Frontiers in Ab Initio Nuclear Structure Theory

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

Interactions from Chiral EFT

Low-Energy QCD

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents
- standard Hamiltonian:
  - NN at N^3LO
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N^2LO
    Navrátil, local, 350...500 MeV cutoff

From QCD to Nuclear Structure

Nuclear Structure

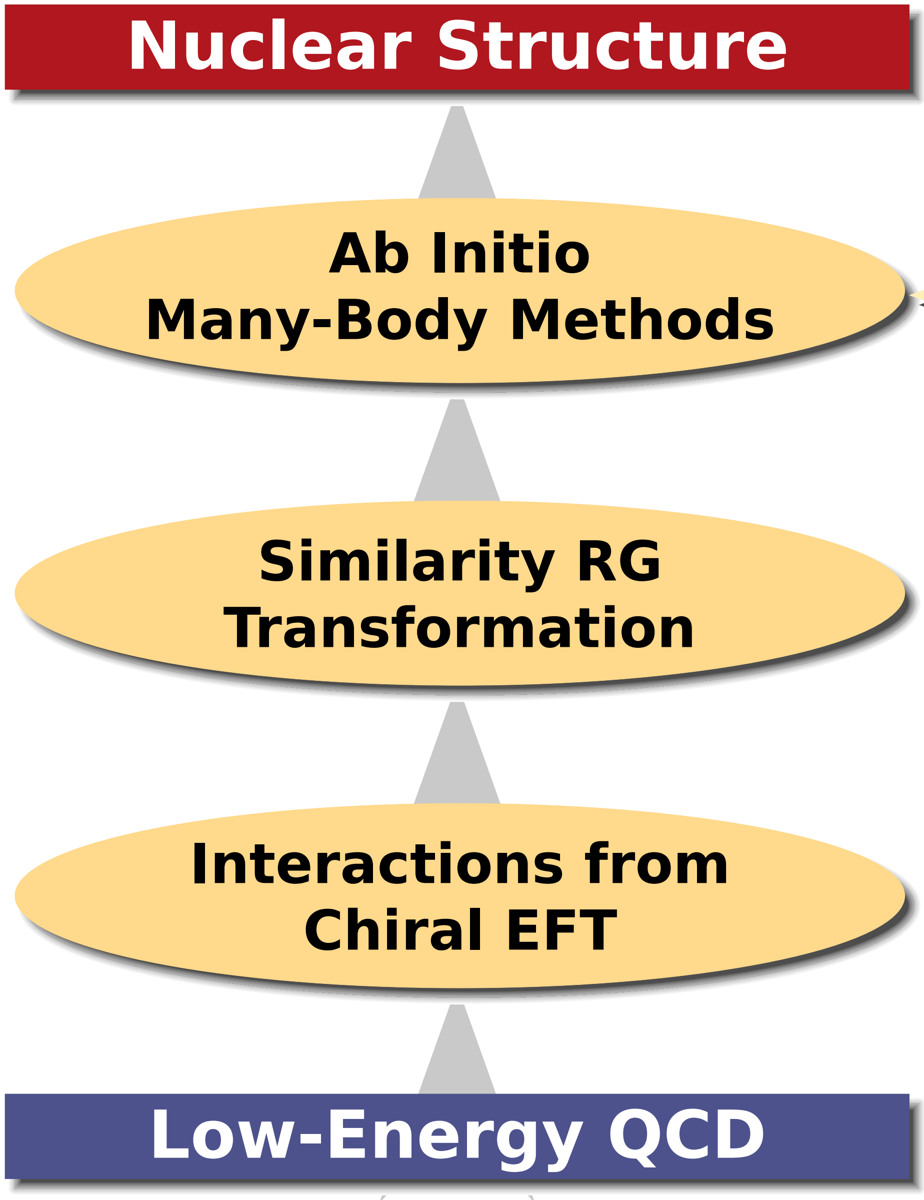
Similarity RG Transformation

Interactions from Chiral EFT

Low-Energy QCD

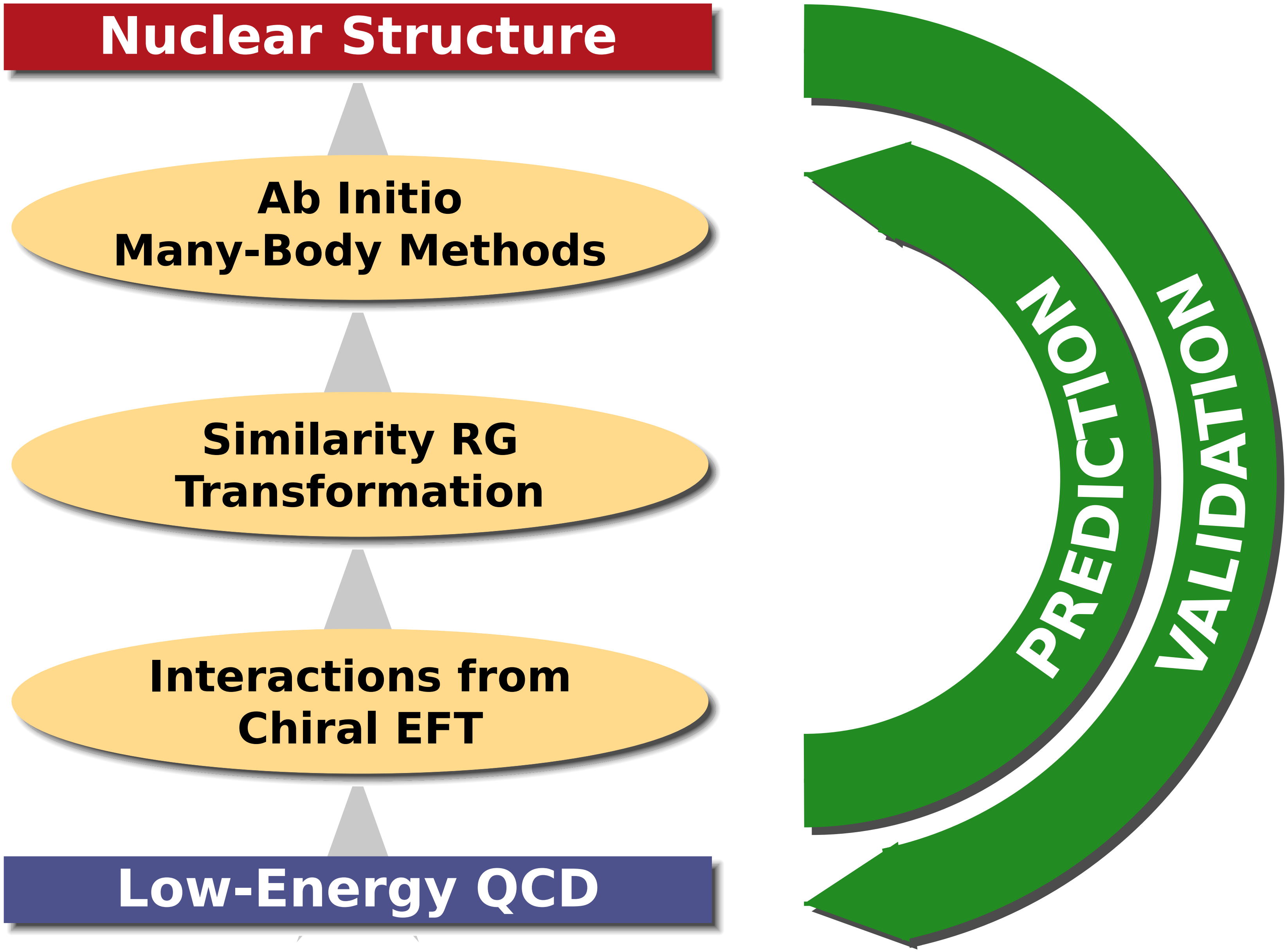
- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- consistent SRG evolution of Hamiltonian & observables up to the 3N (or 4N) level
- probe omitted multi-nucleon interactions by varying flow parameter α

From QCD to Nuclear Structure



- accurate solution of the many-body problem
  - quantified uncertainties
  - systematically improvable
- 'light' nuclei: complete access to all states & observables
  (NCSM & friends)
- medium-mass & beyond: selected states & observables
  (CC, IM-SRG, SCGF, MBPT,...)

From QCD to Nuclear Structure



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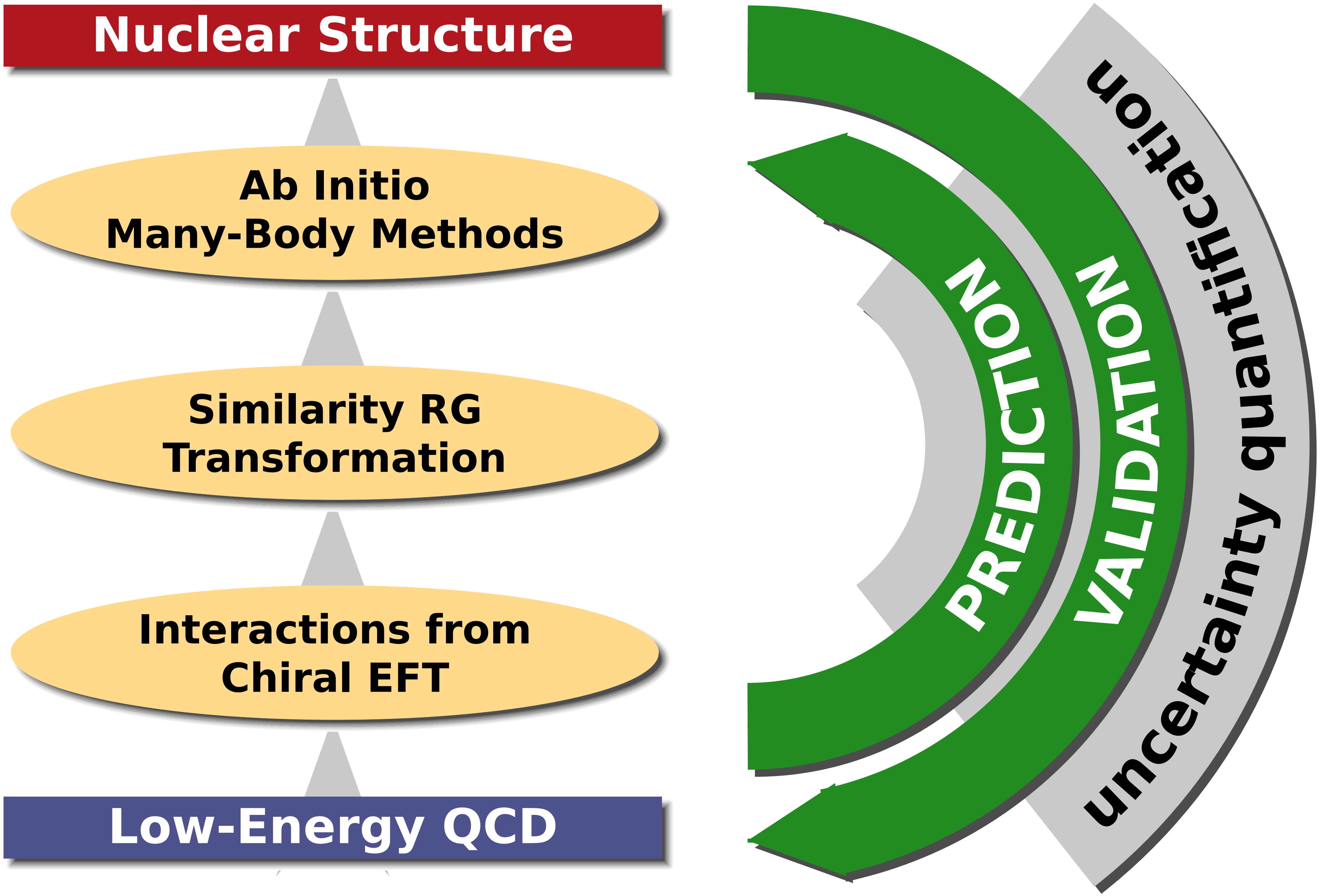


‘Light’ Nuclei

Importance-Truncated NCSM

Barrett, Vary, Navratil, Maris, Nogga, Roth,...

NCSM is one of the most powerful and universal exact ab-initio methods

- compute low-lying eigenvalues of the Hamiltonian in a **model space of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of basis with $N_{\max}$ & A
- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states

Ground States of 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)

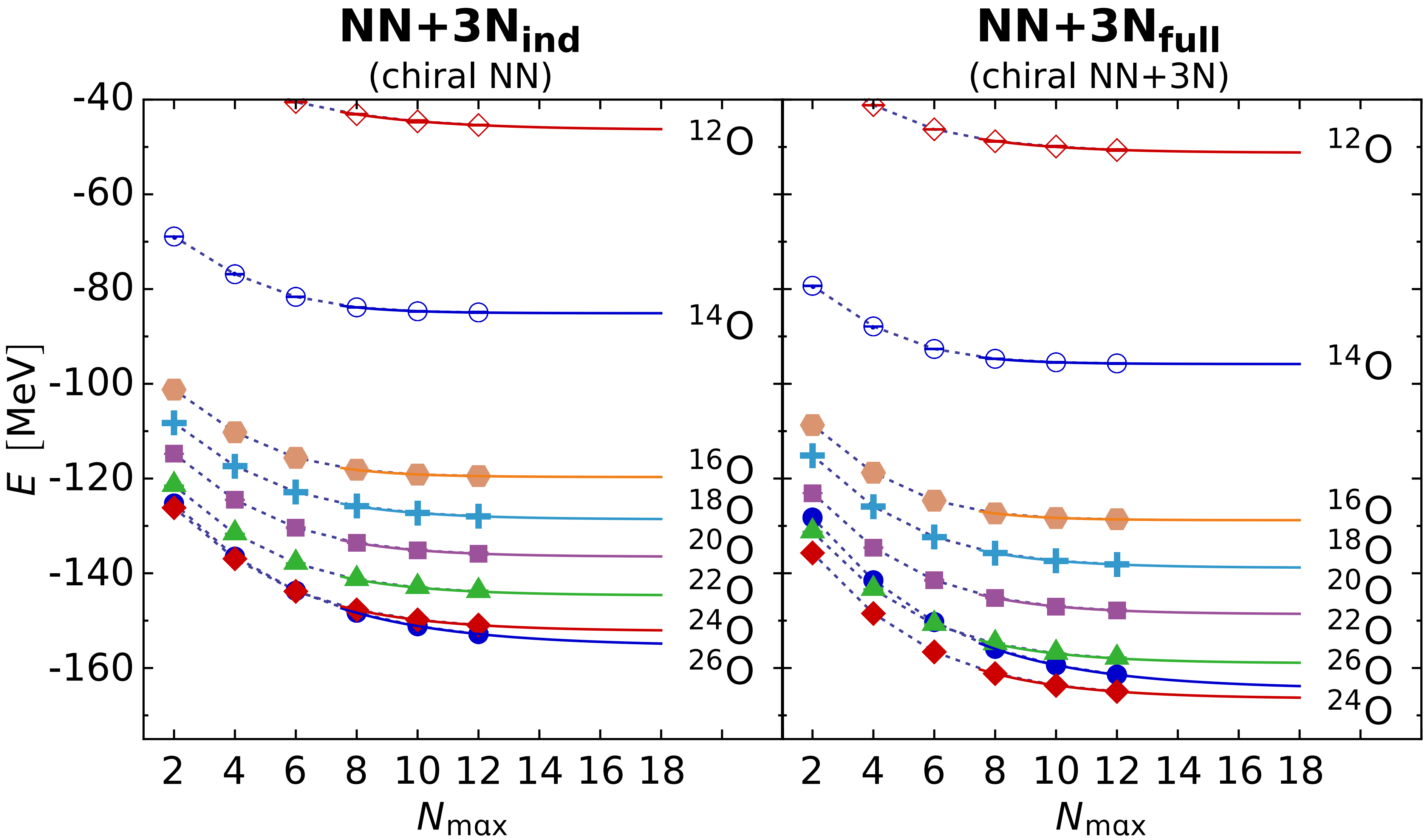
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

Cipollone, Barbieri, Navrátil, PRL 111, 062501 (2013)
Bogner, Hergert, Holt, Schwenk, Binder, Calci, Langhammer, Roth, arXiv:1402.1407

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

Ground States of Oxygen Isotopes

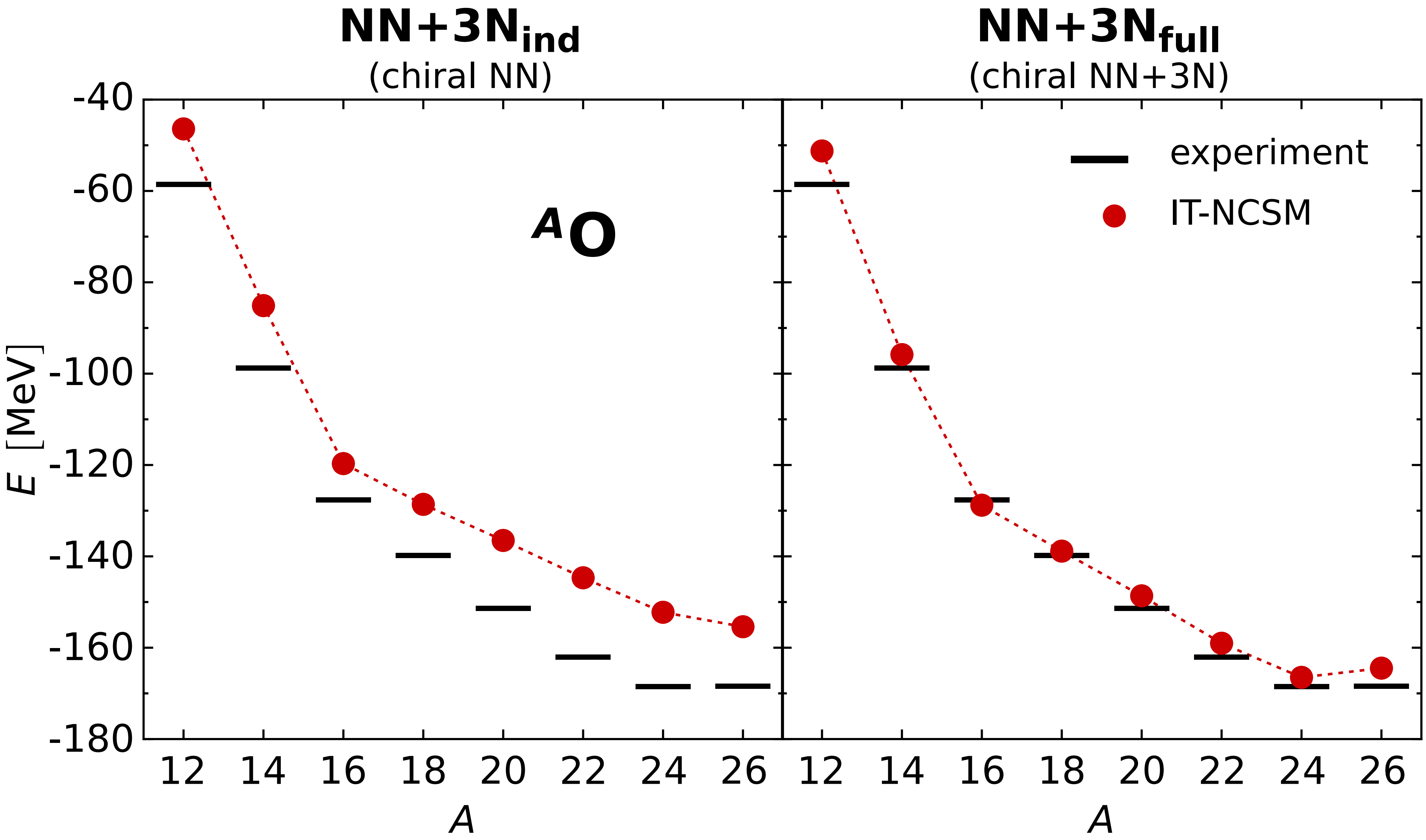
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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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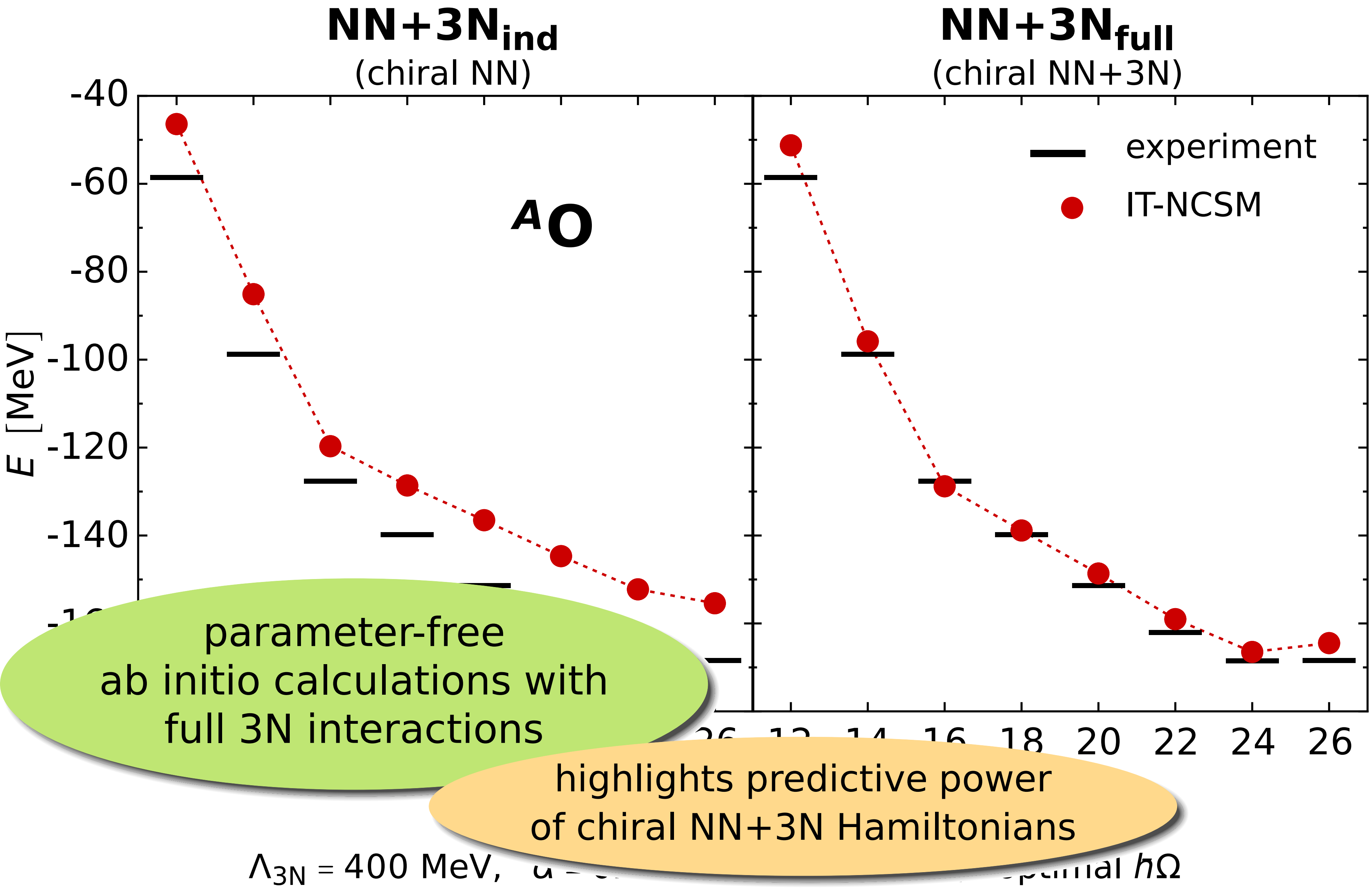
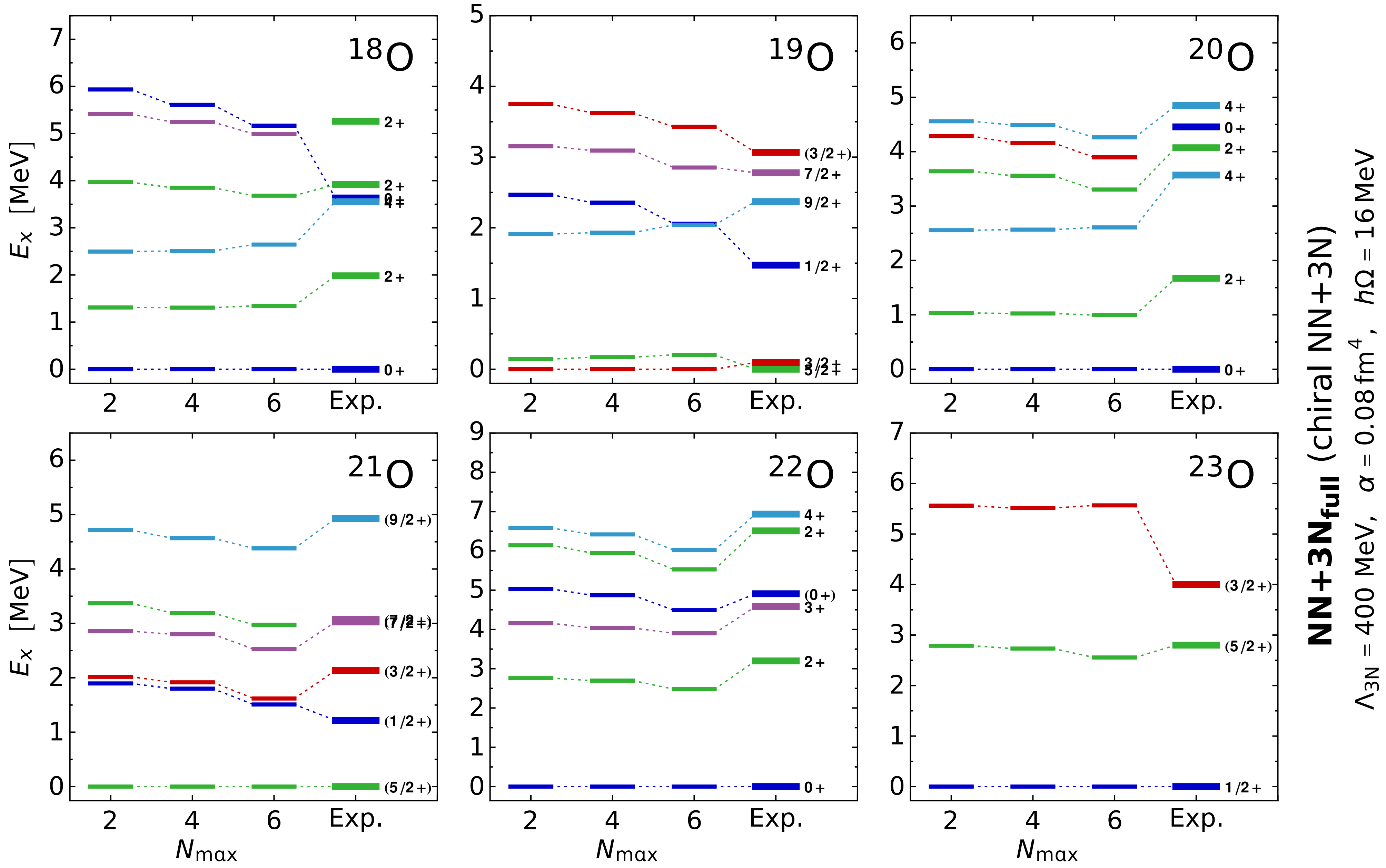


parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

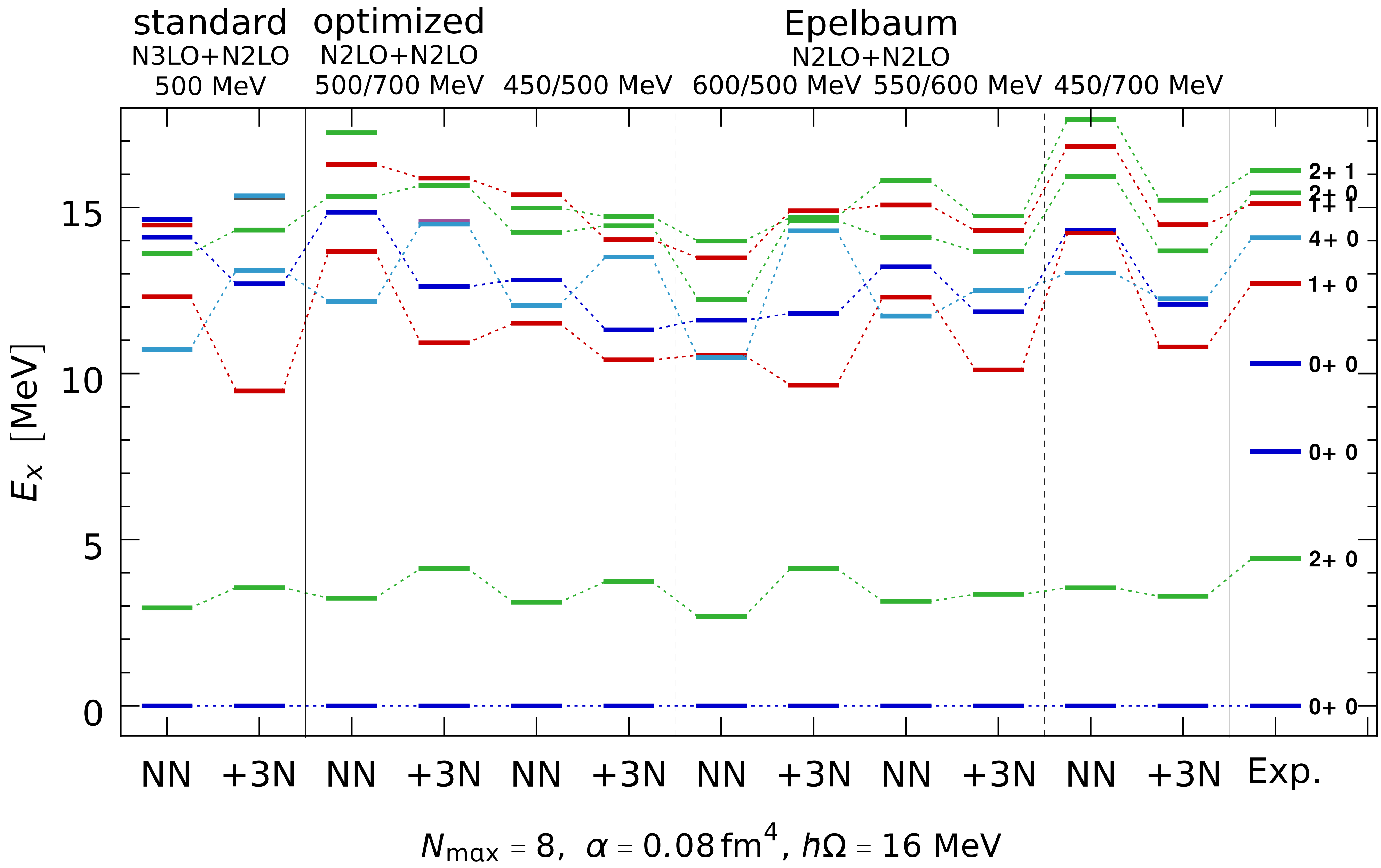
Outlook: Oxygen Spectroscopy

Bogner et al., arXiv:1402.1407 & Roth et al., in prep.



Outlook: Testing Chiral Hamiltonians

Calci et al., in prep.



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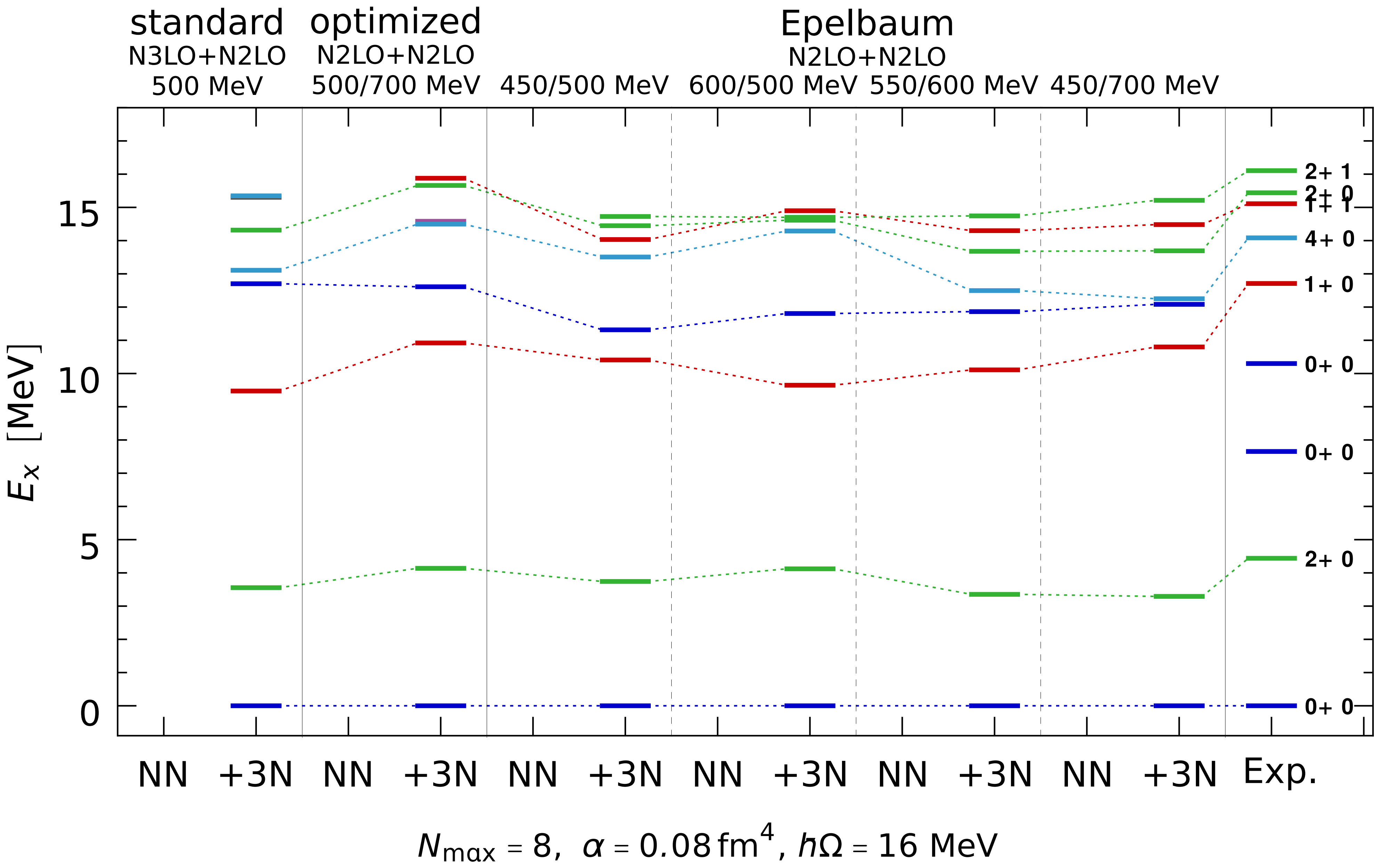

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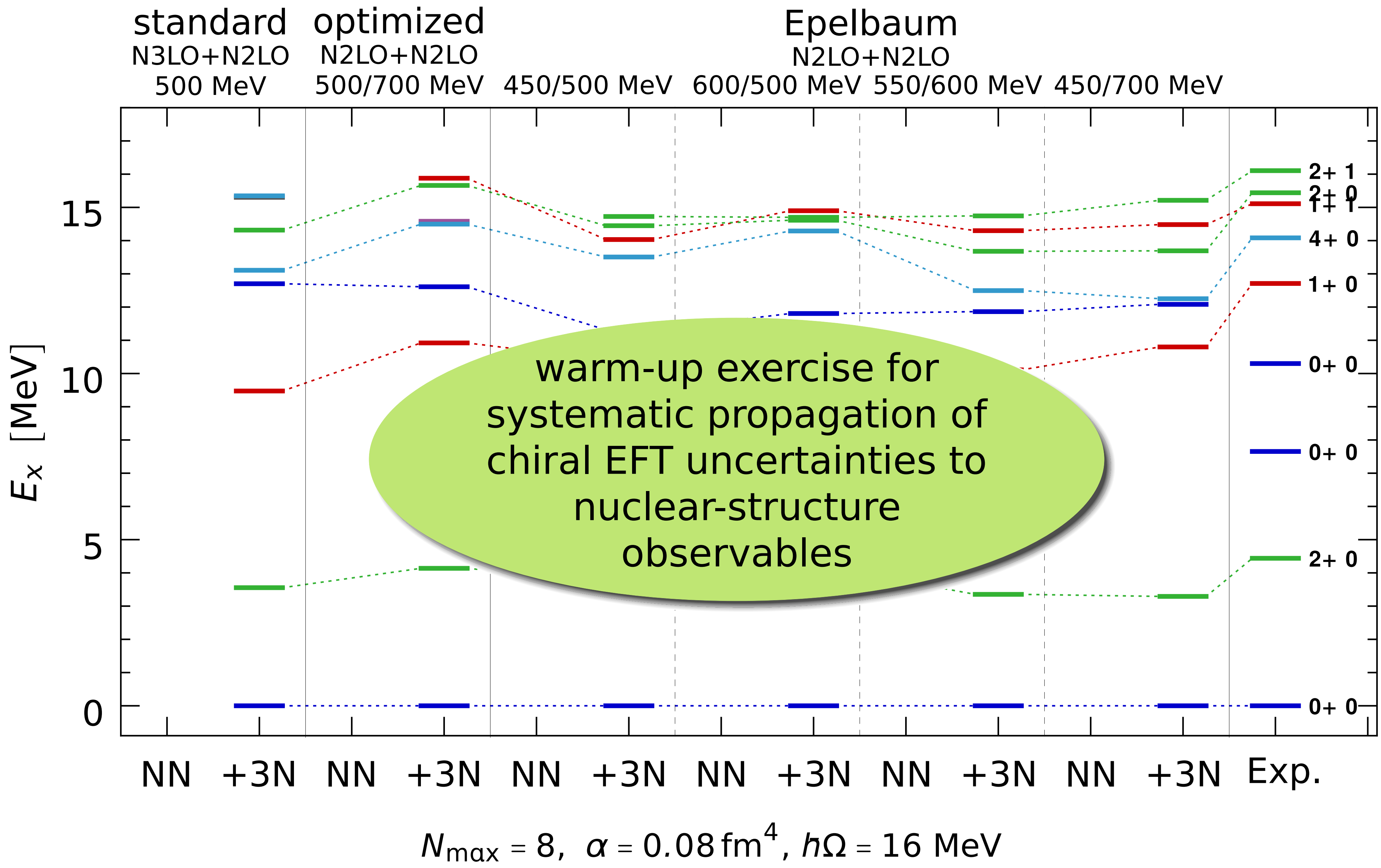

Medium-Mass & Beyond

Medium-Mass & Beyond

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...

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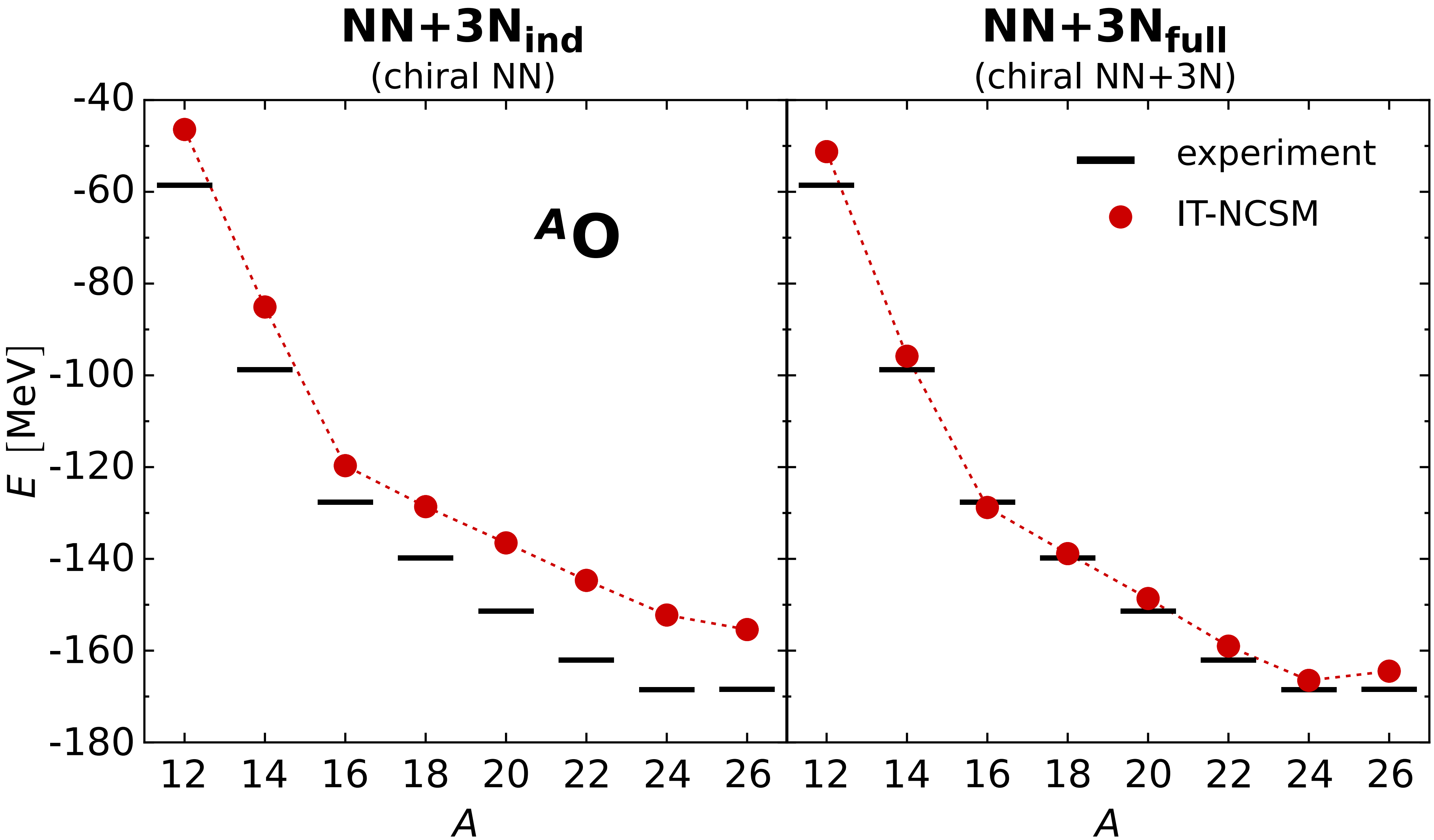
controlling and quantifying the uncertainties due to various truncations is major challenge

Ground States of Oxygen Isotopes

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



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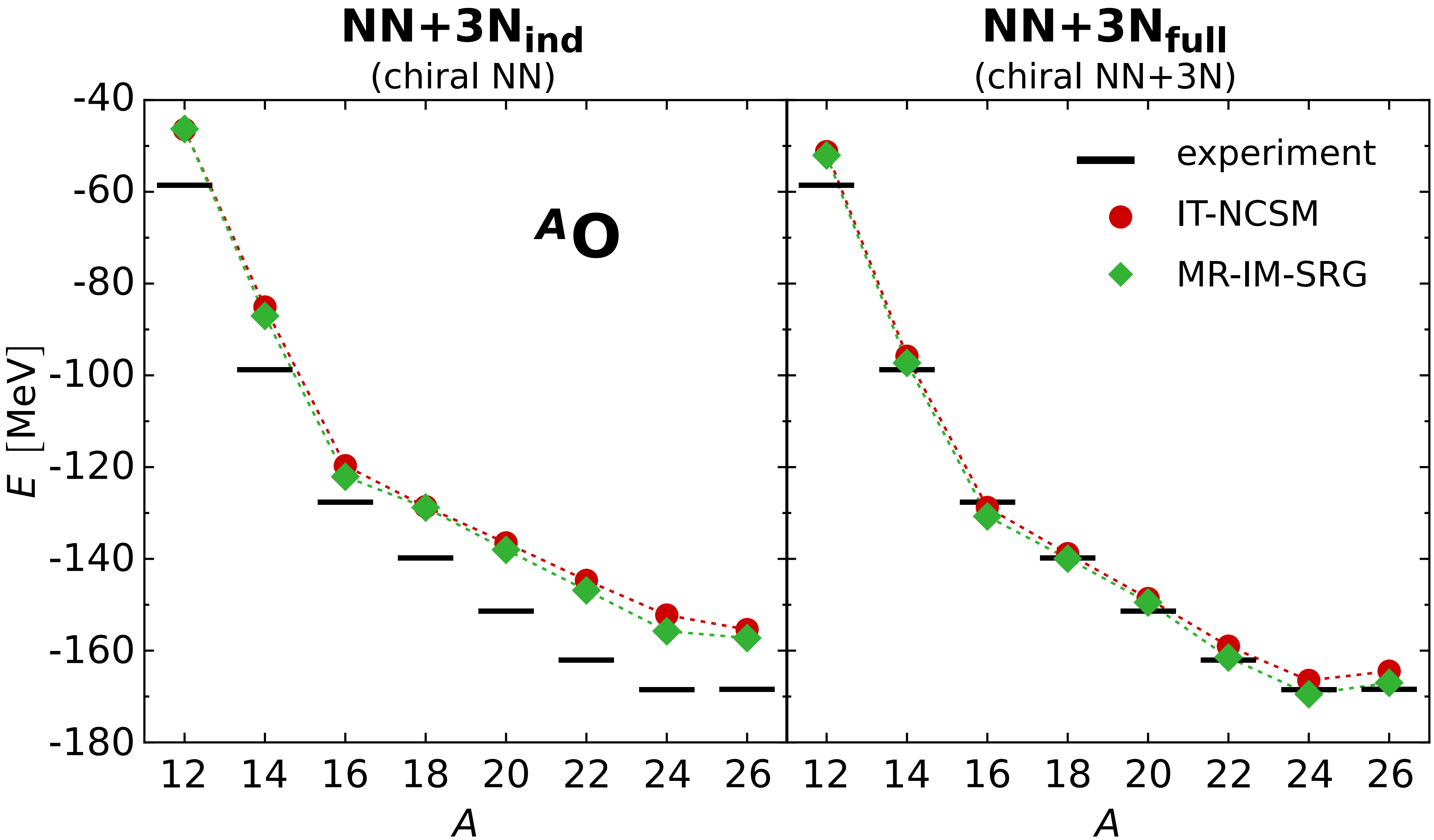

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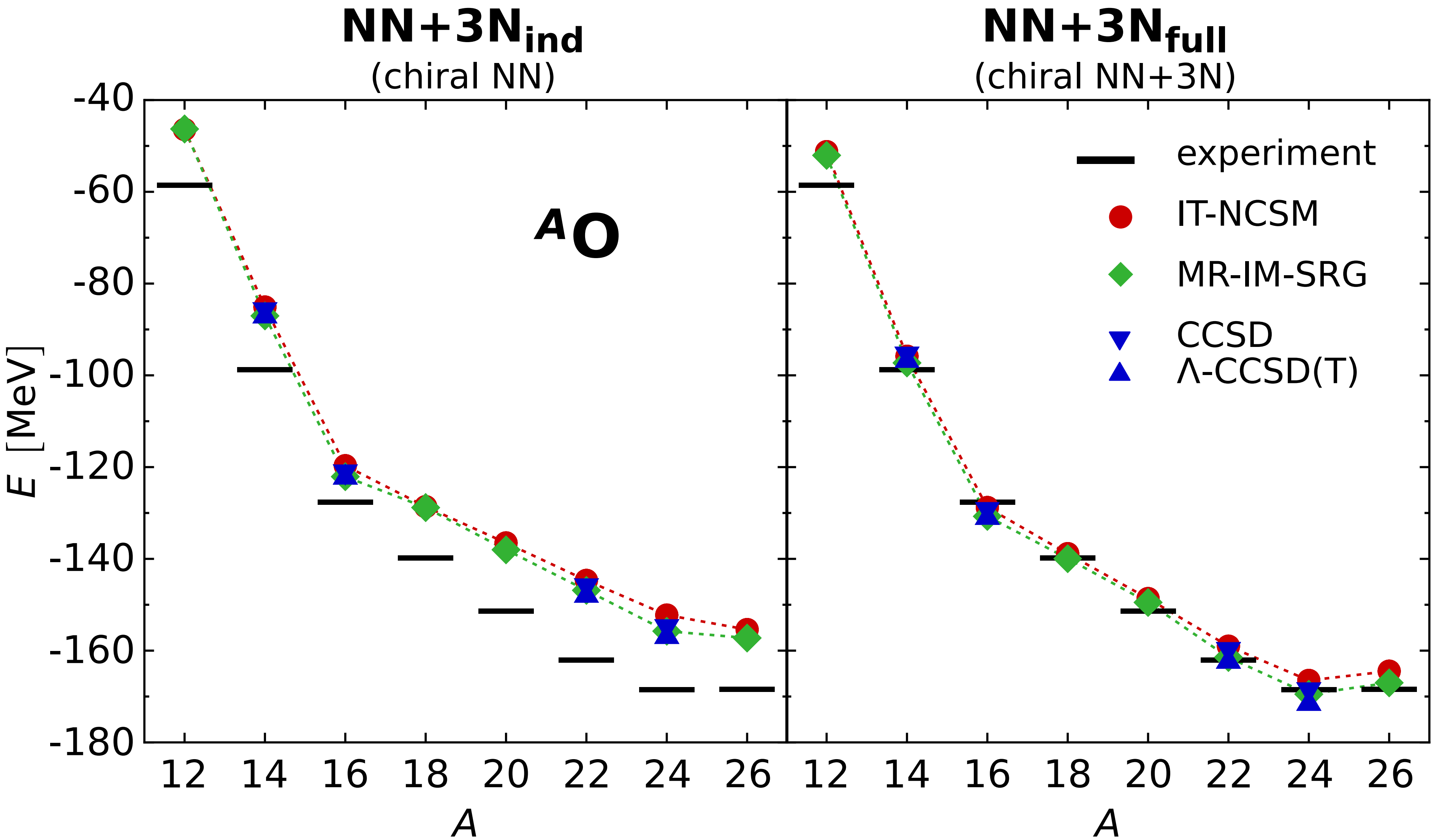

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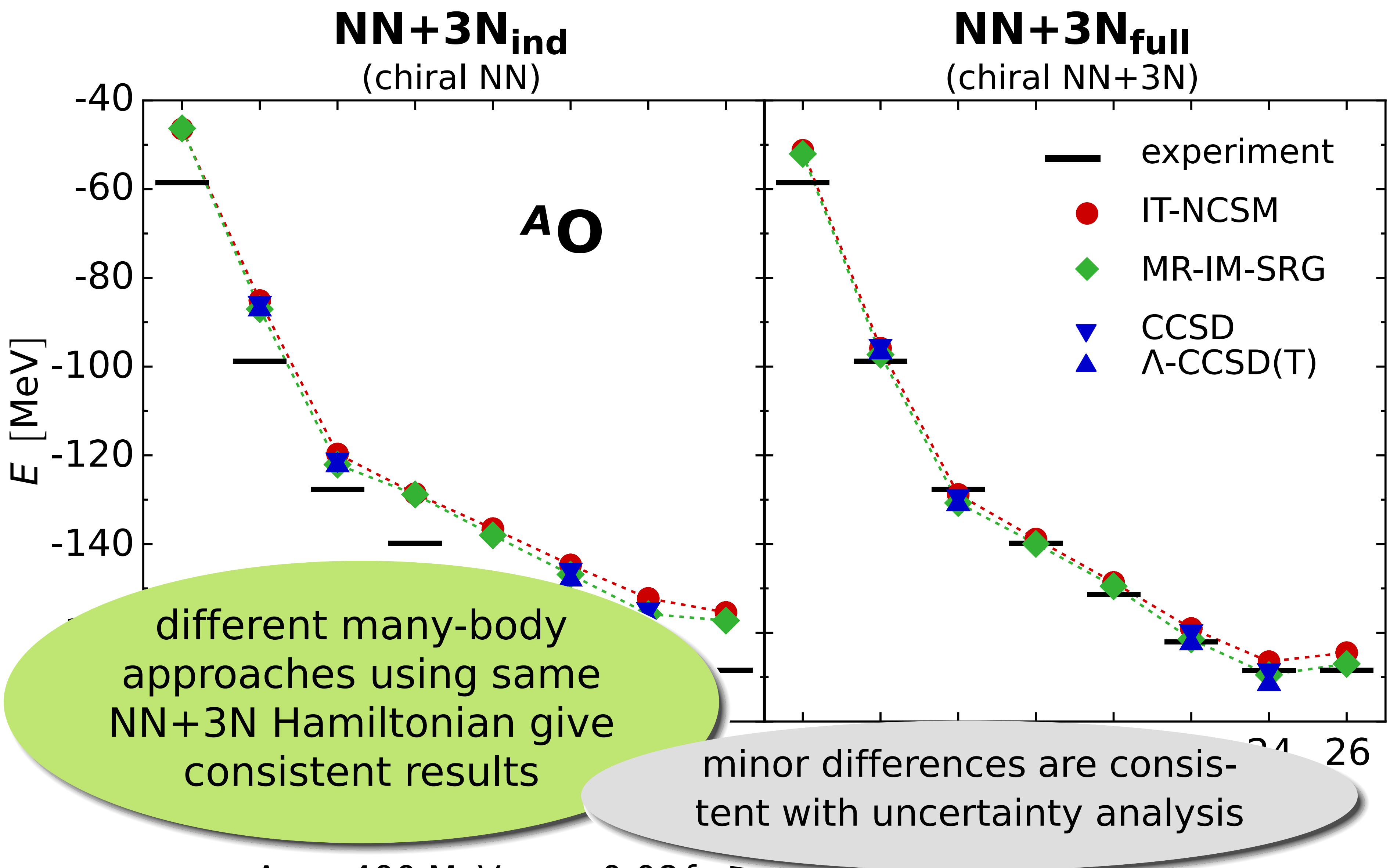

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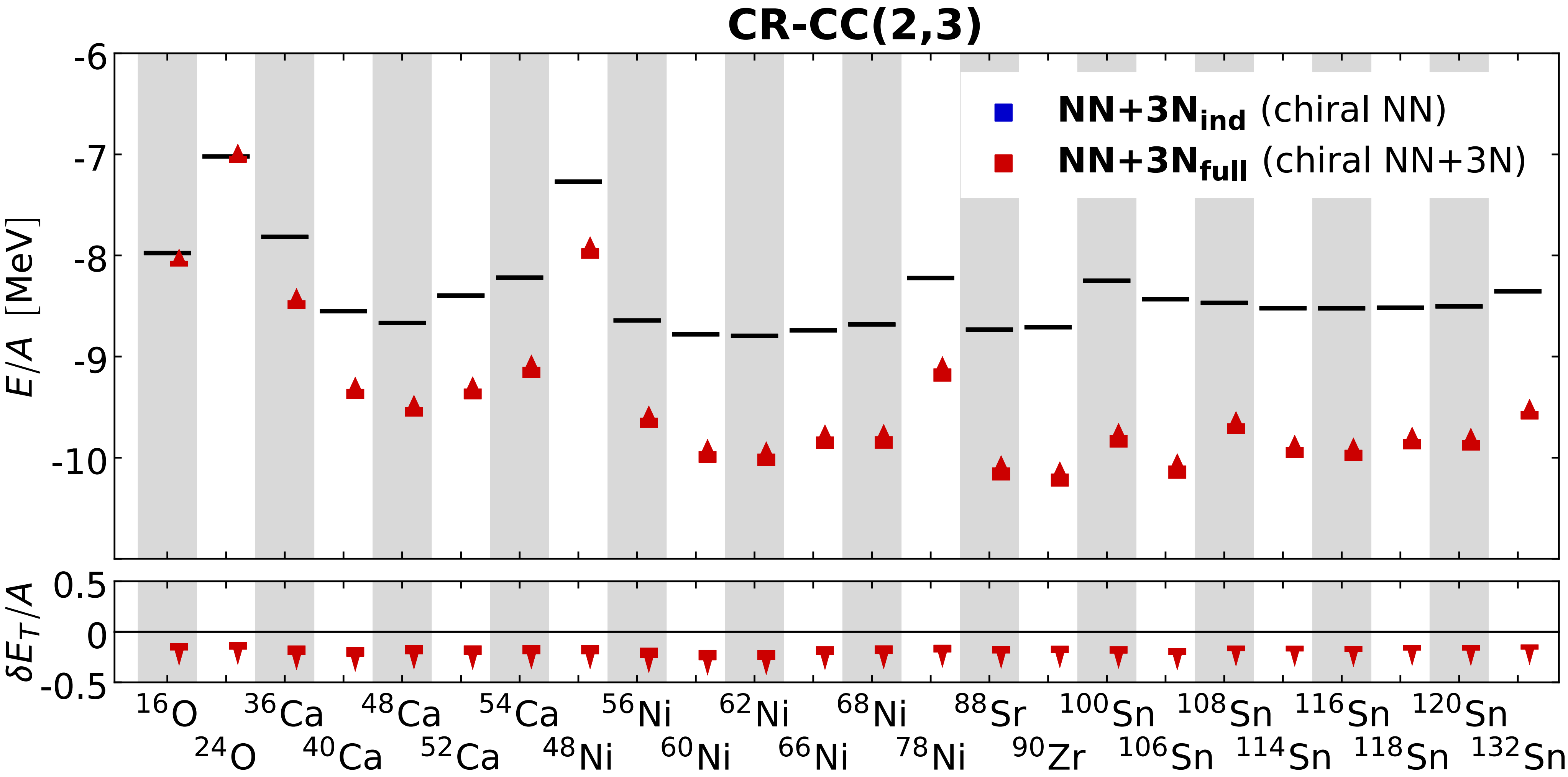
Towards Heavy Nuclei - Ab Initio ?

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013); PRC 88, 054319 (2013); PLB 736, 119 (2014)

- calculations for medium-mass and heavy nuclei are **computationally feasible** with CC or IM-SRG
- however, many of the **technical truncations** that are good in light nuclei **fail for heavier systems**
- we **analysed and improved** all of these truncations...
- **2% residual uncertainty** of the many-body approach for $A \lesssim 130$

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 $\hbar\Omega$

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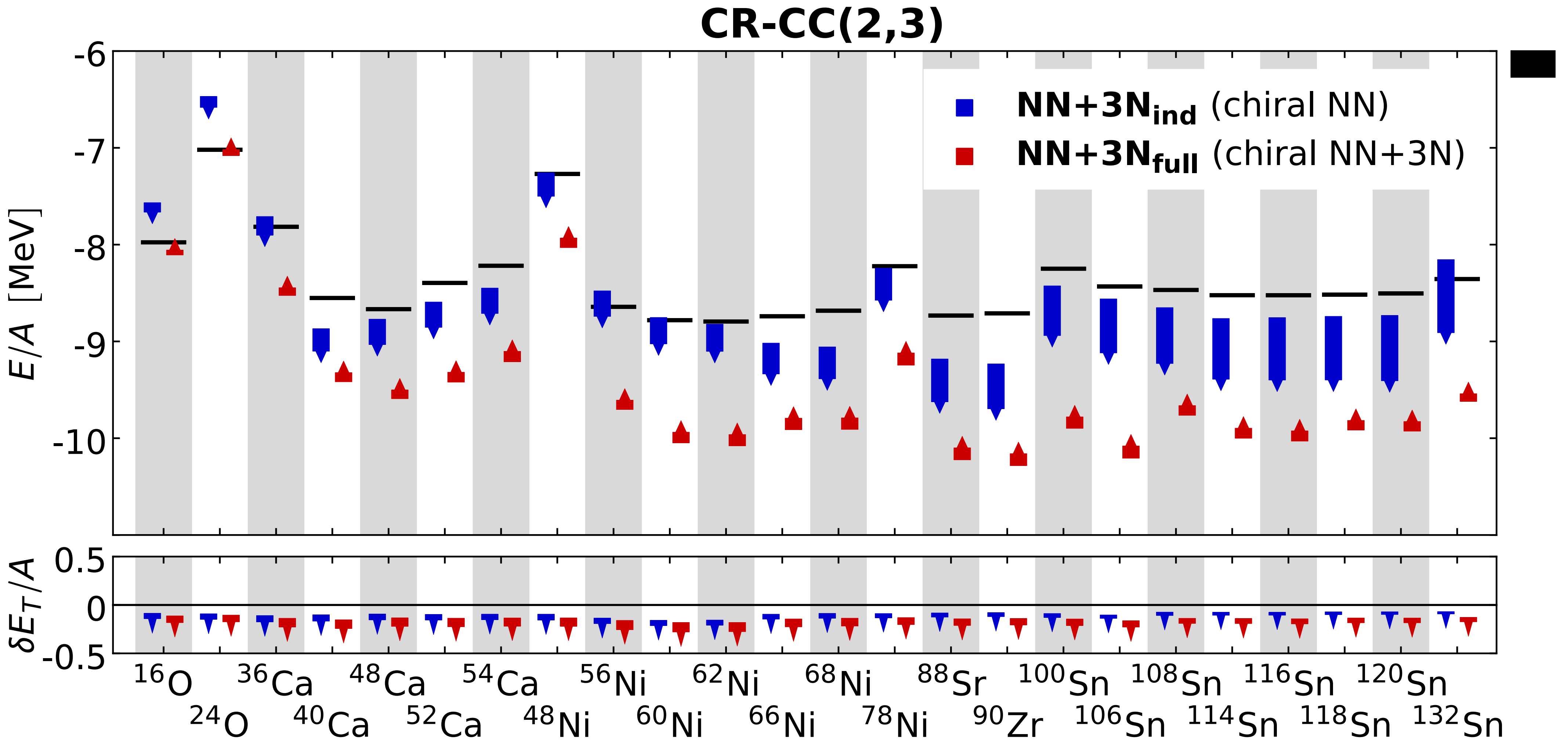
Binder et al., PLB 736, 119 (2014)



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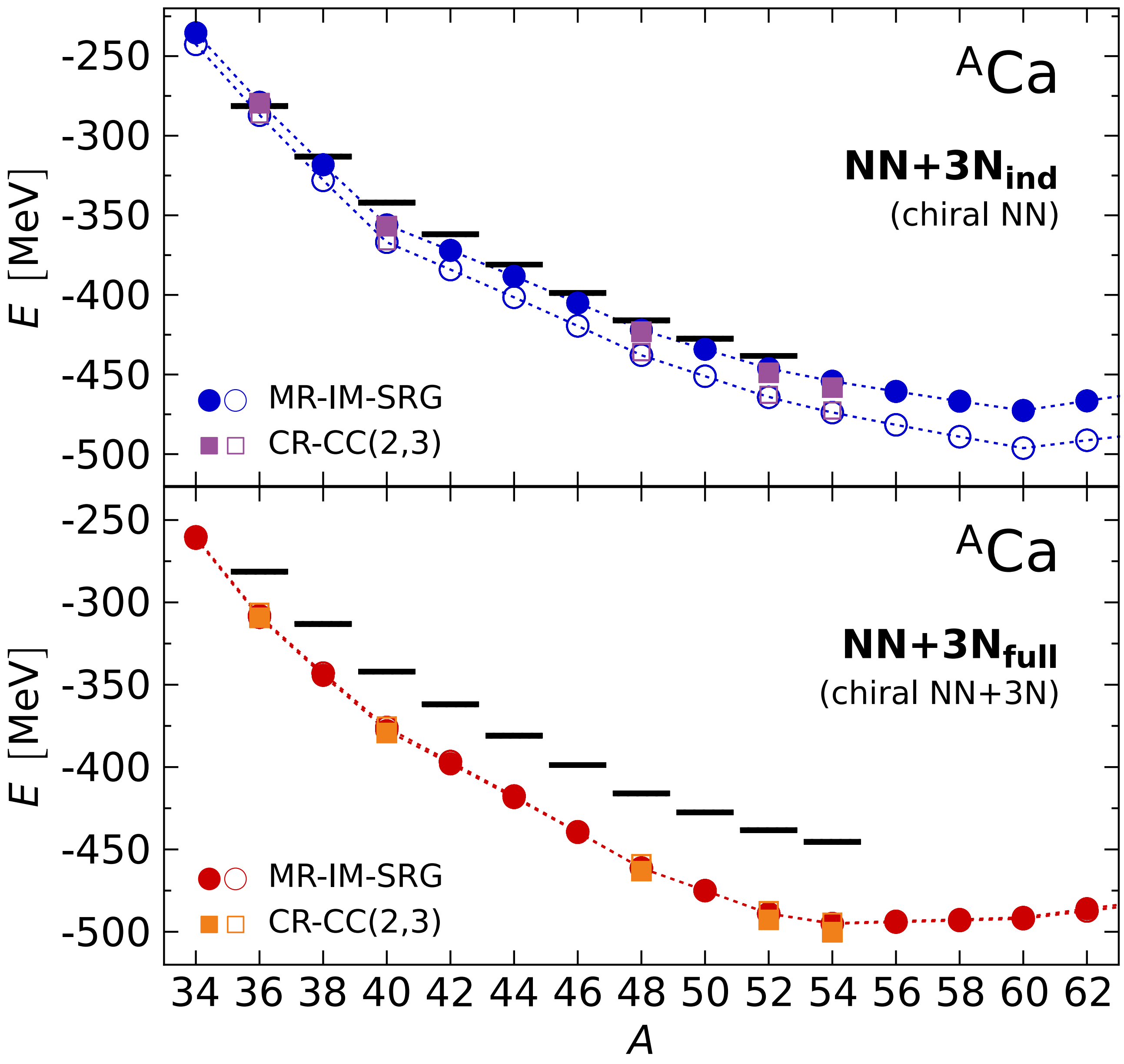
Outlook: Open-Shell Medium-Mass Nuclei

Hergert et al, arXiv:1407.xxxx



- 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

Outlook: Open-Shell Medium-Mass Nuclei

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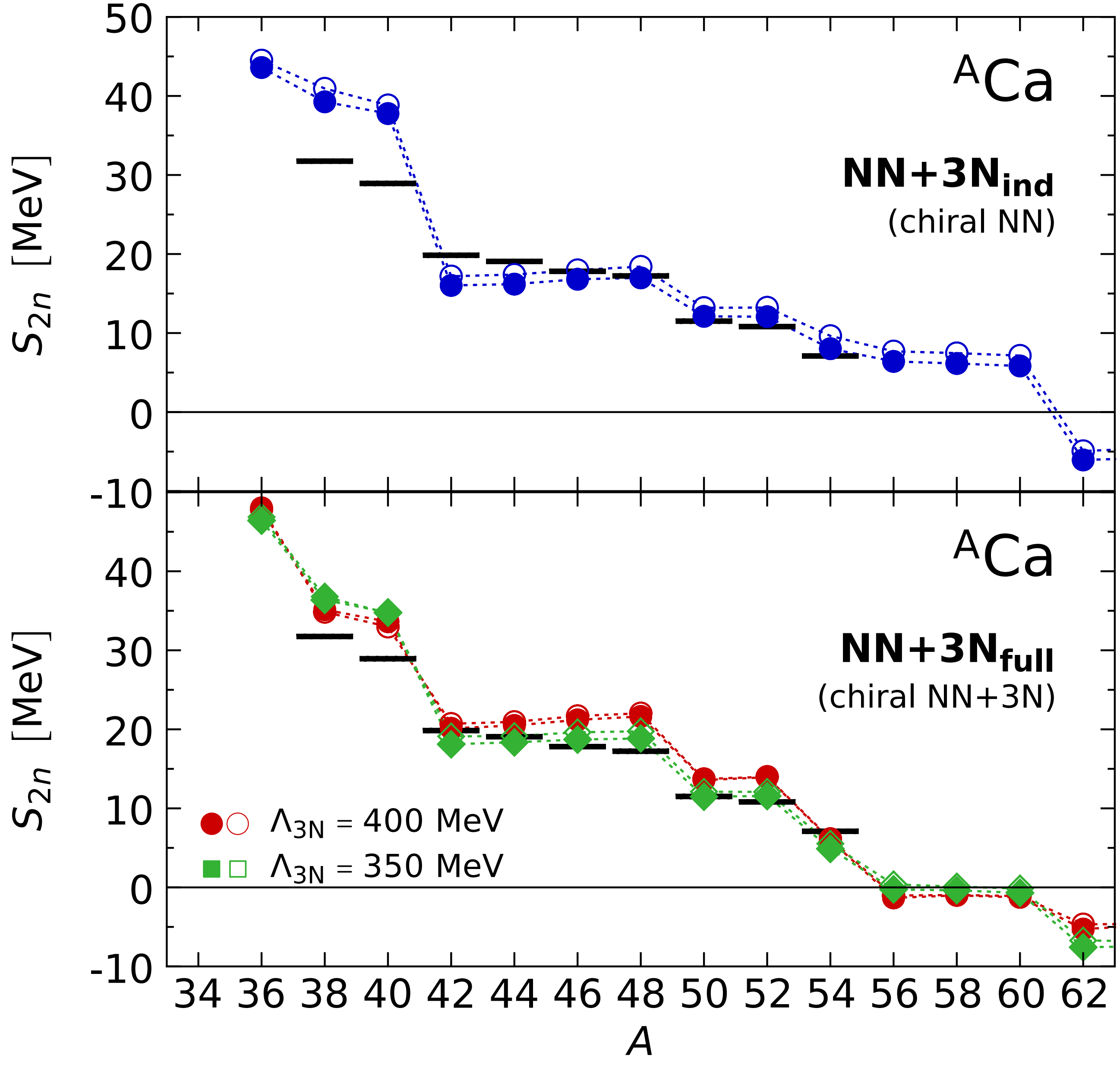

- two-neutron separation energies hide overall energy shift
- compares well to updated Gro'kov-GF results

  talk by C. Barbieri

- chiral 3N interaction generates magicity of ^{54}Ca and defines dripline

all MR-IM-SRG

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Outlook: Open-Shell Medium-Mass Nuclei

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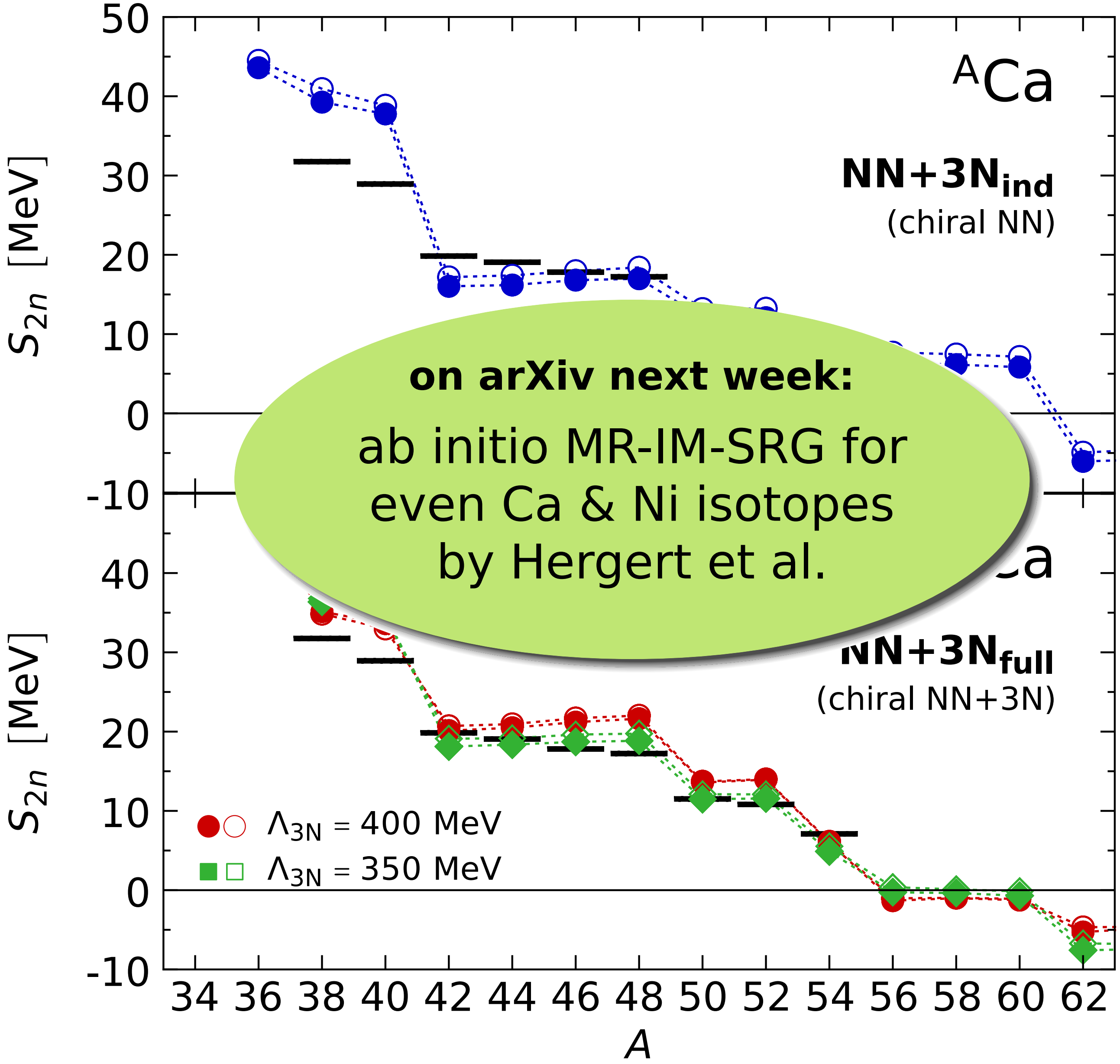

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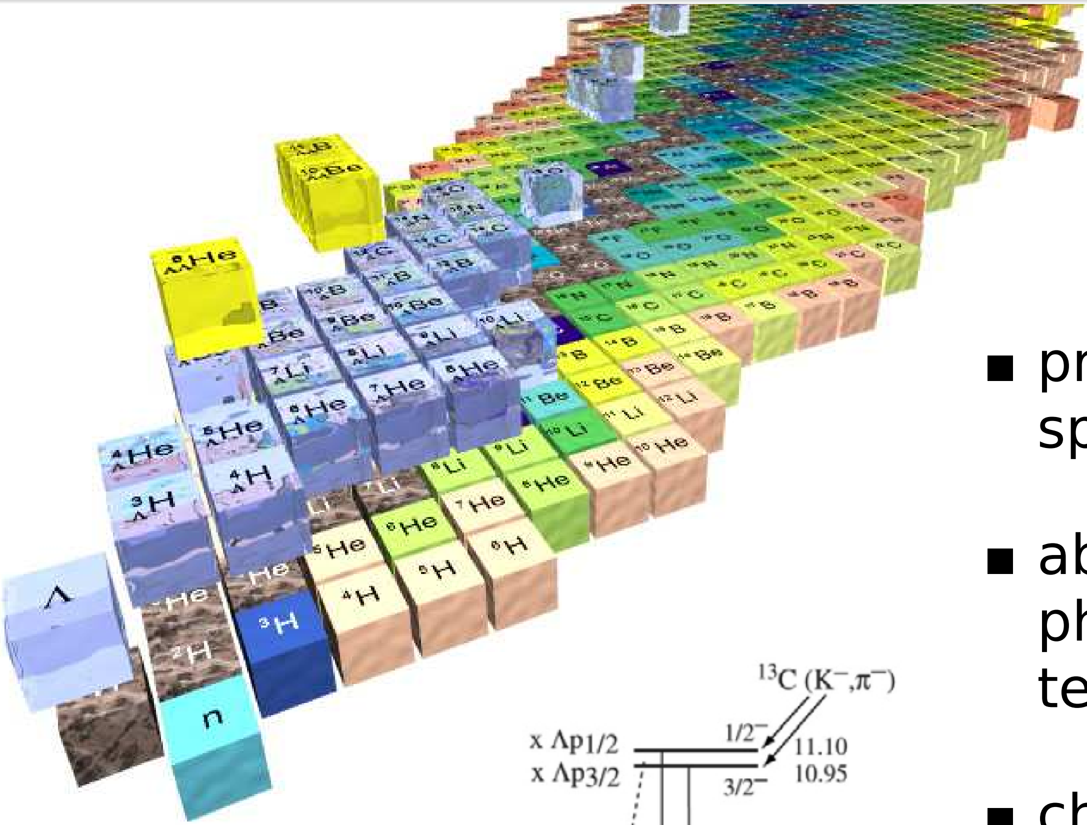
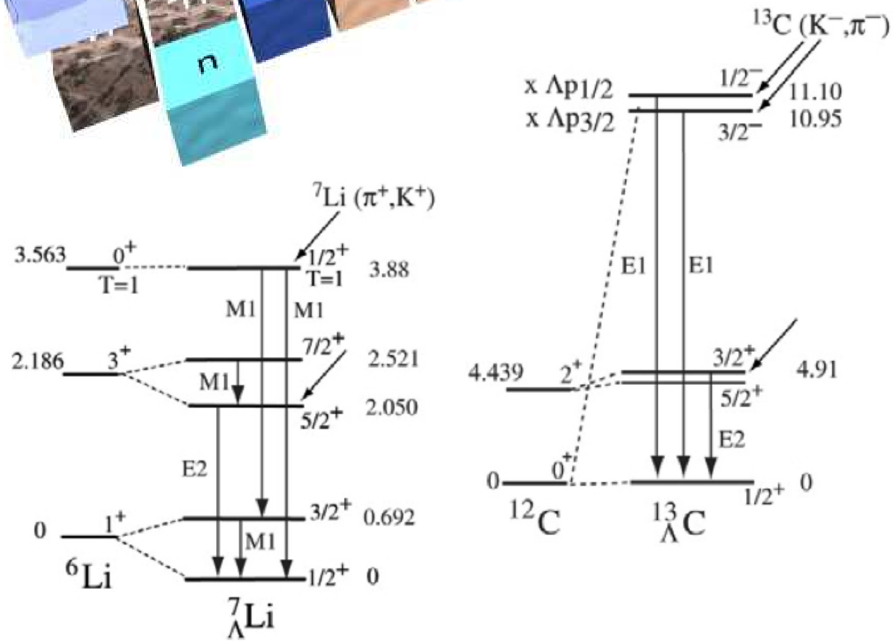
Hypernuclei

Ab Initio Hypernuclear Structure



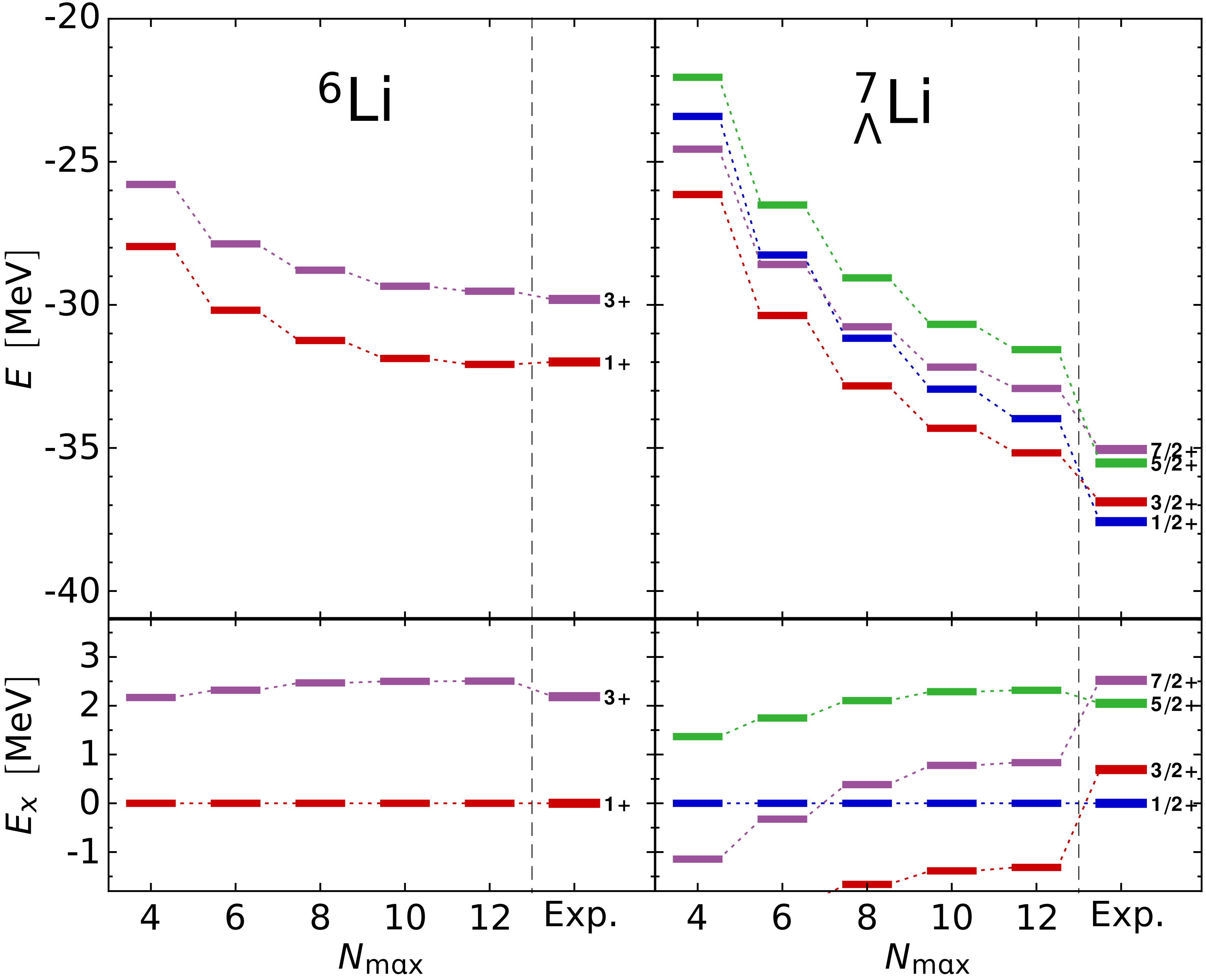


- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body ($A \lesssim 4$) and phenomenological shell or cluster model calculations
- chiral YN & YY interactions at (N)LO are available

time to transfer ab initio toolbox to hypernuclei

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

Wirth et al., arXiv:1403.3067



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

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

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

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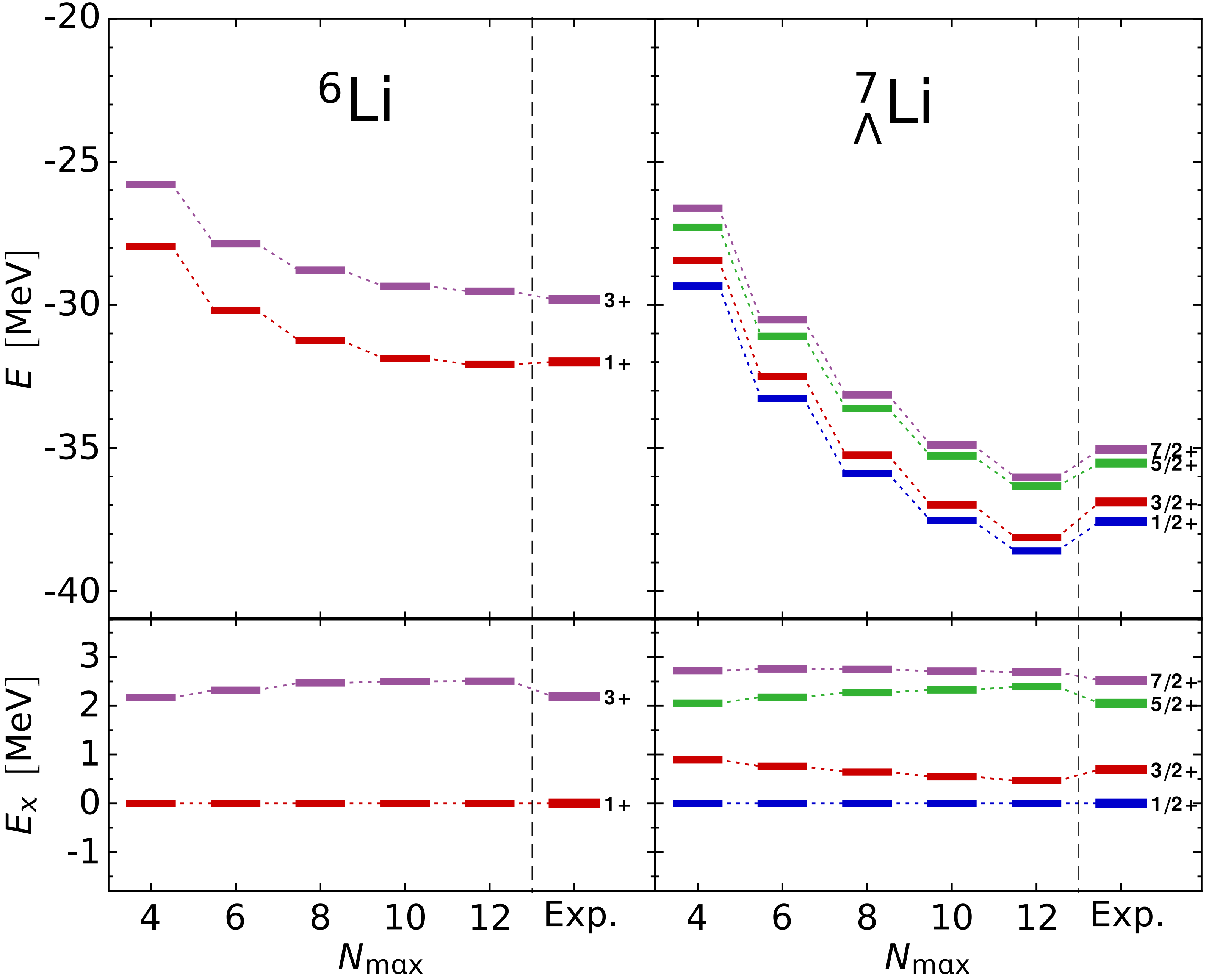

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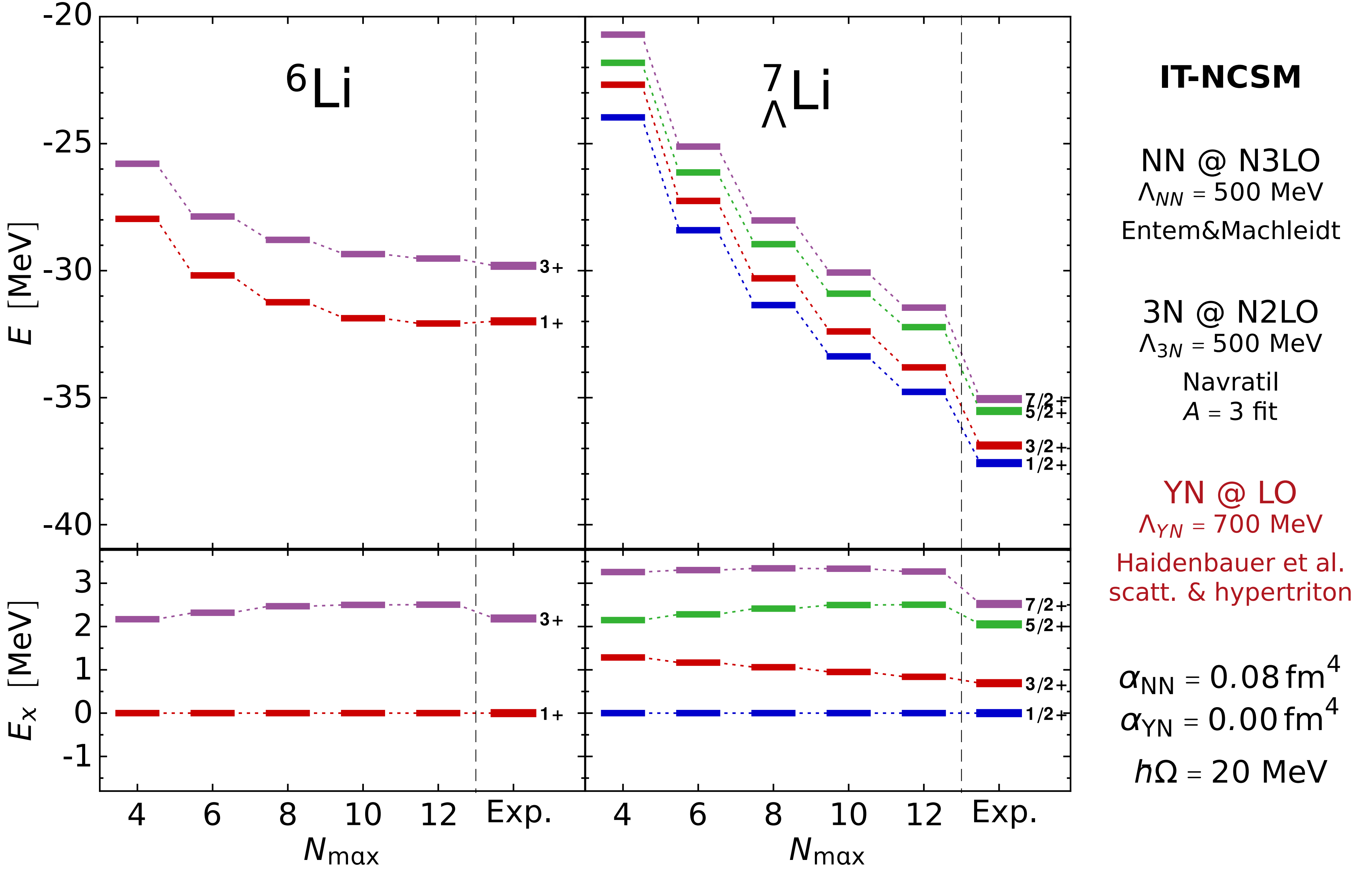

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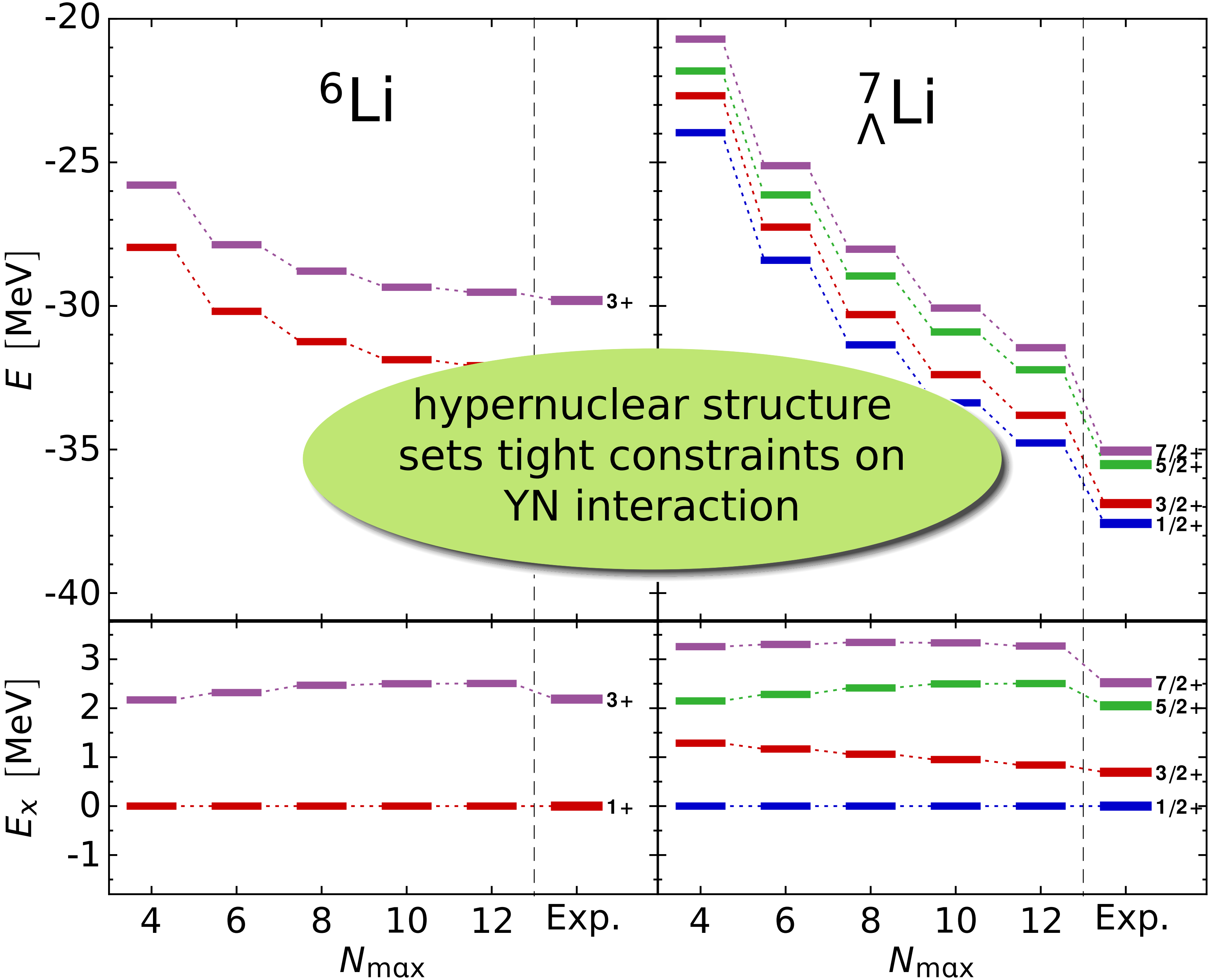

IT-NCSM

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

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

Frontiers

- **ab initio theory is entering new territory...**

  - **QCD frontier** *talks by A. Gezerlis, G. Hagen*
    nuclear structure connected systematically to QCD via chiral EFT
  - **precision frontier** *talk by G. Hagen*
    precision spectroscopy of light nuclei, including current contributions
  - **mass frontier** *talks by G. Hagen, C. Barbieri*
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier** *talks by J. Holt, G. Hagen, C. Barbieri*
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum frontier** *talks by S. Quaglioni, P. Navrátil*
    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 & my collaborators**
  - S. Binder, J. Braun, A. Calci, S. Fischer, E. Gebrerufael, H. Spiess, J. Langhammer, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth, K. Vobig
    Institut für Kernphysik, TU Darmstadt
  - P. Navrátil
    TRIUMF Vancouver, Canada
  - J. Vary, P. Maris
    Iowa State University, USA
  - S. Quaglioni, G. Hupin
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert
    Ohio State University, USA
  - P. Papakonstantinou
    IBS/RISP, Korea
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

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