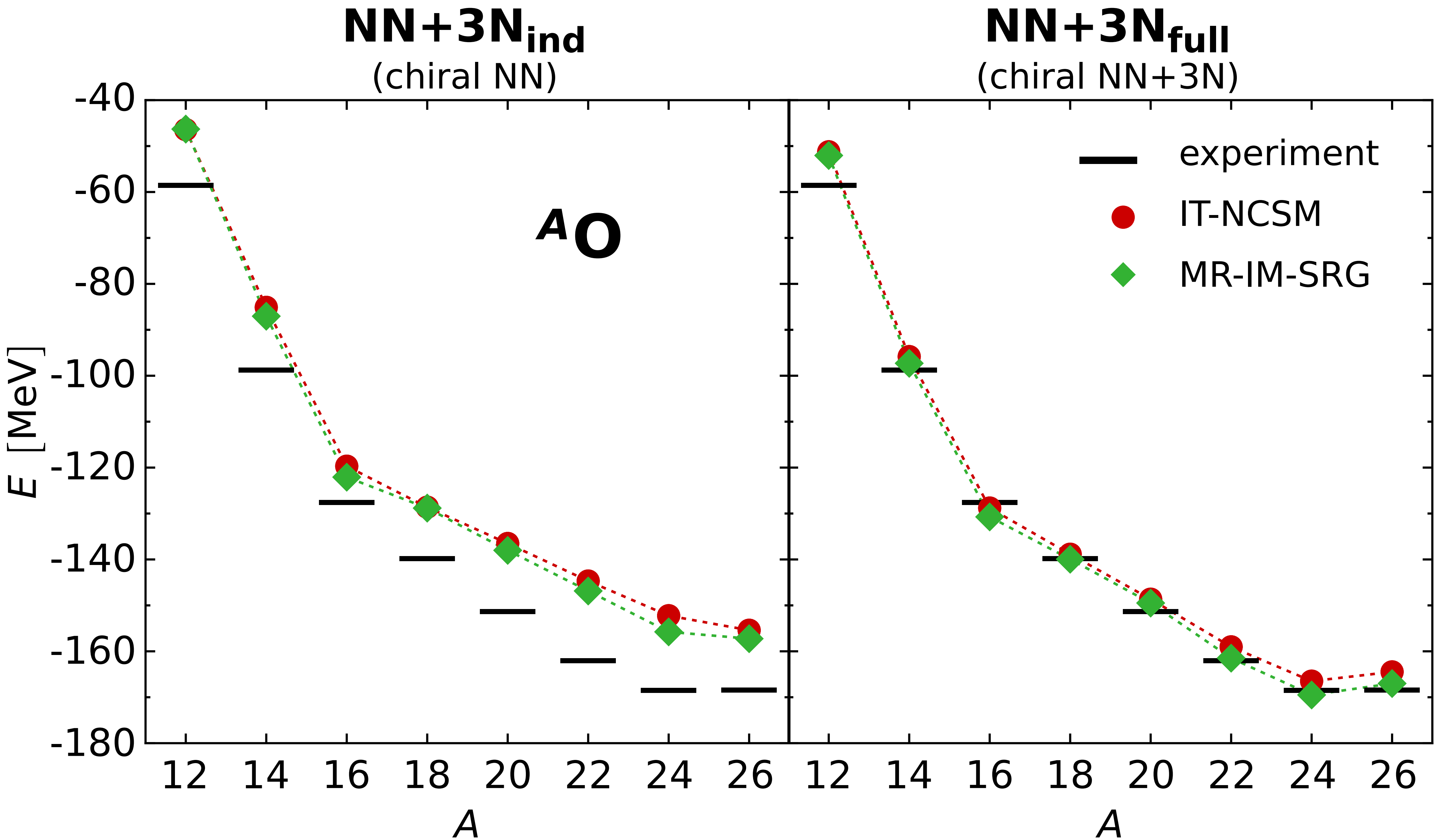
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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)



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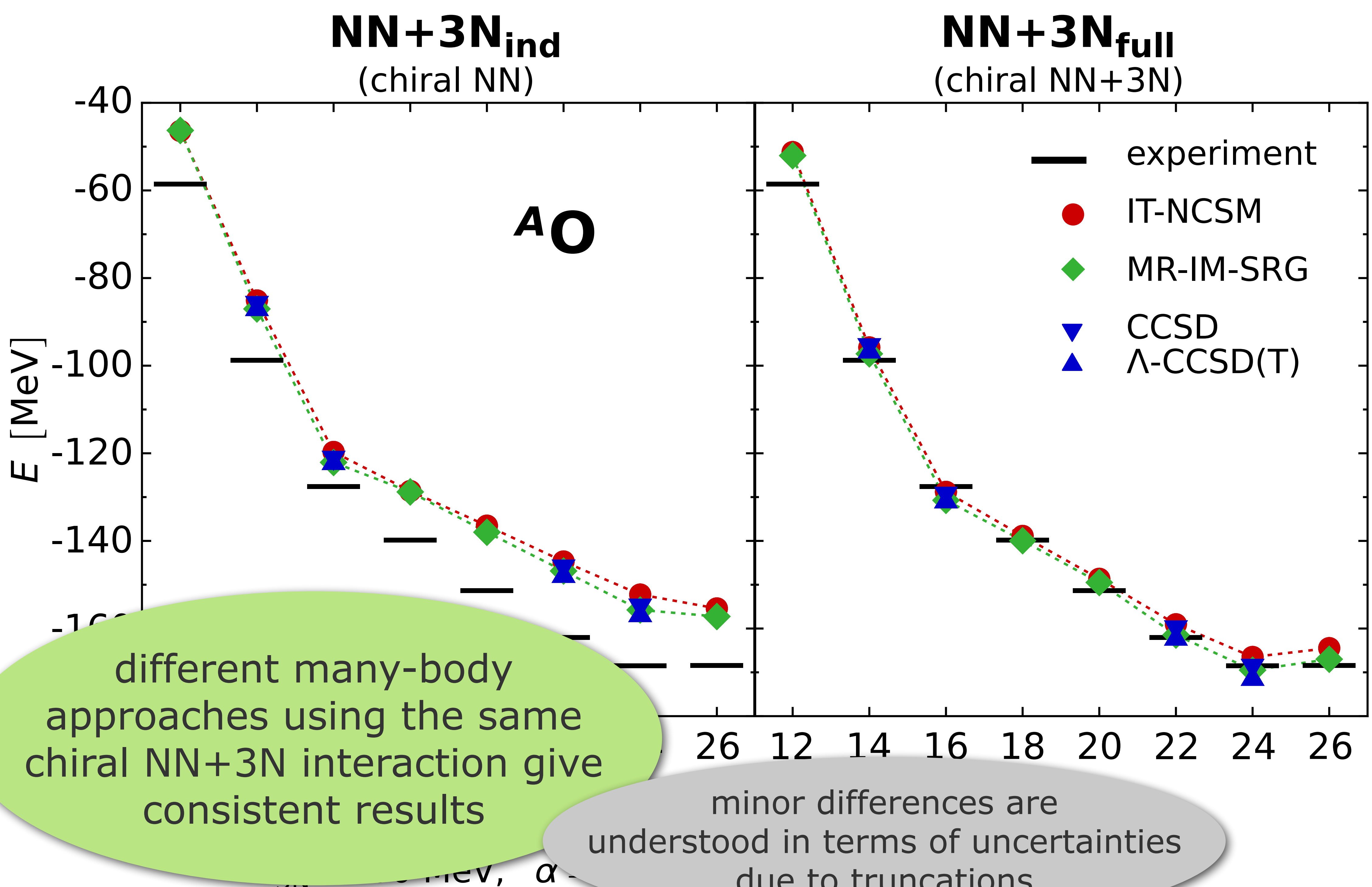
Ground States of Oxygen Isotopes

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

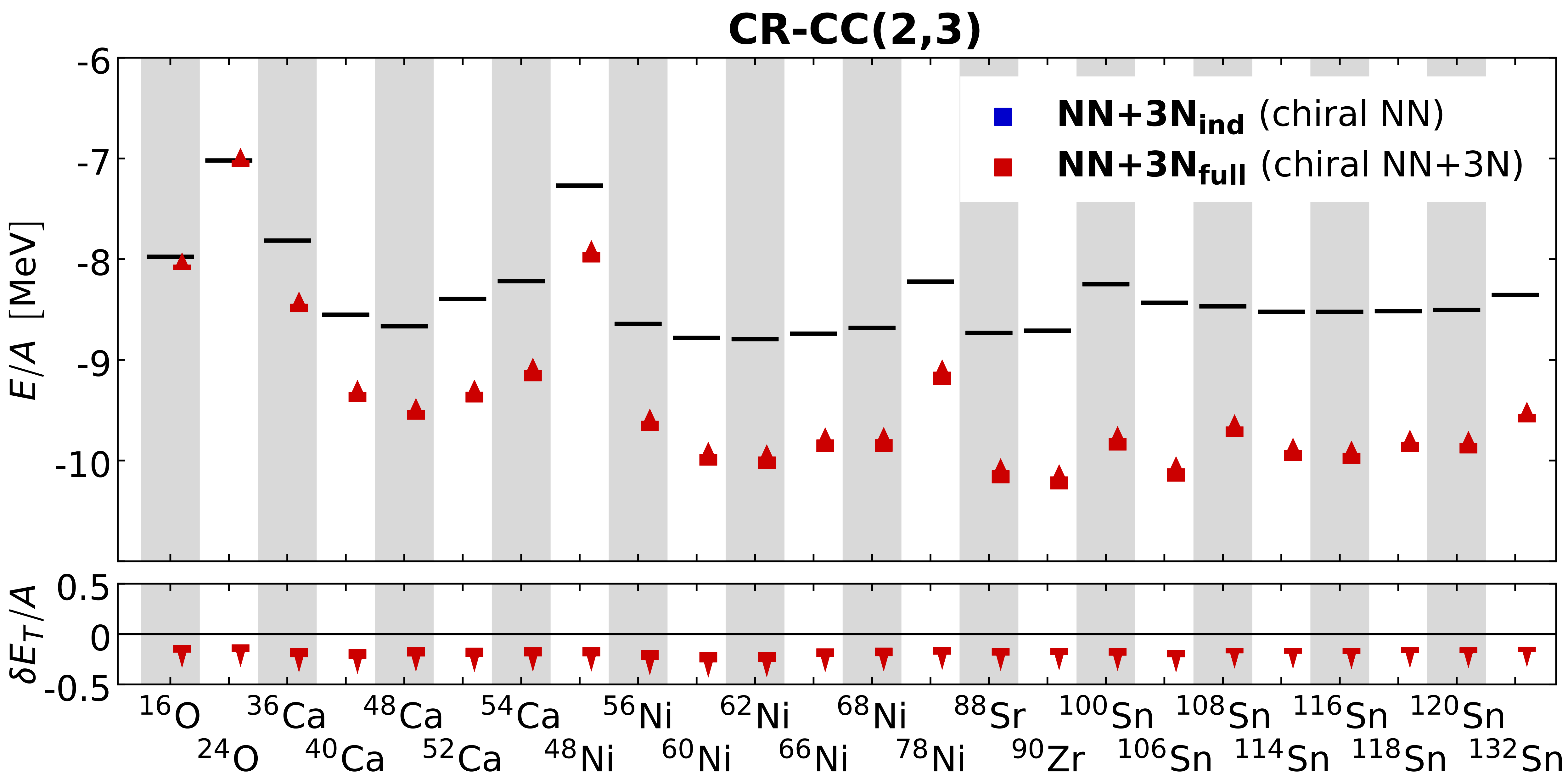


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Towards Heavy Nuclei - Ab Initio

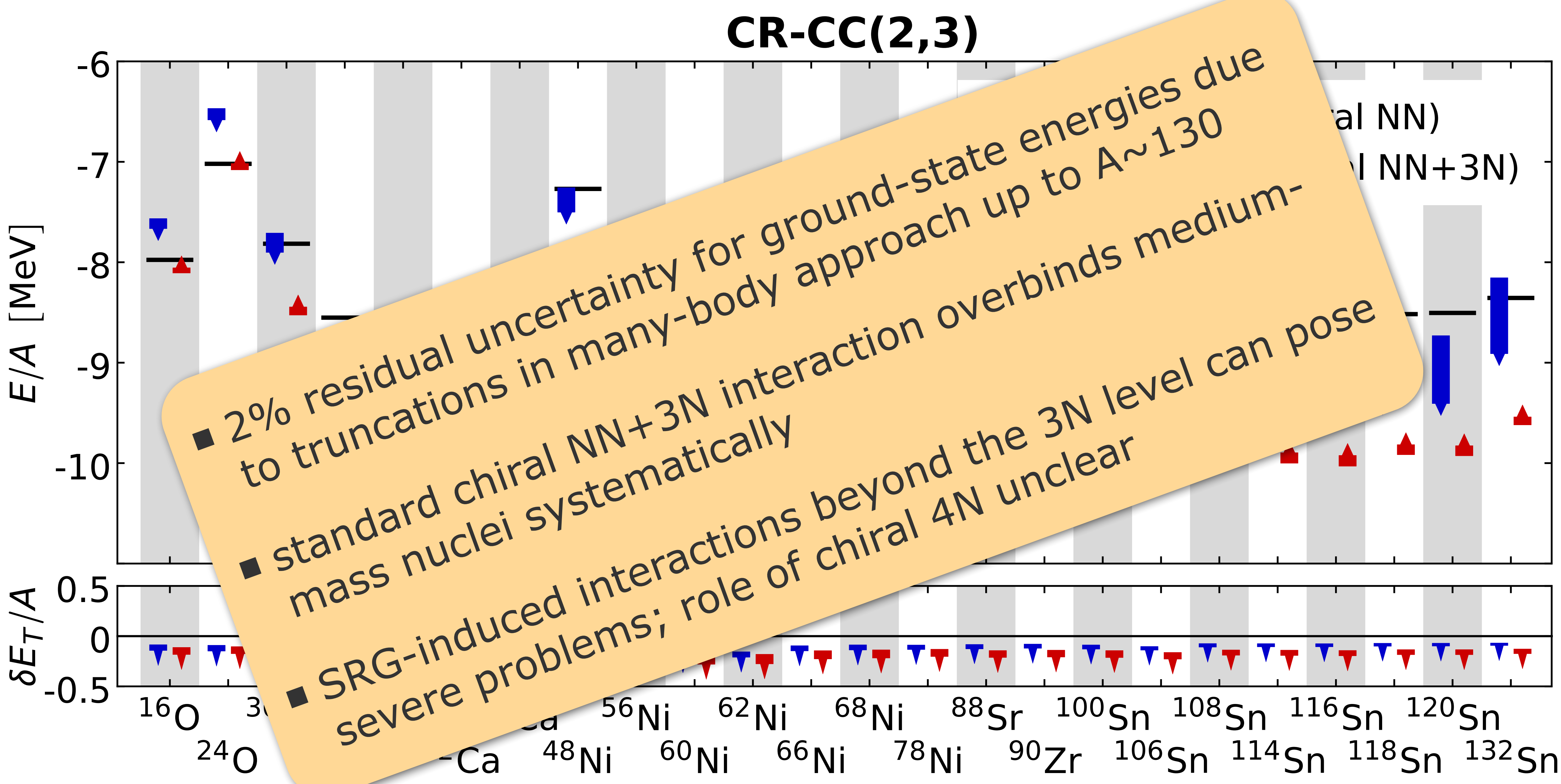
Binder et al., PLB 736, 119 (2014)



$\Lambda_{3N} = 400$ 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)

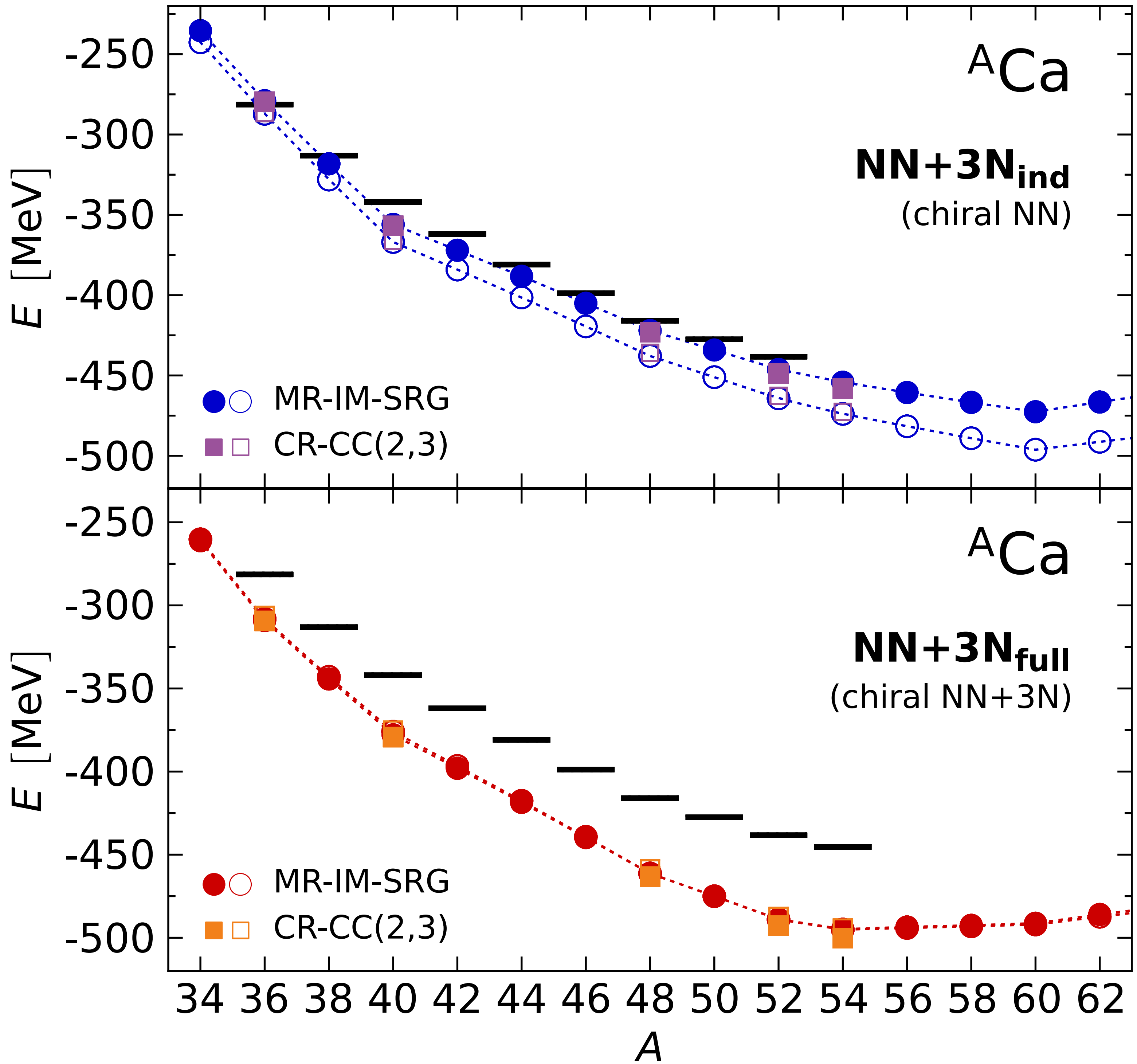


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

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

Open-Shell Medium-Mass Nuclei

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

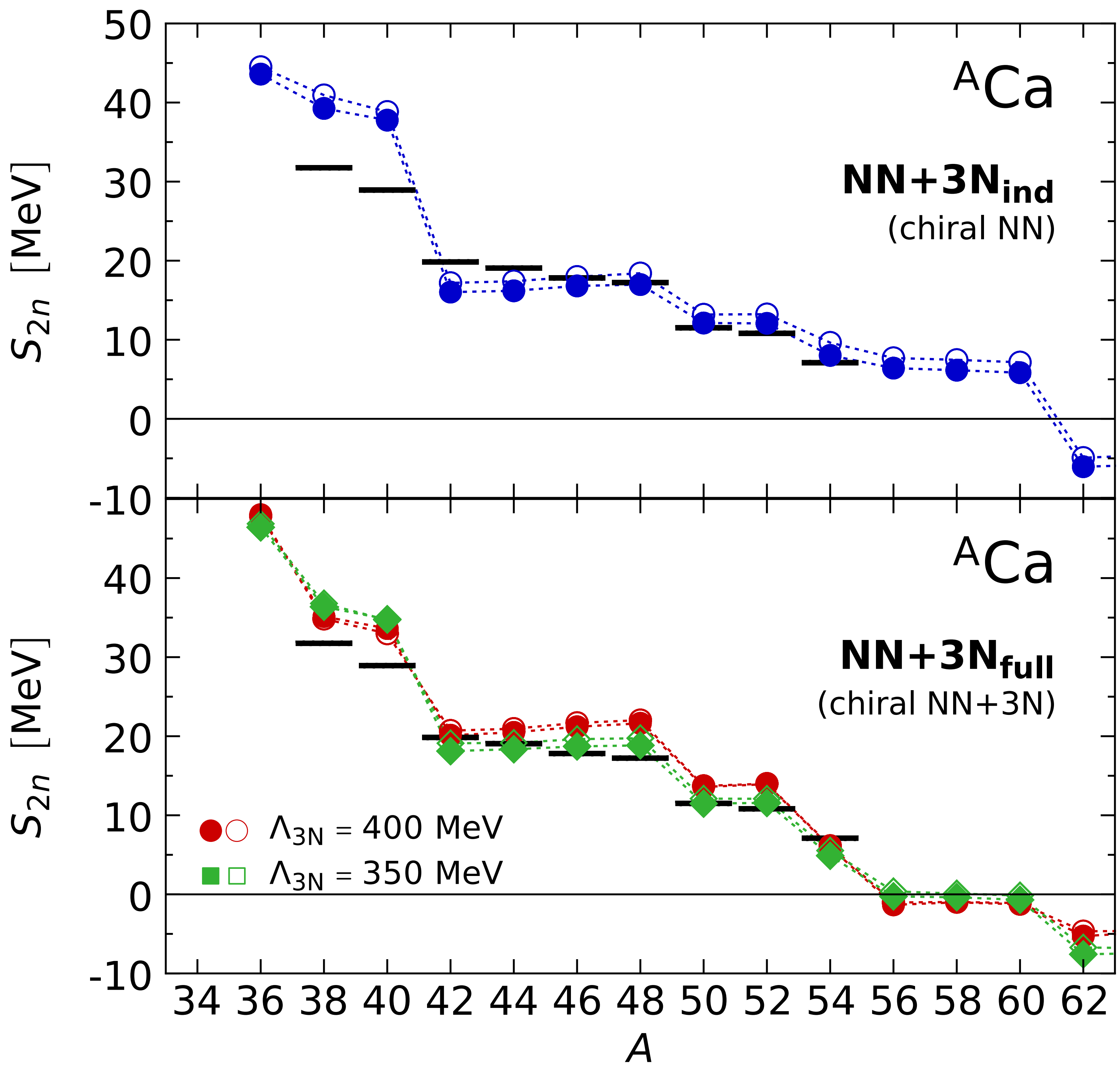


- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

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

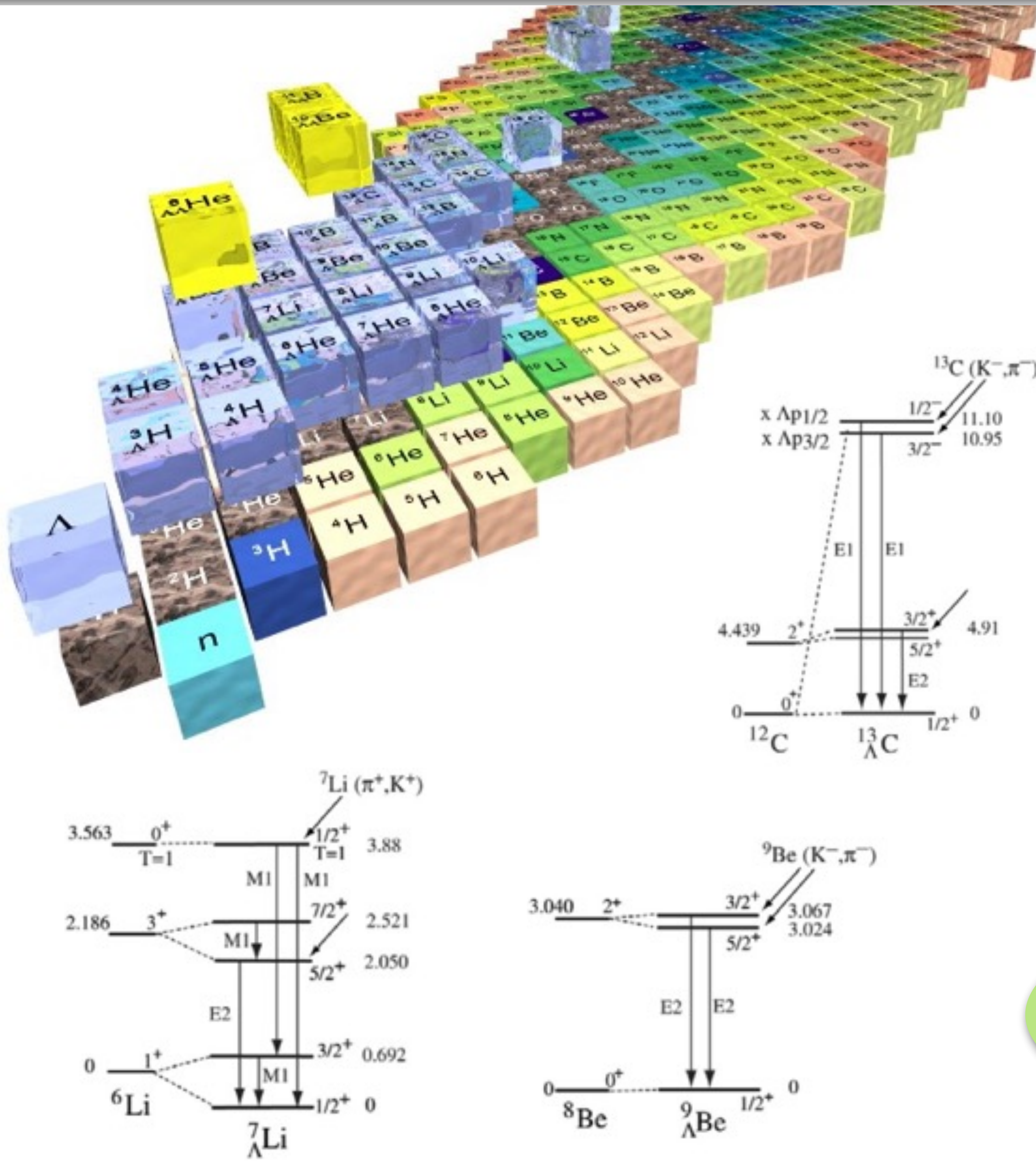
α = 0.04 fm^4 (○)
0.08 fm^4 (●)

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

Many-Body Methods III:

Hypernuclei

Ab Initio Hypernuclear Structure

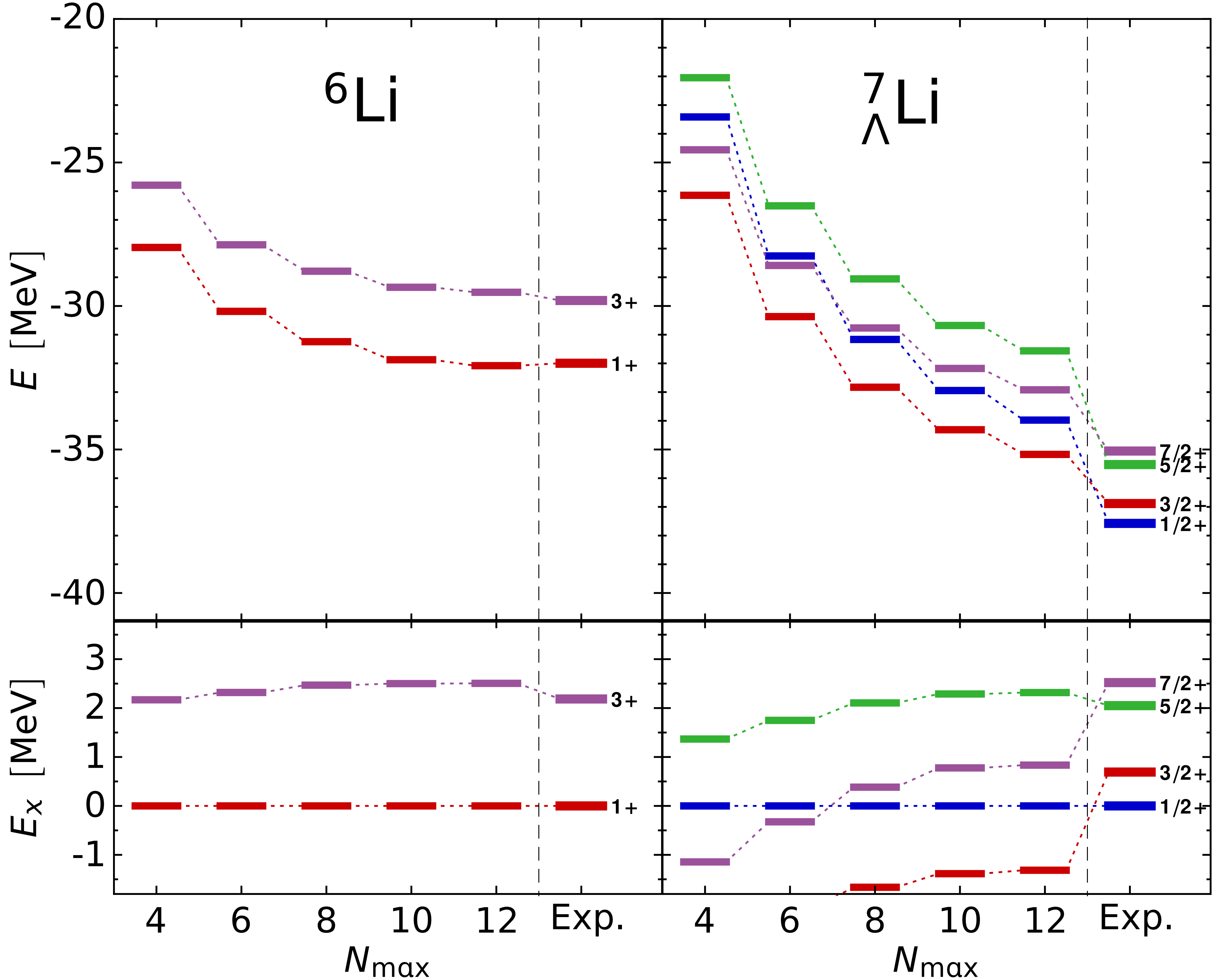


- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body ($A \lesssim 4$) and phenomenological shell or cluster model calculations so far
- chiral YN & YY interactions at (N)LO are available

time to transfer ab initio toolbox to hypernuclei

Application: $^{7}_{\Lambda}$Li

Wirth et al., PRL 113, 192502 (2014)



IT-NCSM

NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

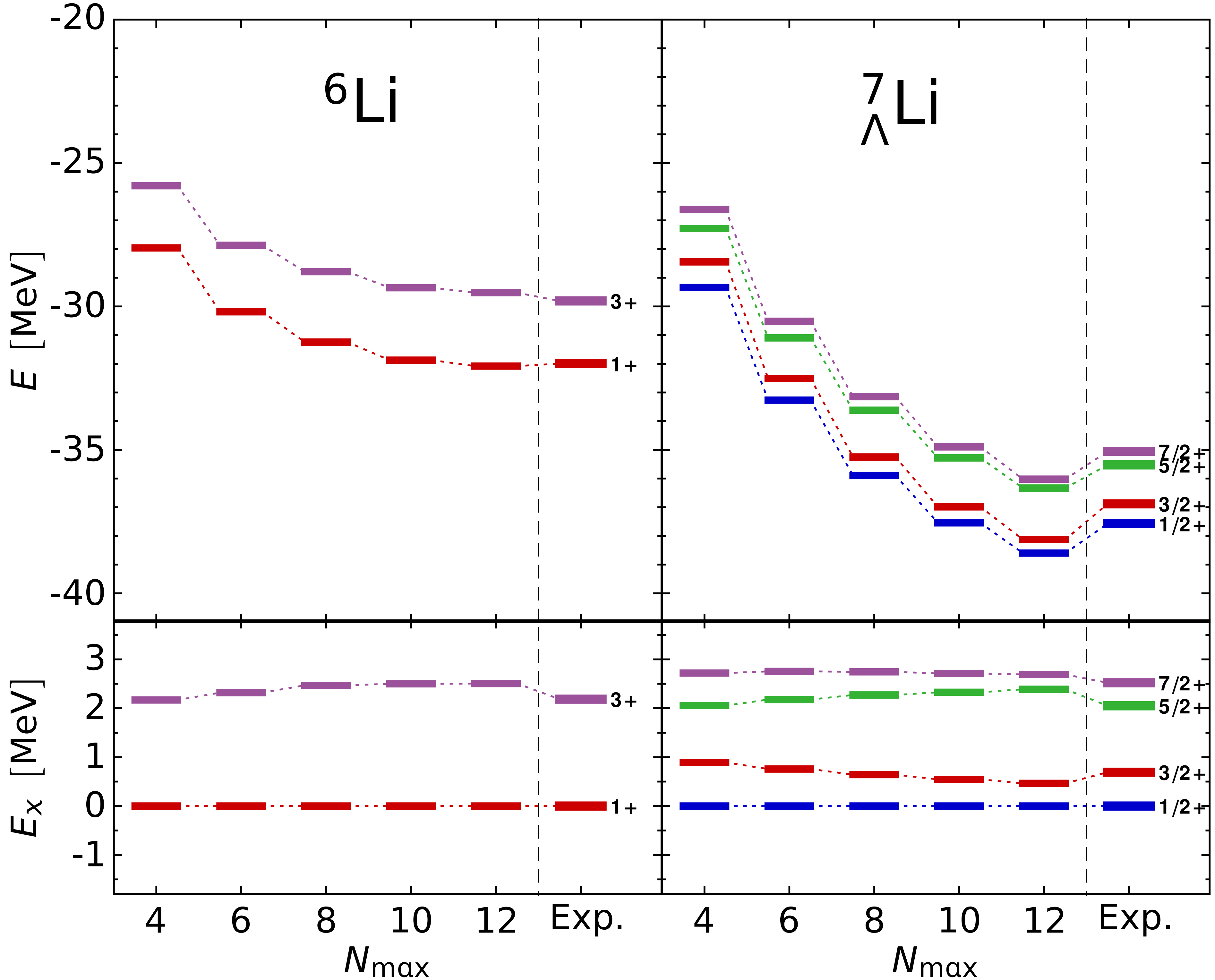
3N @ N2LO
Λ_{3N} = 500 MeV
Navratil
A = 3 fit

Jülich'04
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

Application: ${}^{7}_{\Lambda}$Li

Wirth et al., PRL 113, 192502 (2014)



IT-NCSM

NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

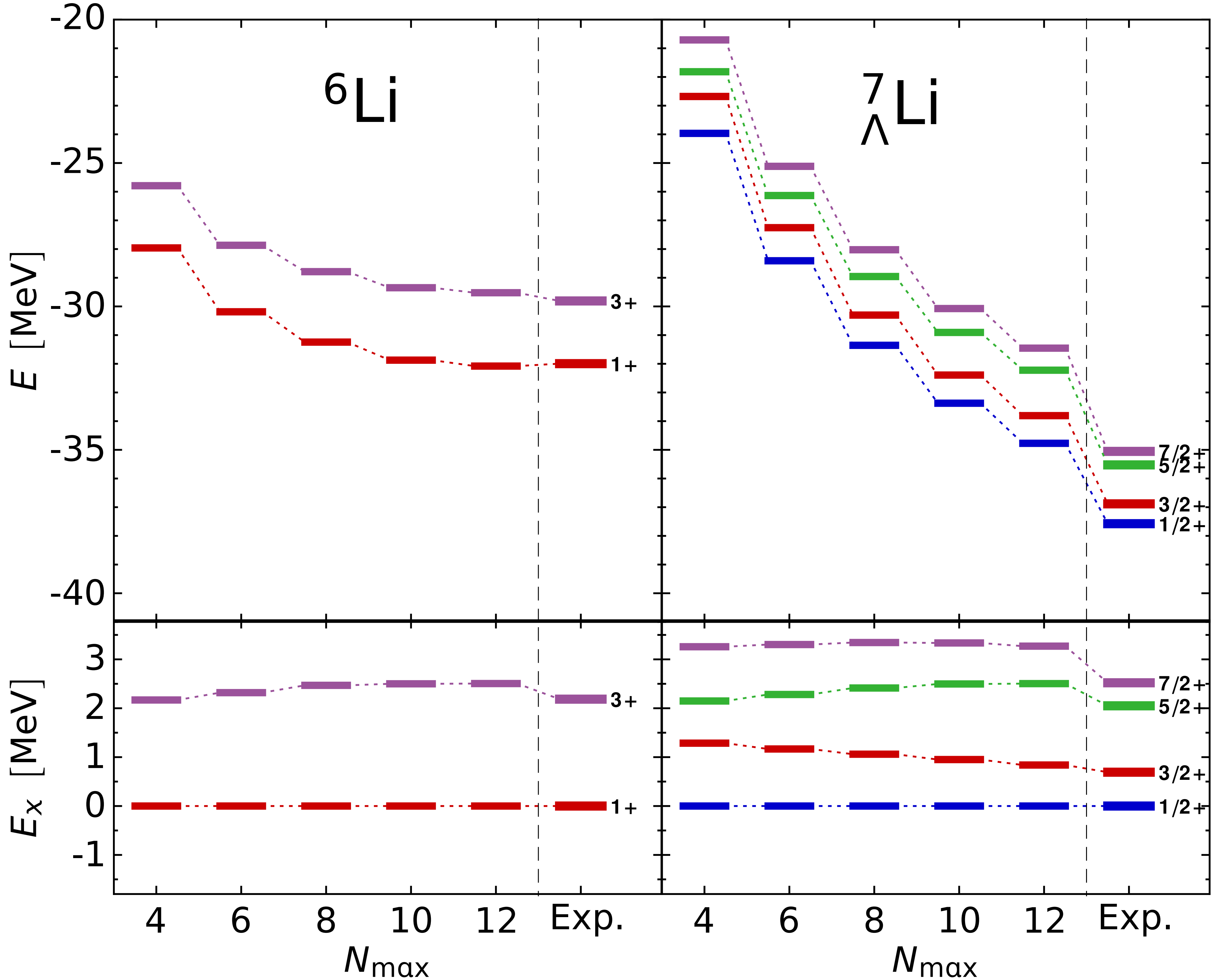
3N @ N2LO
Λ_{3N} = 500 MeV
Navratil
A = 3 fit

YN @ LO
Λ_{YN} = 600 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

Application: $^{7}_{\Lambda}$Li

Wirth et al., PRL 113, 192502 (2014)



IT-NCSM

NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

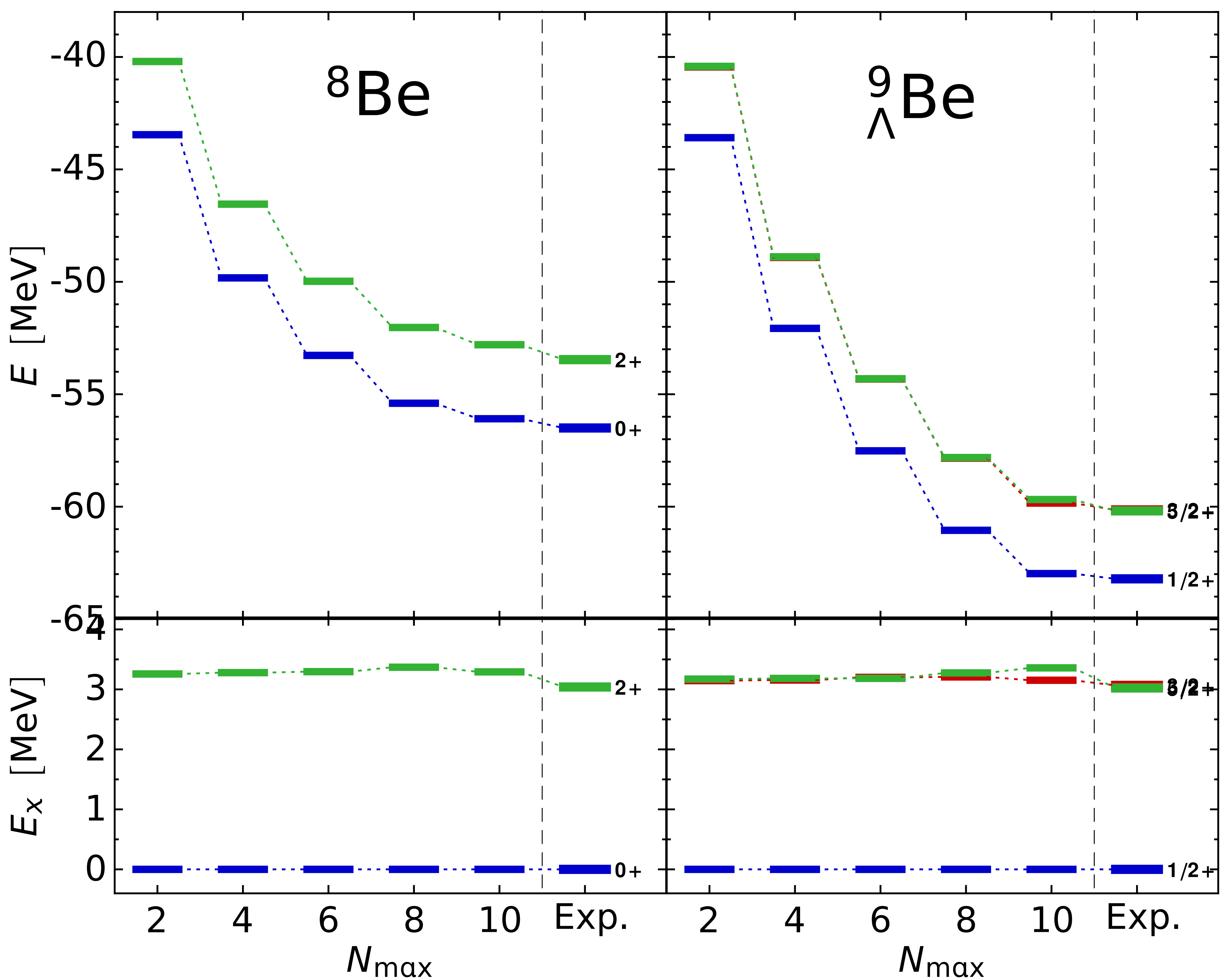
3N @ N2LO
Λ_{3N} = 500 MeV
Navratil
A = 3 fit

YN @ LO
Λ_{YN} = 700 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

Application: $^{9}_{\Lambda}$Be

Wirth et al., PRL 113, 192502 (2014)



NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

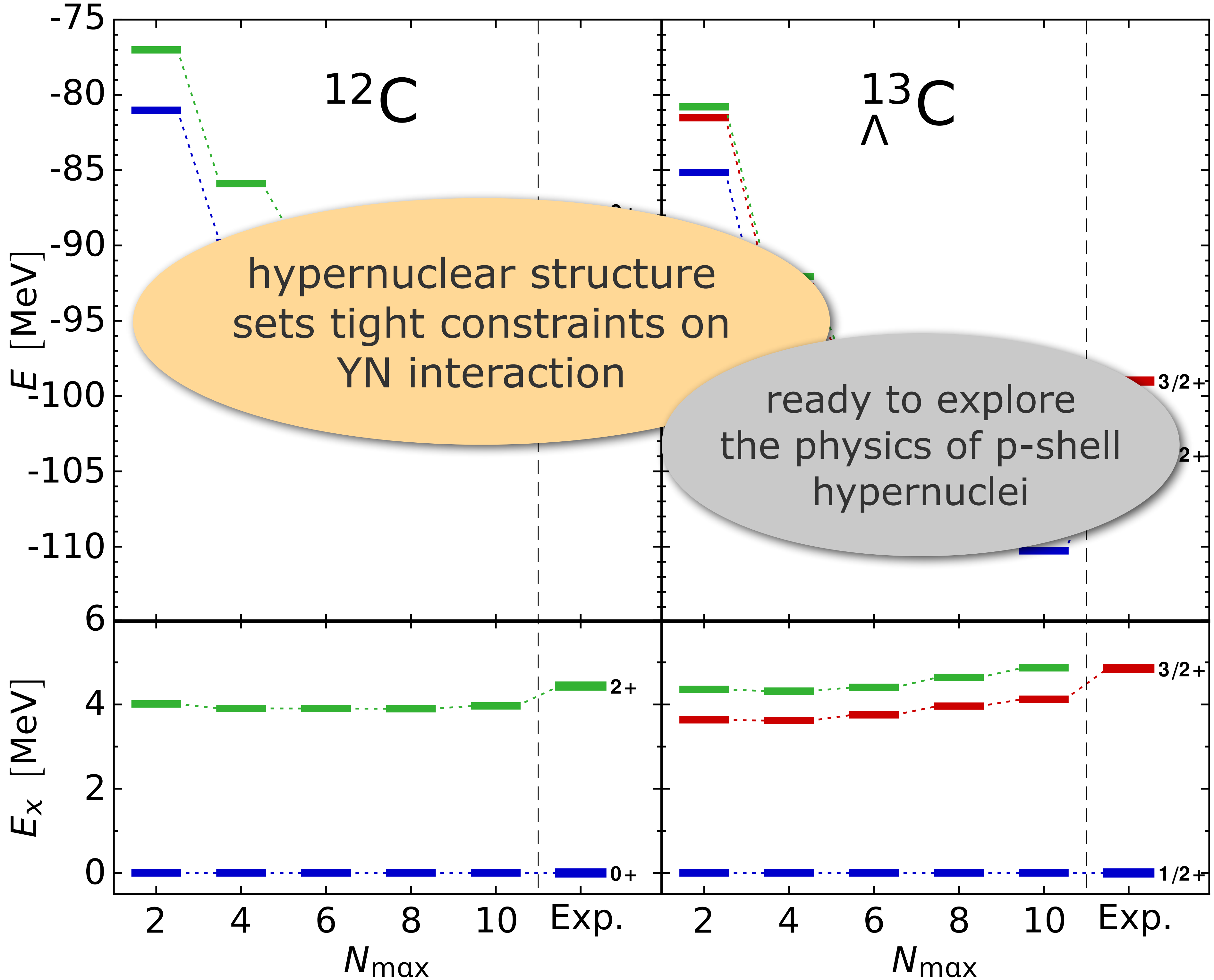
3N @ N2LO
Λ_{3N} = 500 MeV
Navratil
A = 3 fit

YN @ LO
Λ_{YN} = 600 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

Application: ${}^{13}_{\Lambda}C$

Wirth et al., PRL 113, 192502 (2014)



NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

3N @ N2LO
Λ_{3N} = 500 MeV
Navratil
A = 3 fit

YN @ LO
Λ_{YN} = 600 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\text{fm}^4$
$\alpha_{YN} = 0.00\,\text{fm}^4$
$\hbar\Omega = 20$ MeV

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, 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

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

- rigorous quantification of theoretical uncertainties will play an important role

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

- lots of relevant physics predictions for NUSTAR...

Epilogue

- **thanks to my group and my collaborators**
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    Iowa State University
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    Universität Bochum, ...

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

COMPUTING TIME

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Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung