Ab Initio Nuclear Structure Theory: Beyond the Ordinary

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HIC for FAIR
Helmholtz International Center

Overview

- **Ab Initio Toolbox**
  - Similarity Renormalization Group
  - No-Core Shell Model
  - Medium-Mass Methods

- **Beyond the Ordinary**
  - Hypernuclei
  - Merging NCSM & IM-SRG
  - Sensitivity & Correlations

Ab Initio Toolbox

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

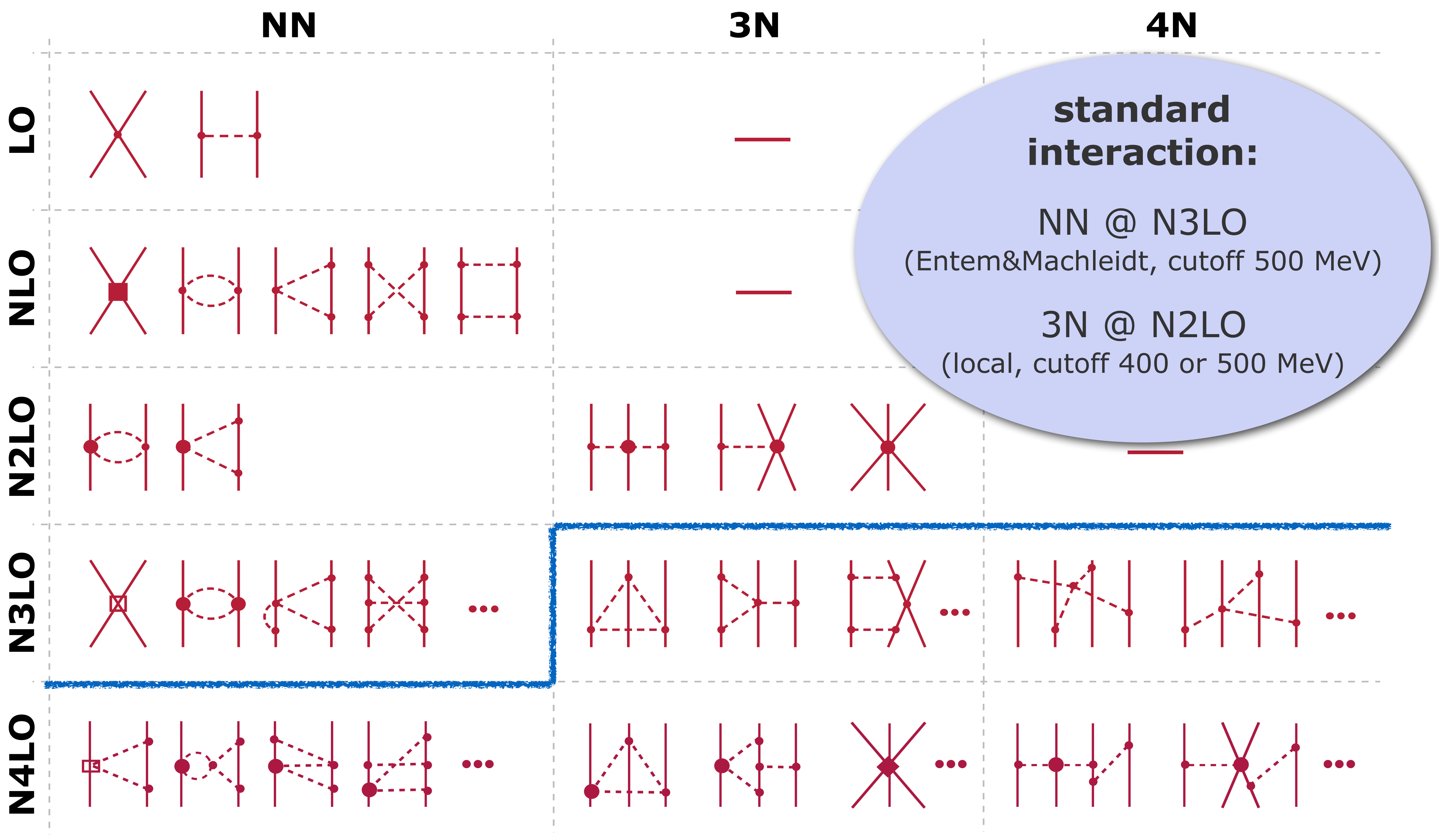
Chiral EFT: Interactions & Operators

Low-Energy QCD

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

Chiral EFT for Nuclear Interactions

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



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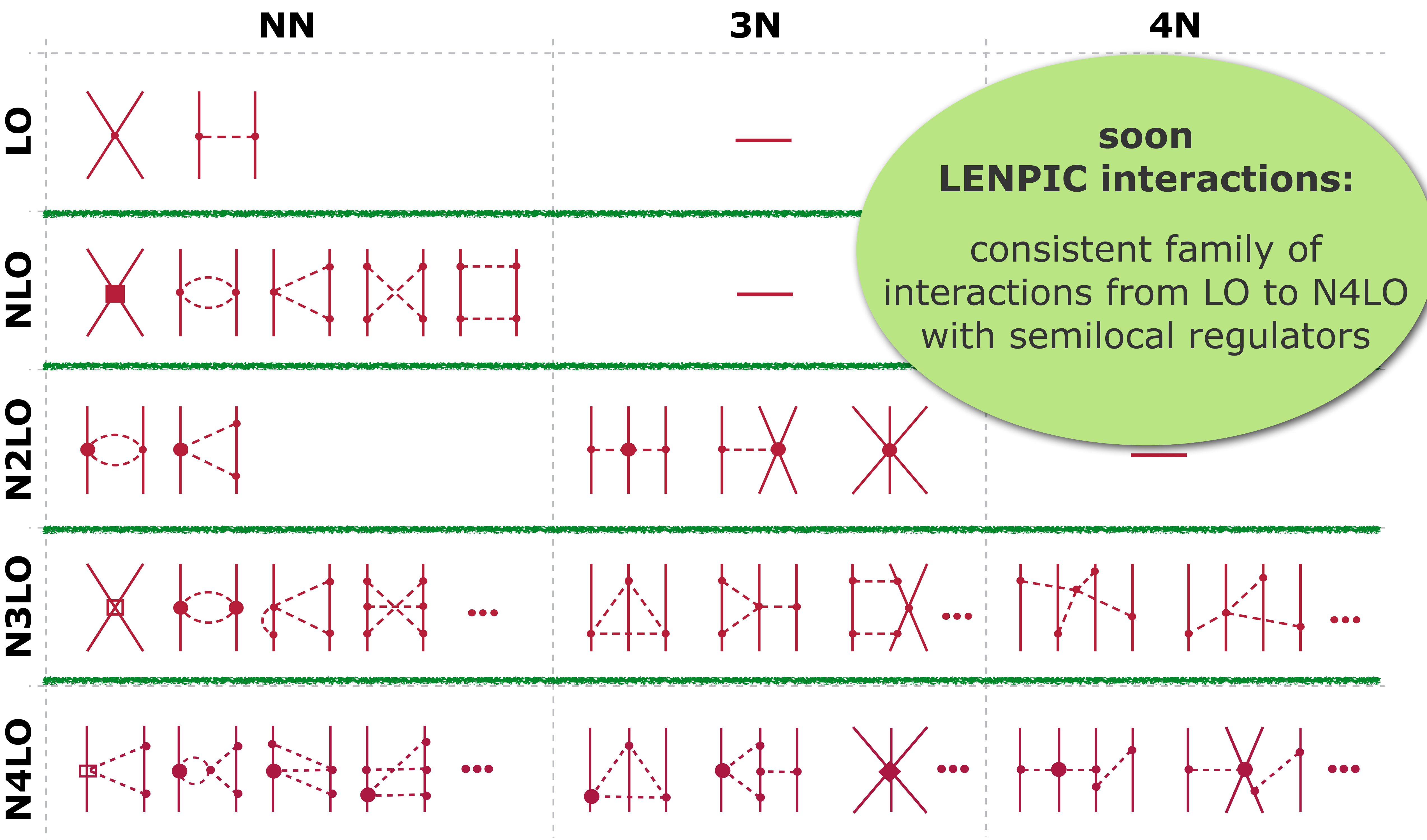


soon
LENPIC interactions:

consistent family of interactions from LO to N4LO with semilocal regulators

Similarity Renormalization Group

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

continuous unitary transformation driving Hamiltonian towards diagonal form

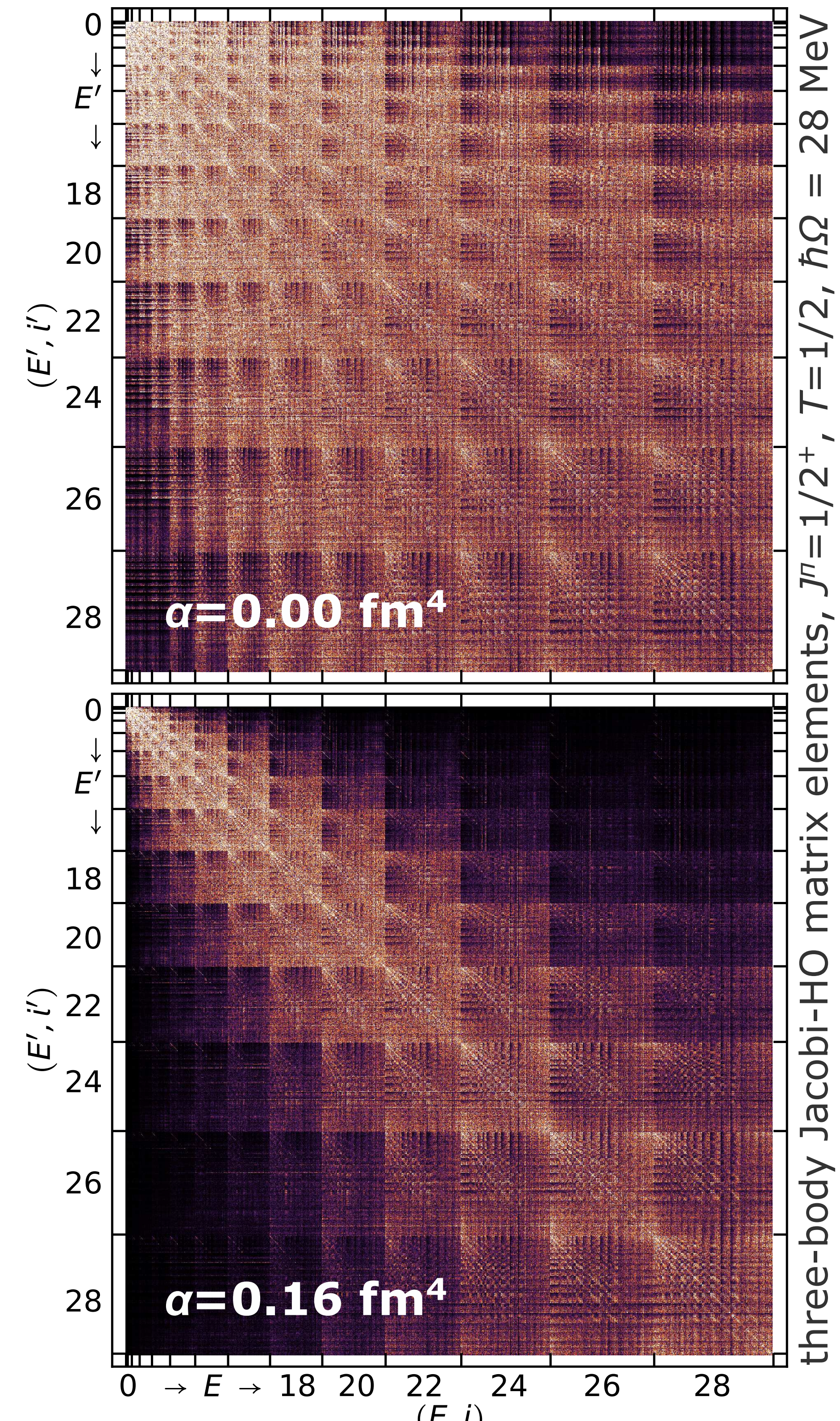
- unitary transformation via flow equation

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

- 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

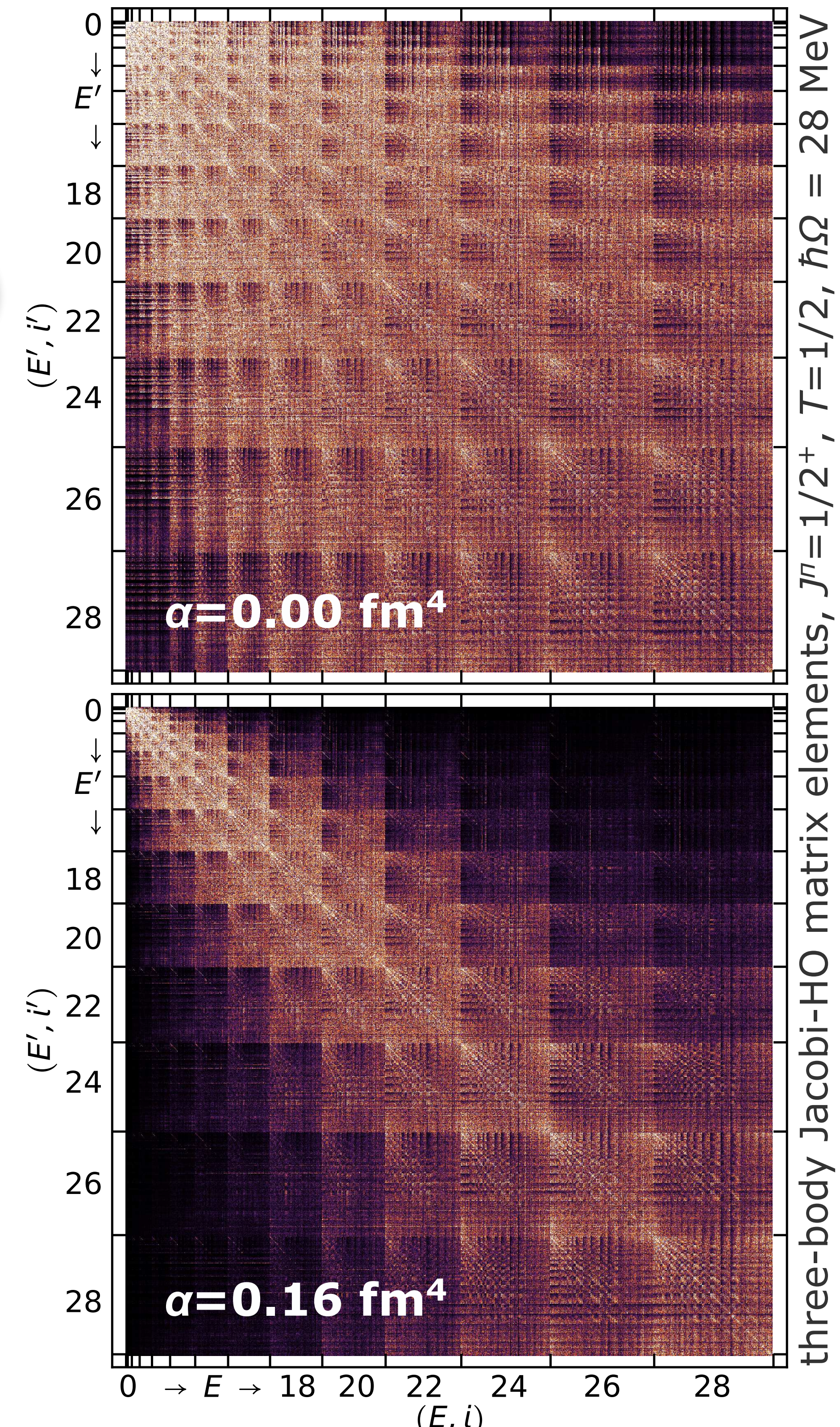
con:
induces many-body
interactions

- need to truncate evolved Hamiltonian

$$\mathrm{H}_\alpha = \mathrm{H}_\alpha^{[1]} + \mathrm{H}_\alpha^{[2]} + \mathrm{H}_\alpha^{[3]} + \mathrm{H}_\alpha^{[4]} + \cdots$$

- 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

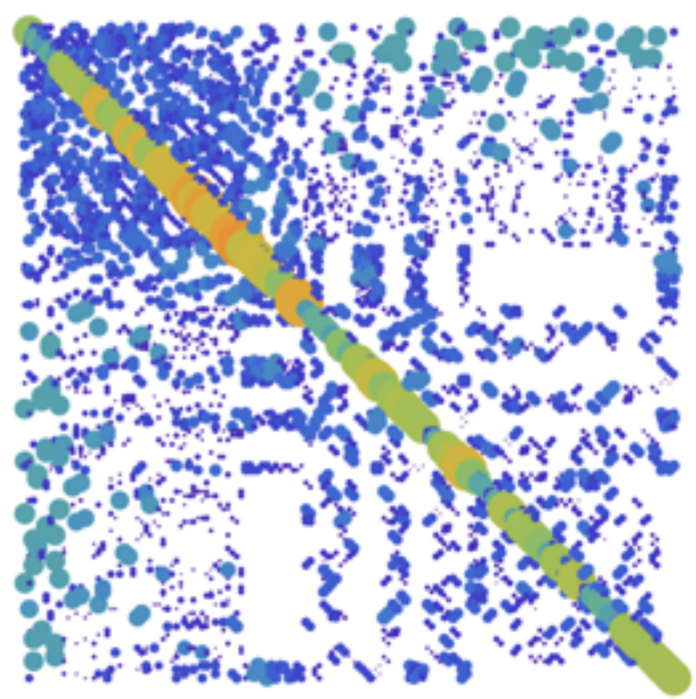


No-Core Shell Model

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

- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$



$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

No-Core Shell Model

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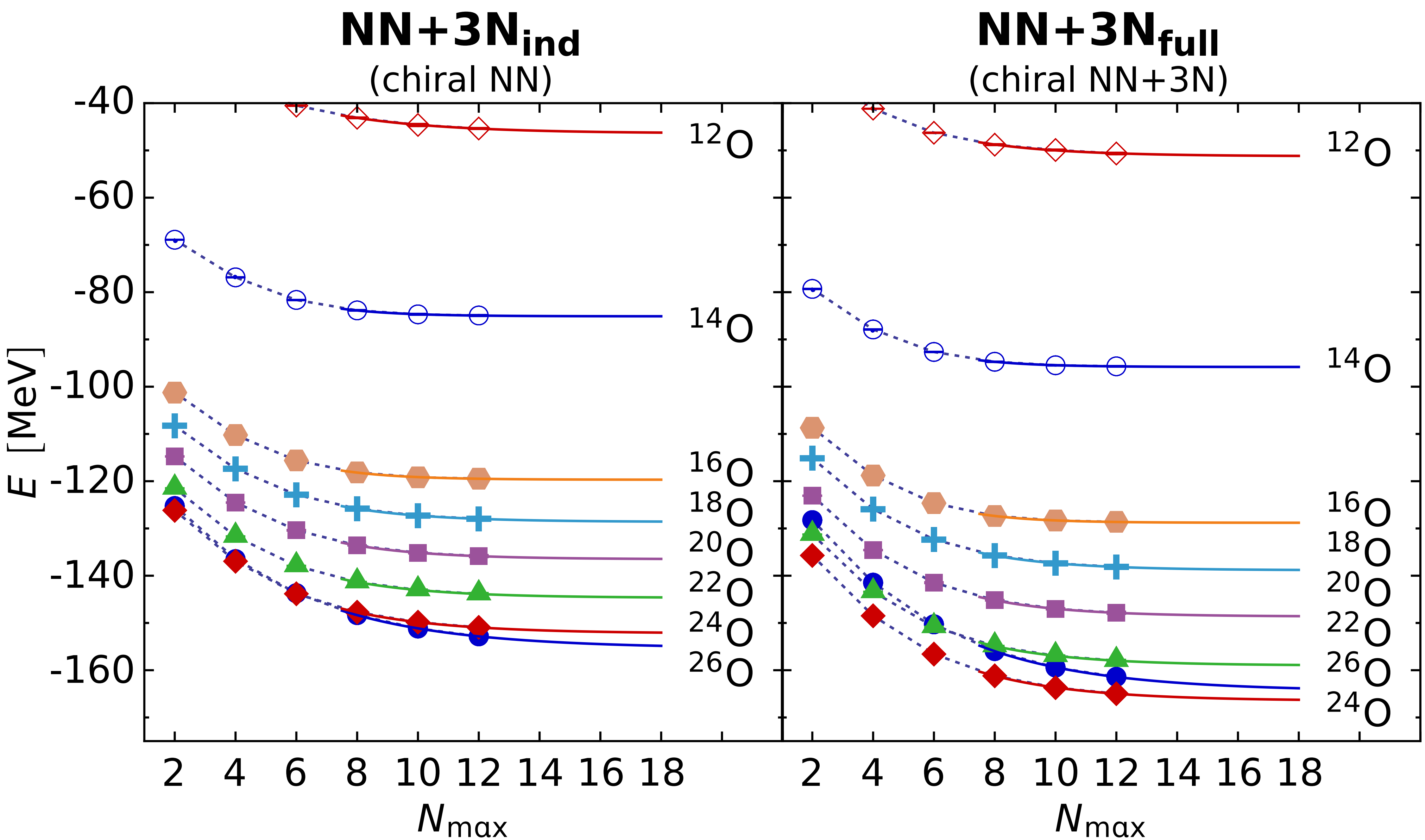
p- and lower sd-shell

- **idea**: 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

(tomorrow's talk by Petr Navrátil)

Ground States of Oxygen Isotopes

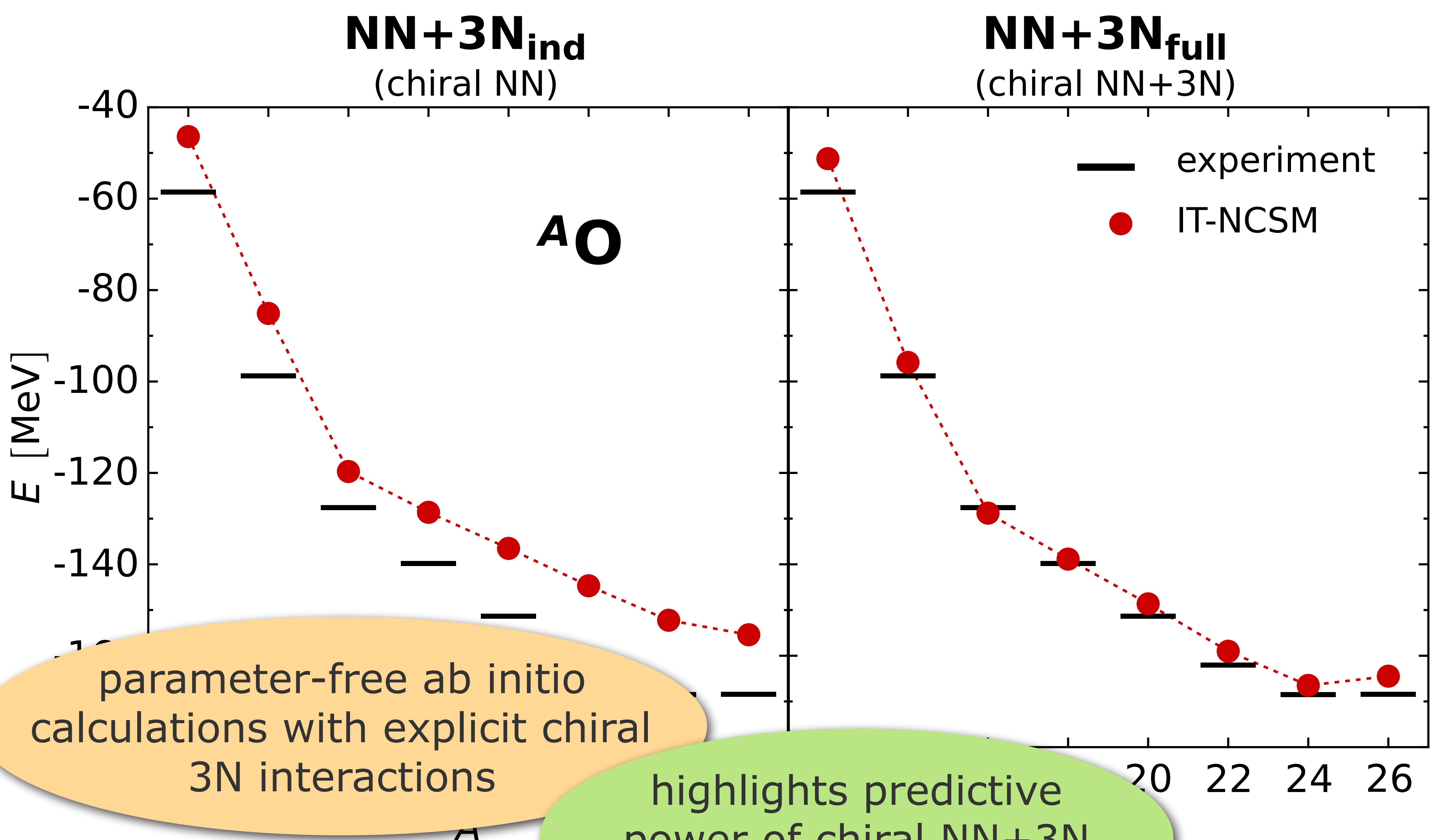
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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)



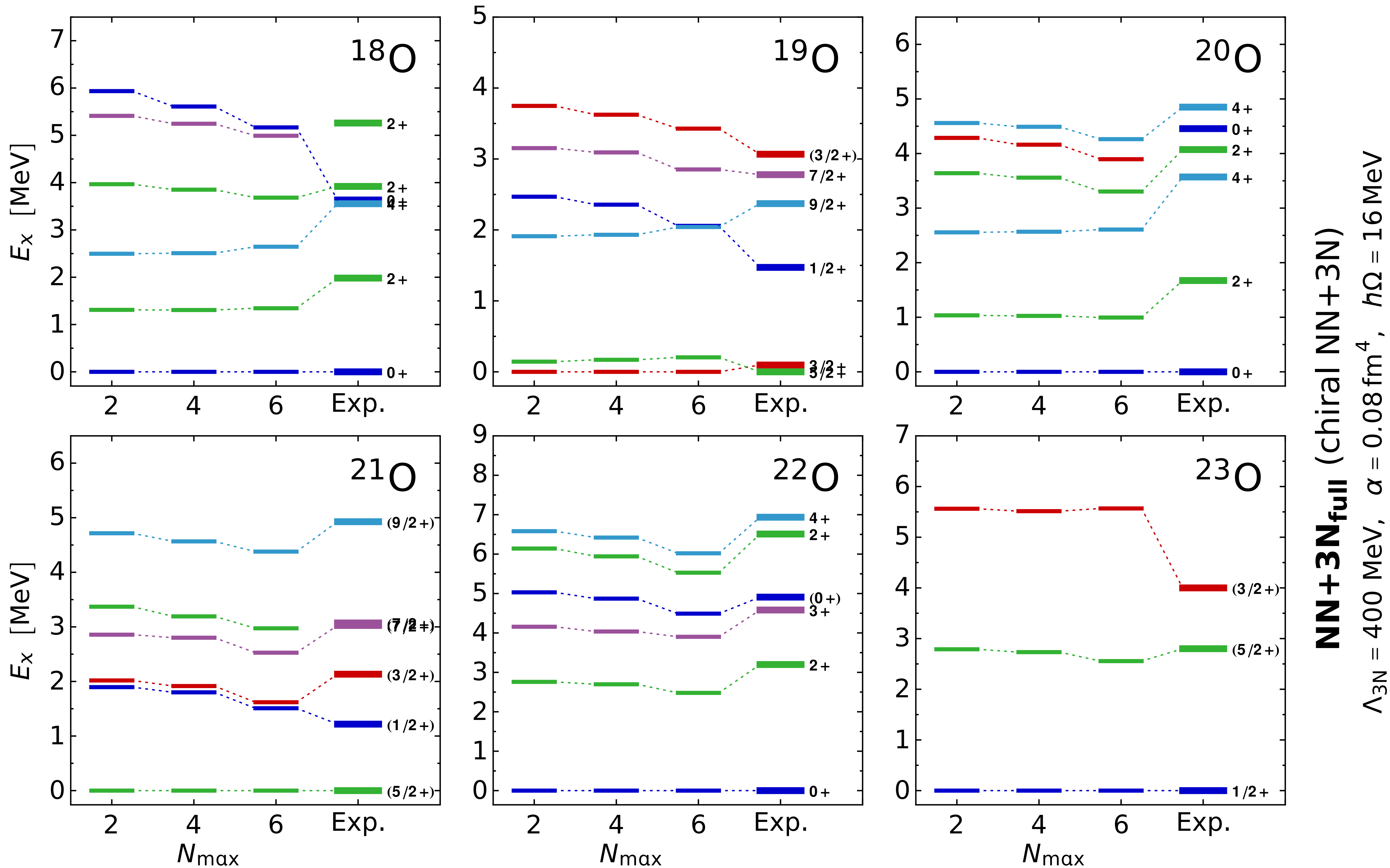
parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

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

Spectra of Oxygen Isotopes

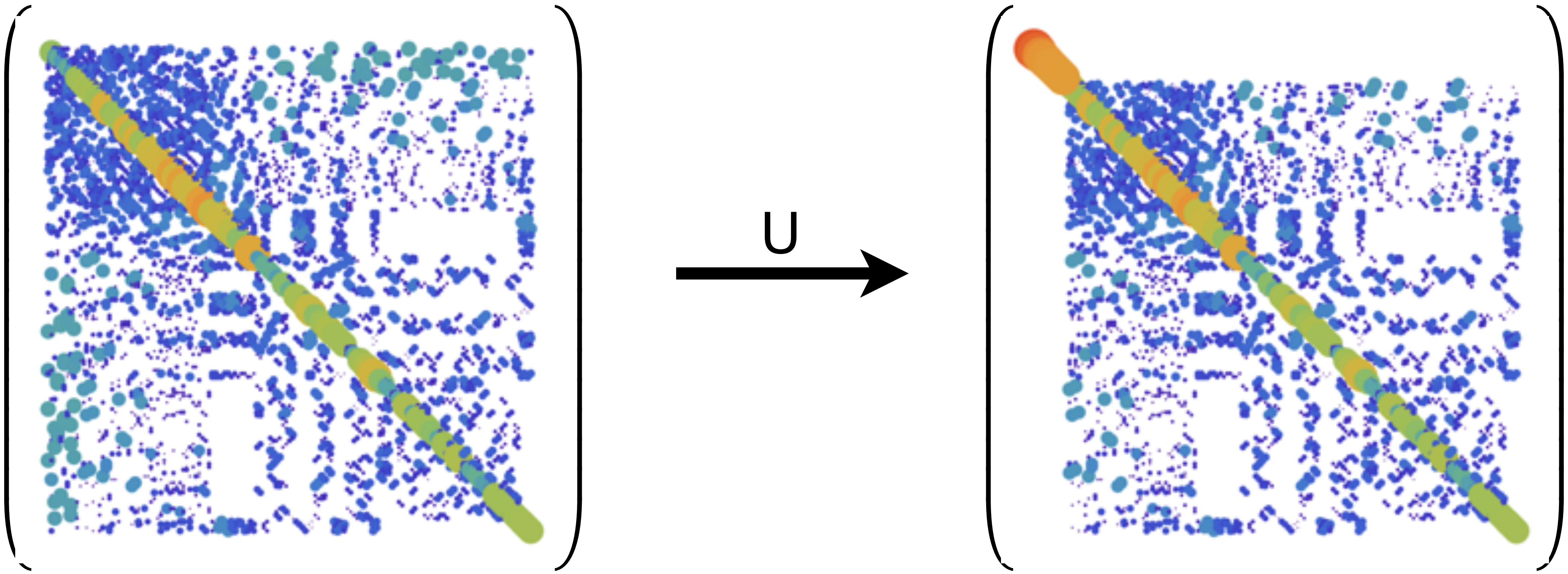
Hergert et al., PRL 110, 242501 (2013) & in prep.



Medium-Mass Methods

advent of novel ab initio approaches
targeting the ground state of medium-mass nuclei
very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian



Medium-Mass Methods

advent of novel ab initio approaches
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- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian

Tsukiyama, Bogner, Schwenk, Hergert,...

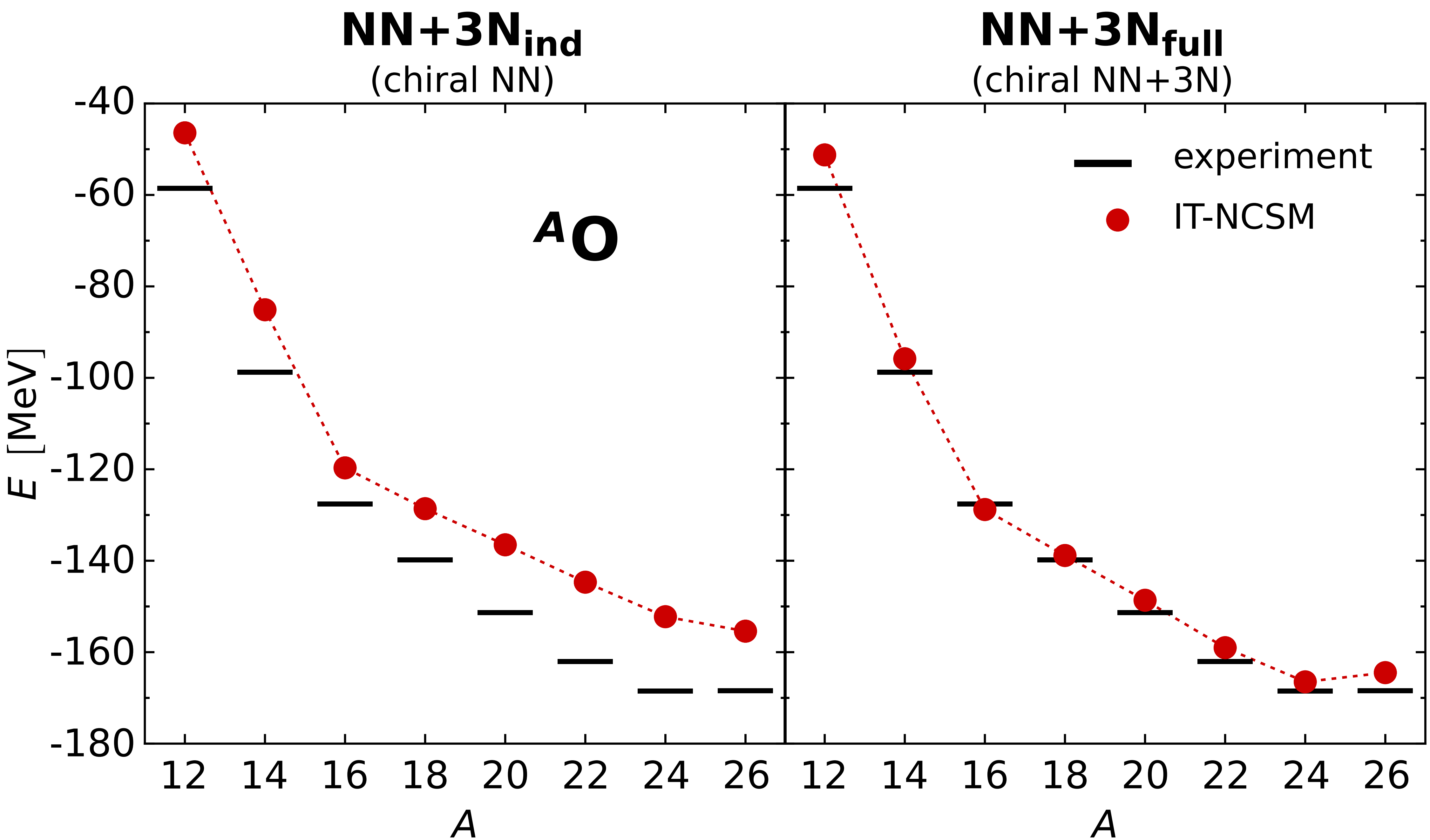
- **In-Medium Similarity Renormalisation Group**: decouple many-body reference state from particle-hole excitations by SRG transformation
  - normal-ordered A-body Hamiltonian truncated at the two-body level
  - open and closed-shell nuclei can be targeted directly

Hagen, Papenbrock, Dean, Piecuch, Binder,...

- **Coupled-Cluster Theory**: ground-state is parametrised by exponential wave operator acting on single-determinant reference state
  - truncation at doubles level (CCSD) with corrections for triples contributions
  - directly applicable for closed-shell nuclei, equations-of-motion methods for open-shell

Ground States of Oxygen Isotopes

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



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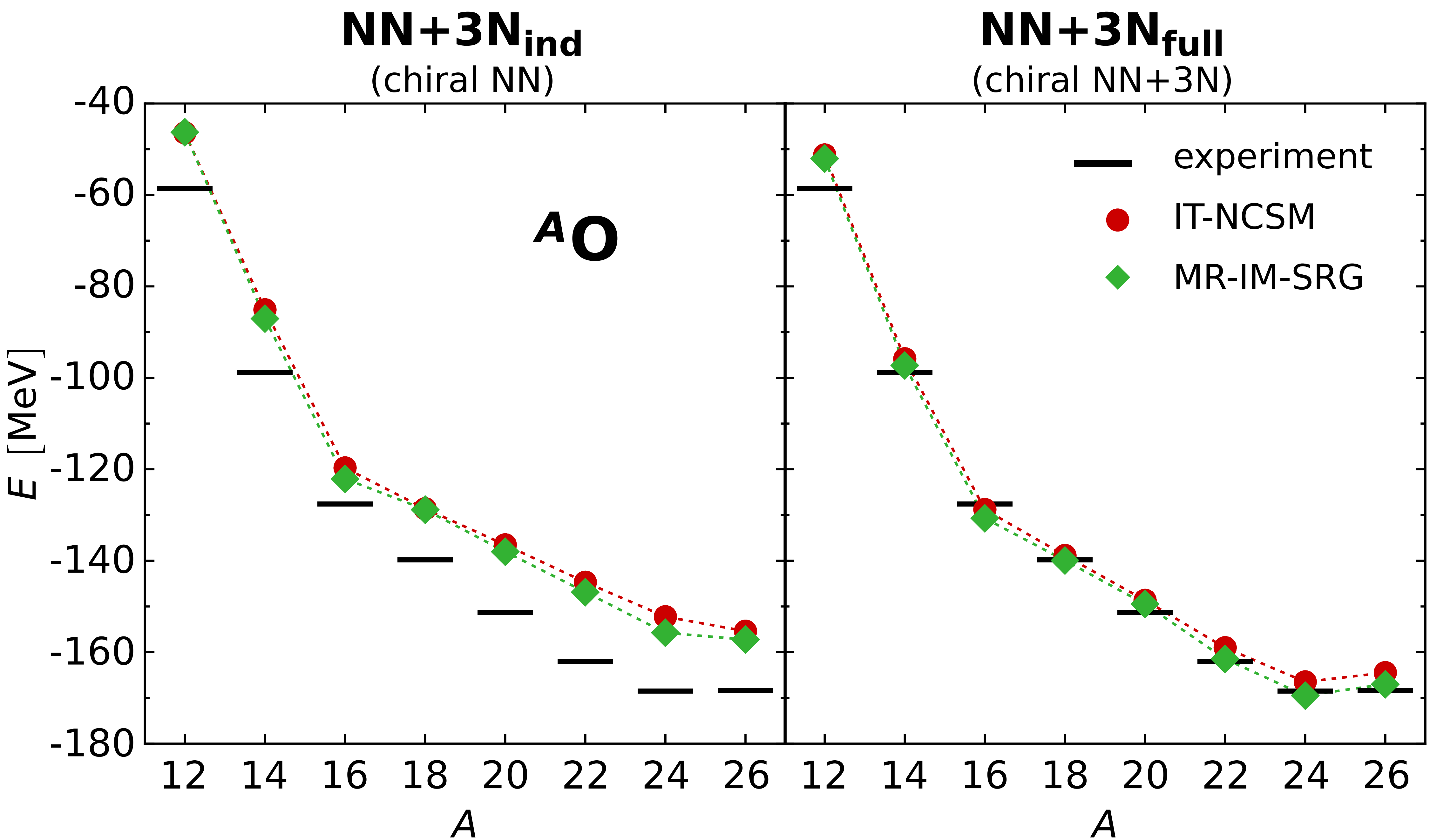

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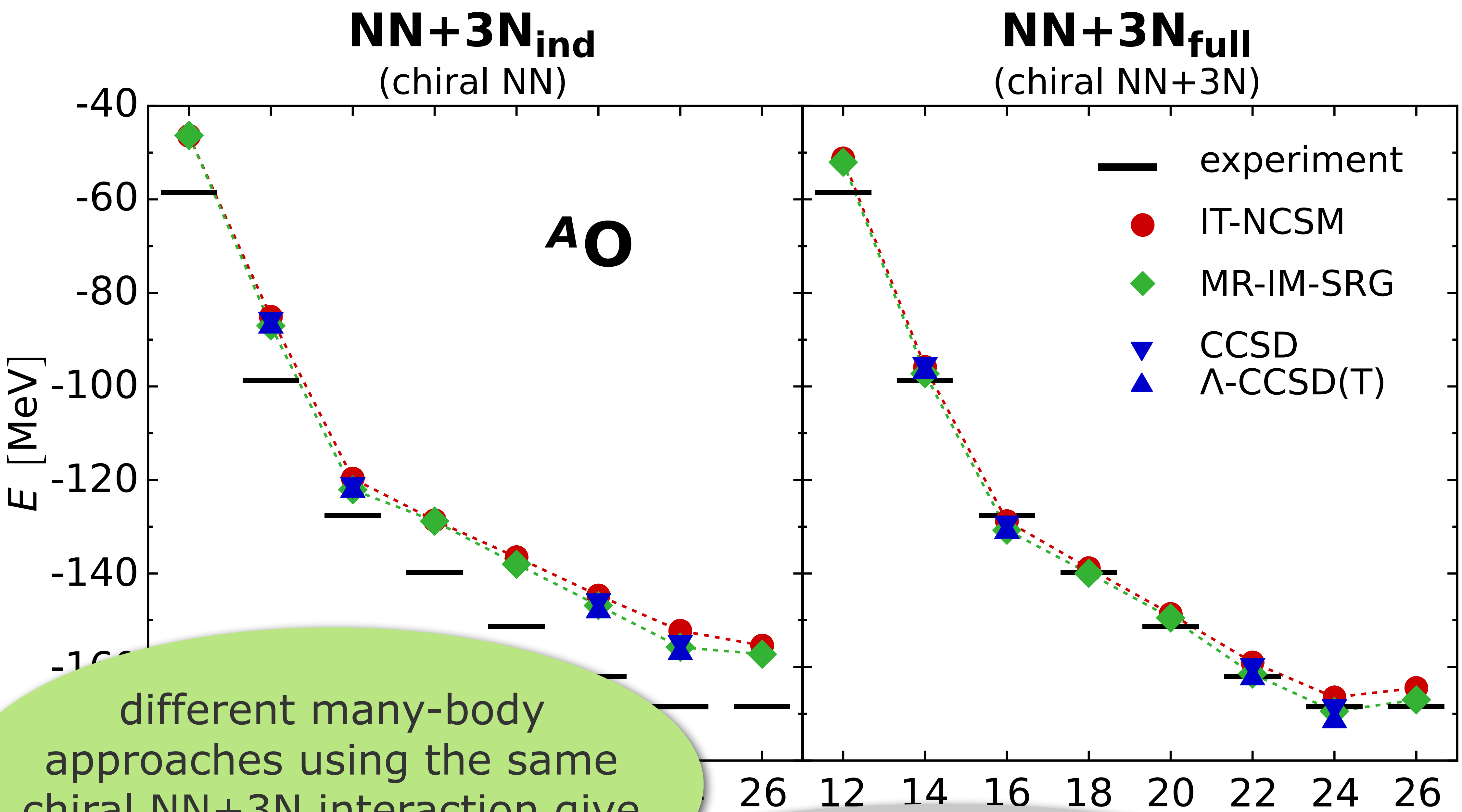
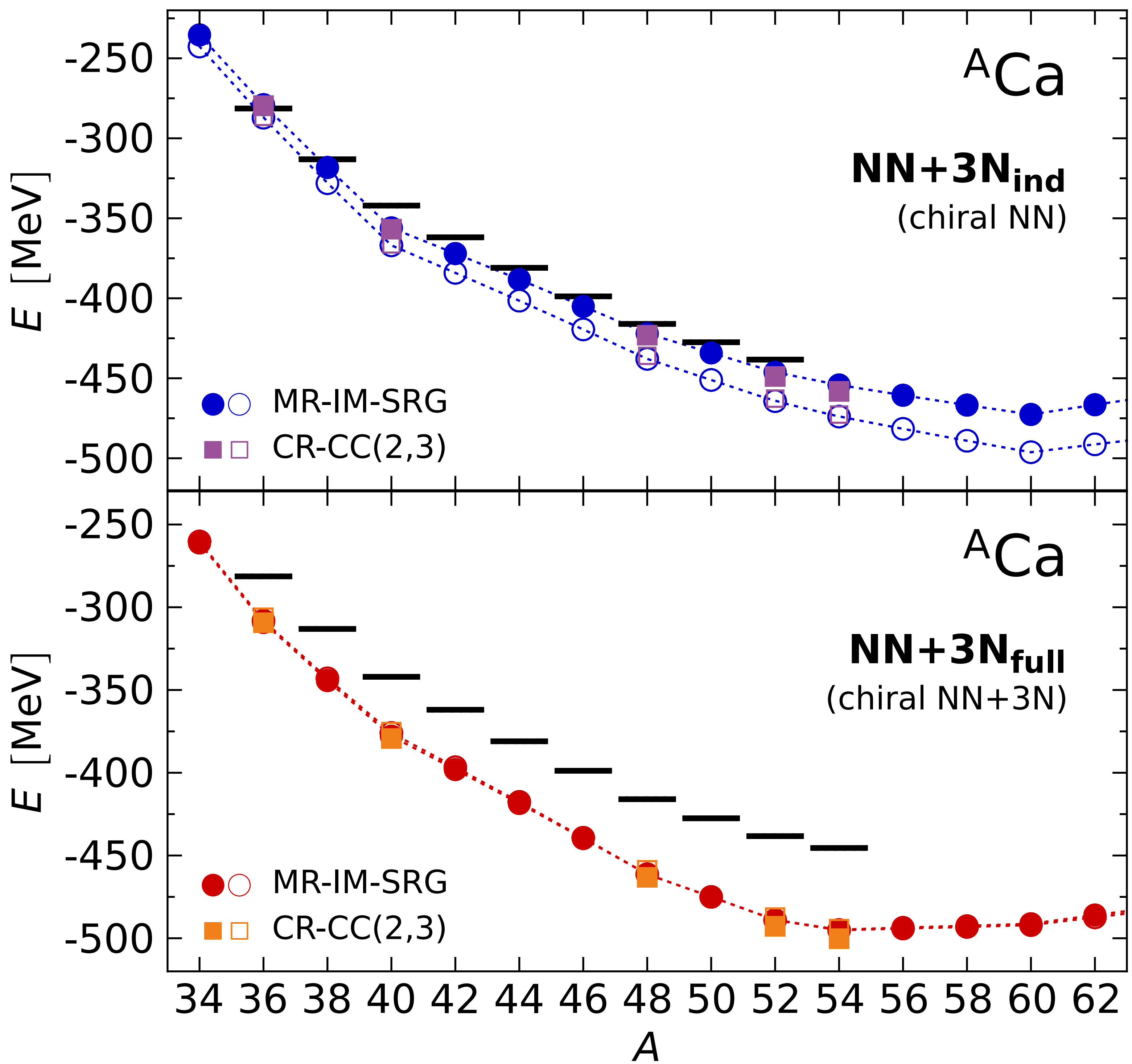


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Open-Shell Medium-Mass Nuclei

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

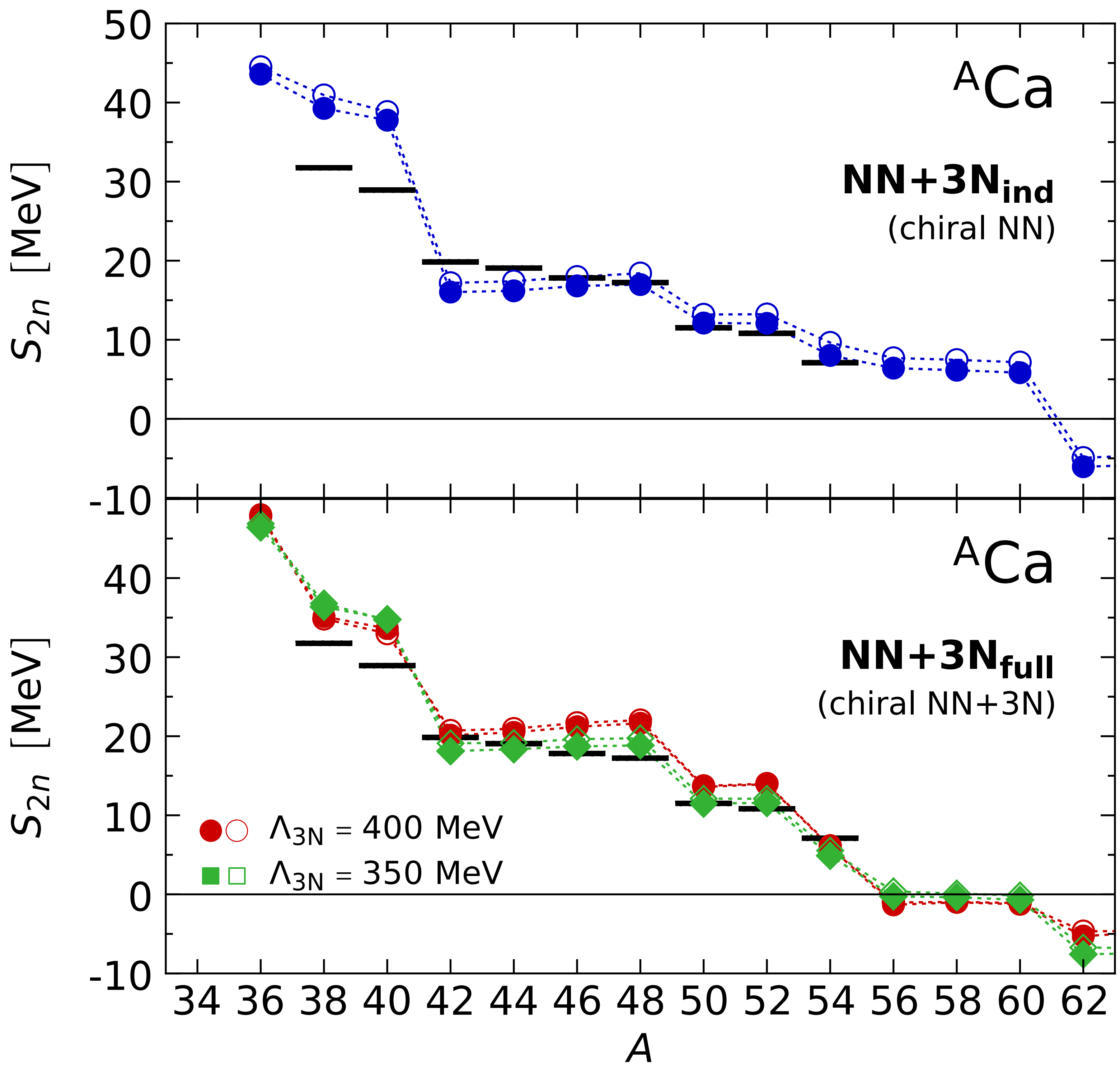


- systematic multi-reference IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

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
- 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

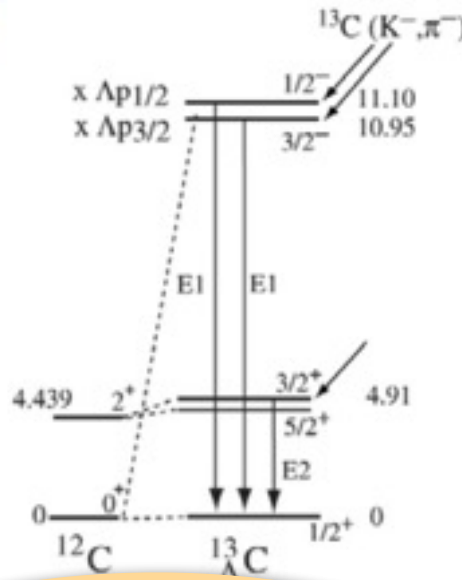
Beyond the Ordinary:

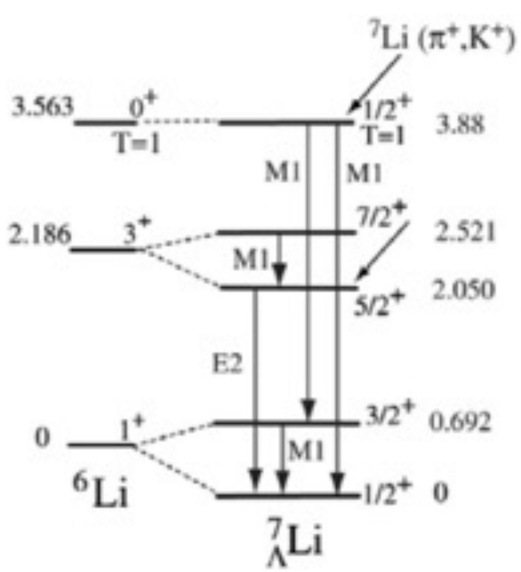
Hypernuclei

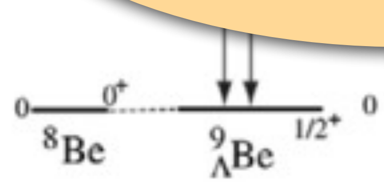
with

Roland Wirth

Ab Initio Hypernuclear Structure





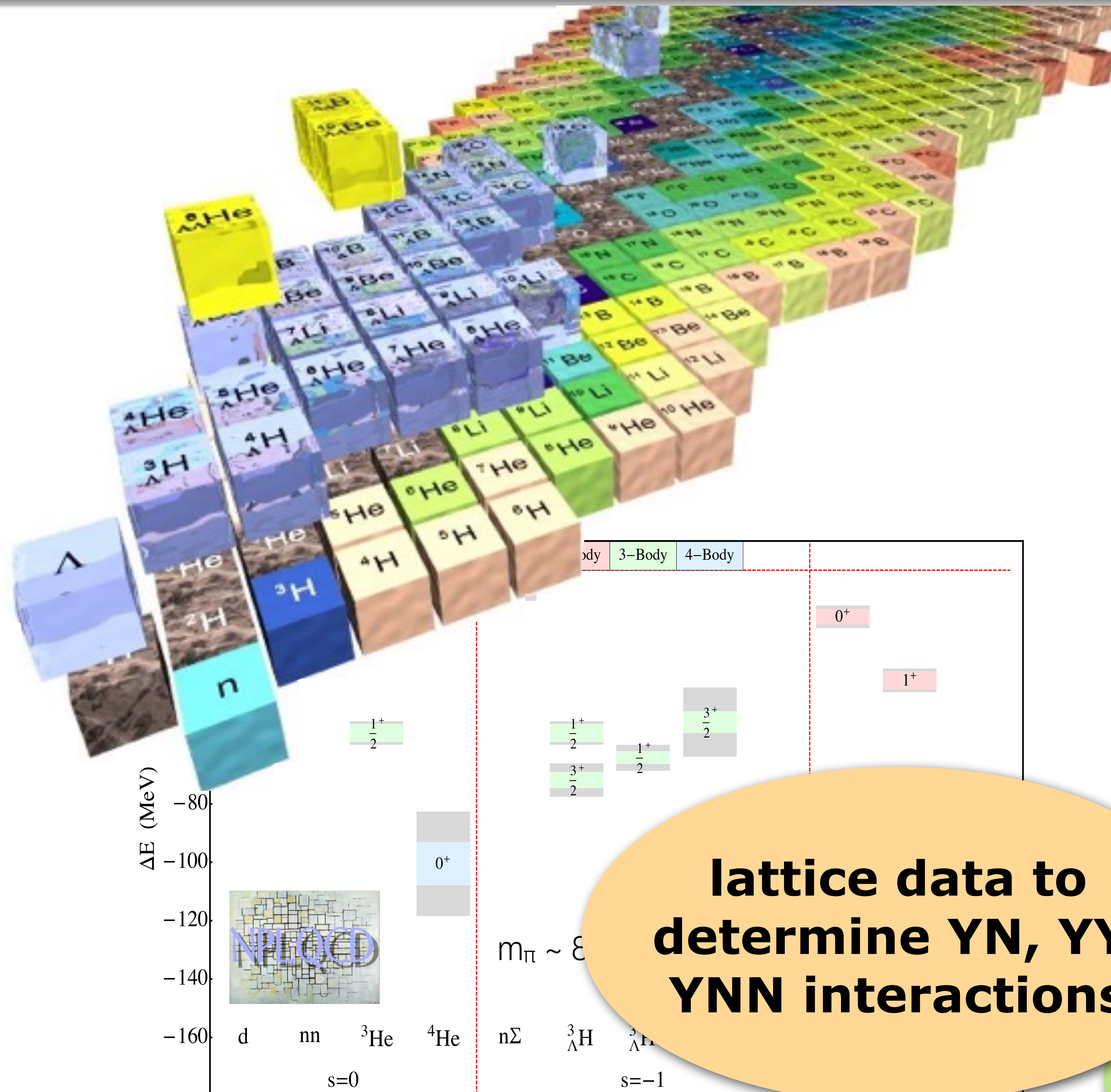


- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body and phenomenological shell or cluster model calculations done so far
- chiral YN & YY interactions at (N)LO are available

constrain YN interactions with hypernuclear spectroscopy

time to transfer ab initio toolbox to hypernuclei

Ab Initio Hypernuclear Structure



- Lattice QCD can be a game changer in hypernuclear physics
- extract YN & YY phase shifts from Lattice QCD, possibly also YNN
- compute light hypernuclei directly on the lattice

lattice data to determine YN, YY, YNN interactions

structure theory for consistency check and access to heavier hypernuclei

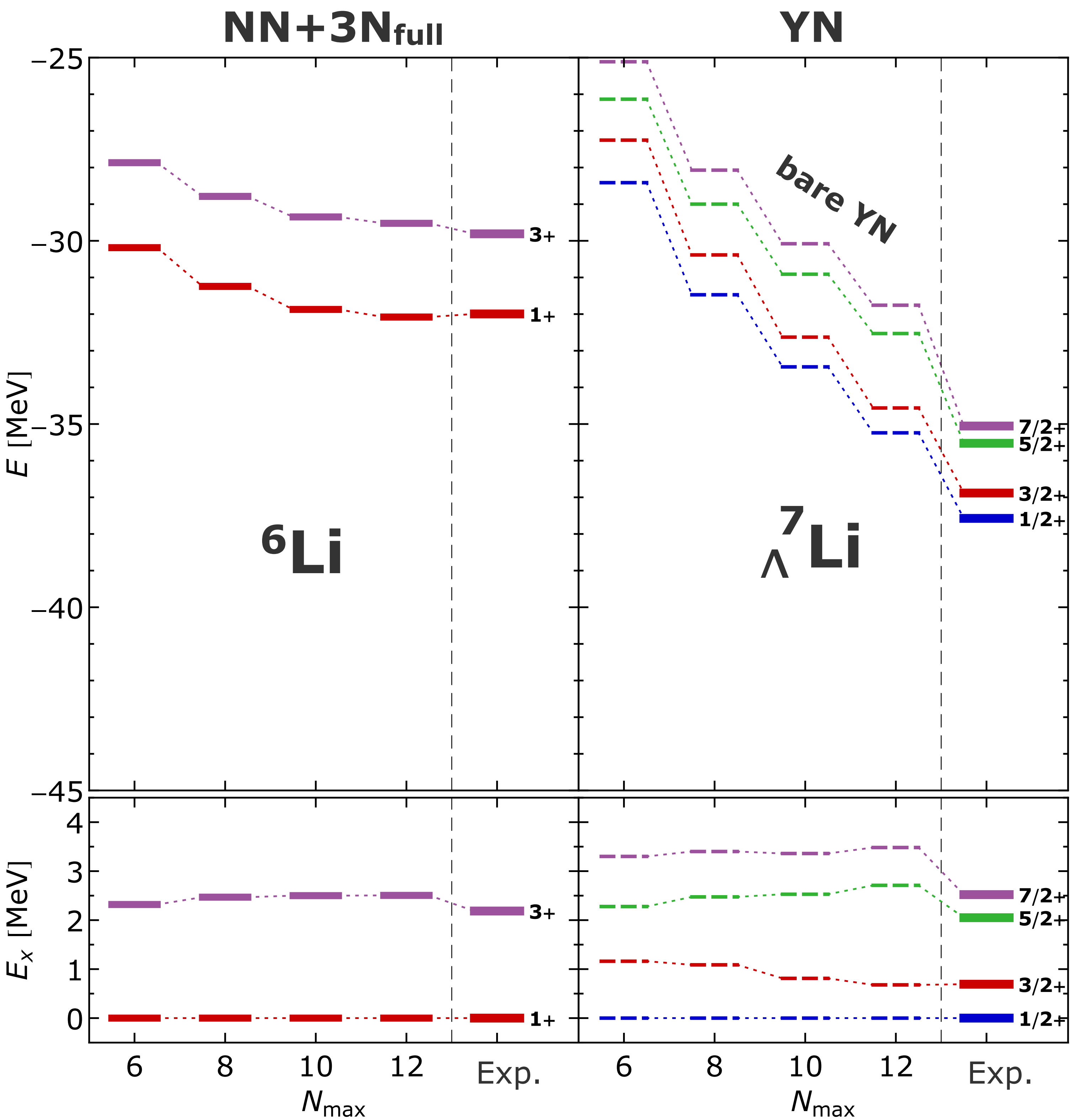
Ab Initio Toolbox for Hypernuclei

Wirth et al., PRL 113, 192502 (2014) & in prep.

- **Hamiltonian from chiral EFT**
  - NN+3N: standard chiral Hamiltonian (Entem&Machleidt, Navrátil)
  - YN: LO chiral interaction (Haidenbauer et al.), NLO in progress
- **Similarity Renormalization Group**
  - consistent SRG-evolution of NN, 3N, YN interactions
  - using particle basis and including ΛΣ-coupling (larger matrices)
  - Λ-Σ mass difference and $p\Sigma^{\pm}$ Coulomb included consistently
- **Importance Truncated No-Core Shell Model**
  - include explicit $(p, n, \Lambda, \Sigma^{+}, \Sigma^{0}, \Sigma^{-})$ with physical masses
  - larger model spaces easily tractable with importance truncation
  - all p-shell single-Λ hypernuclei are accessible

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

Wirth et al., in prep.



IT-NCSM

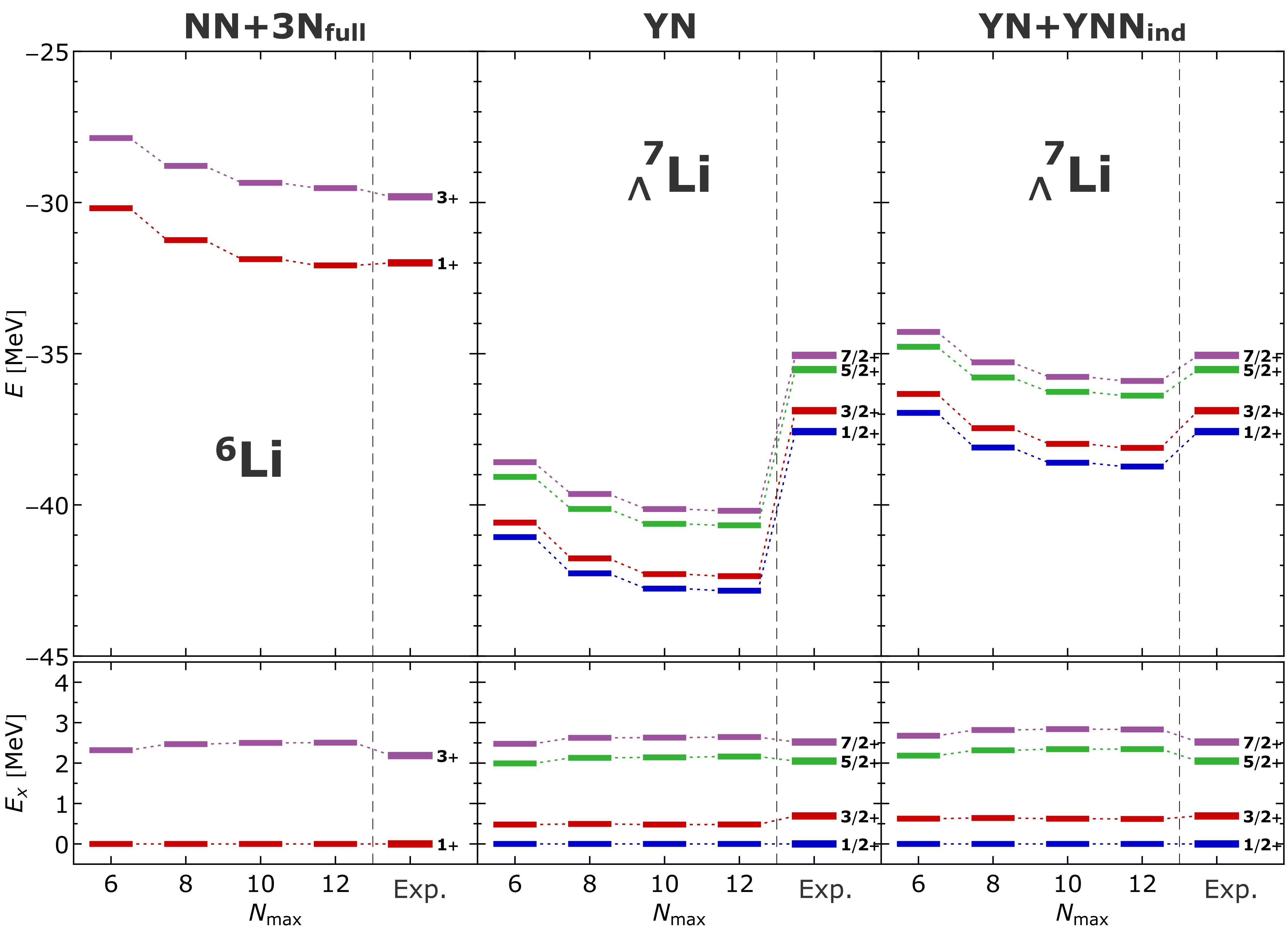
chiral NN+3N
standard
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm^4

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm^4

$\hbar\Omega$=20 MeV

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

Wirth et al., in prep.



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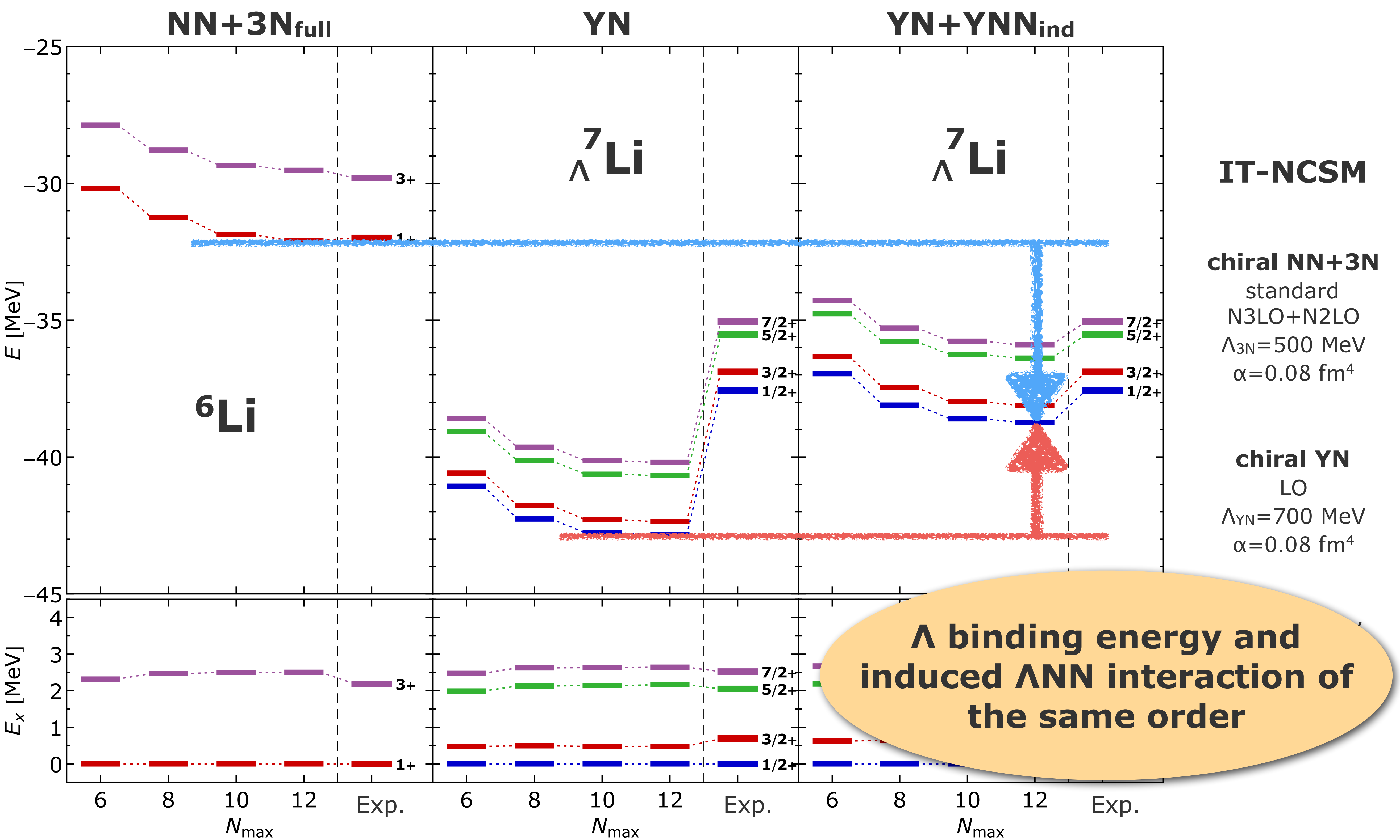

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N3LO+N2LO
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chiral YN
LO
Λ_{YN}=700 MeV
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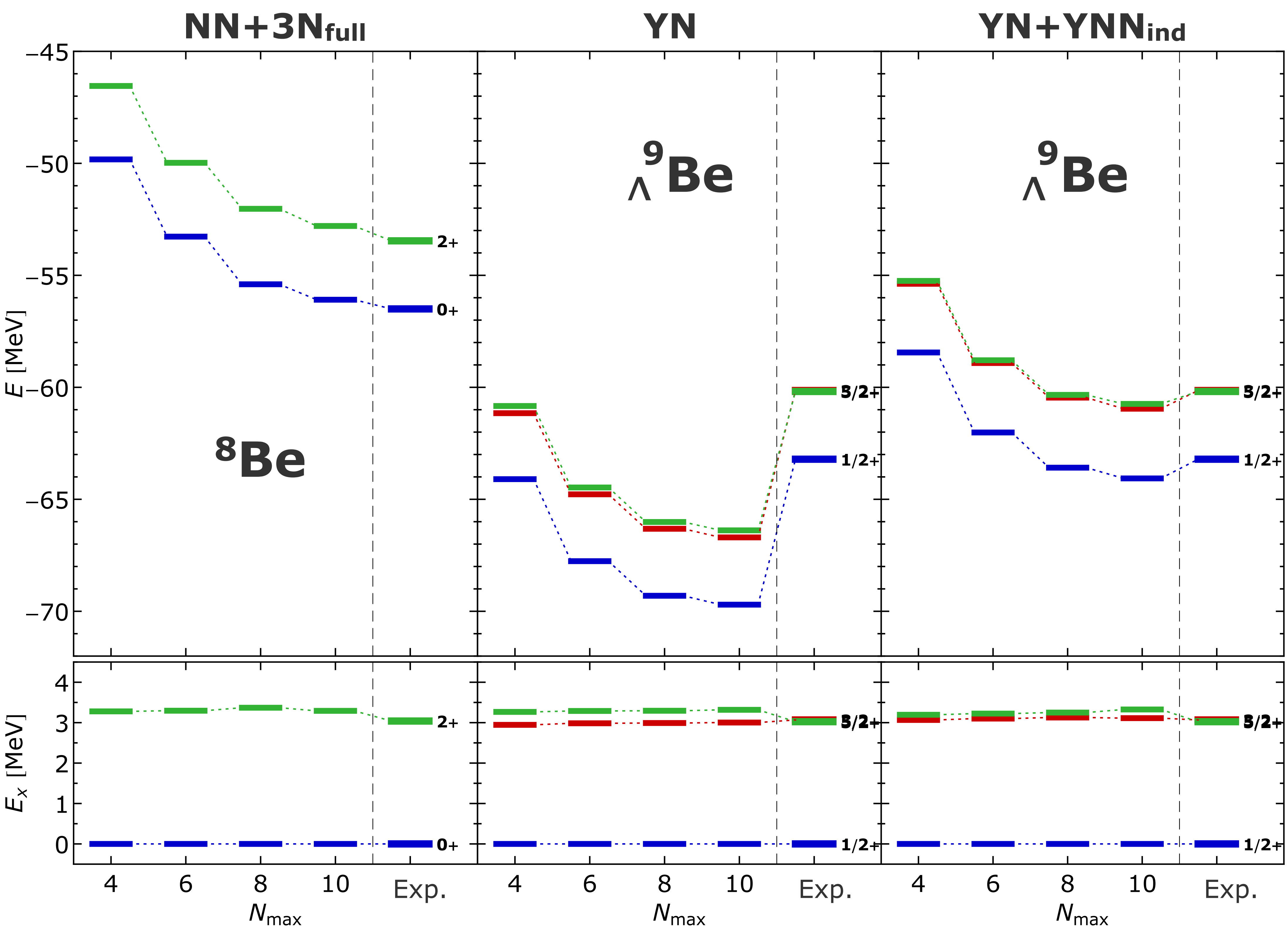
Application: $^{9}_{\Lambda}$Be

Wirth et al., in prep.



IT-NCSM

chiral NN+3N
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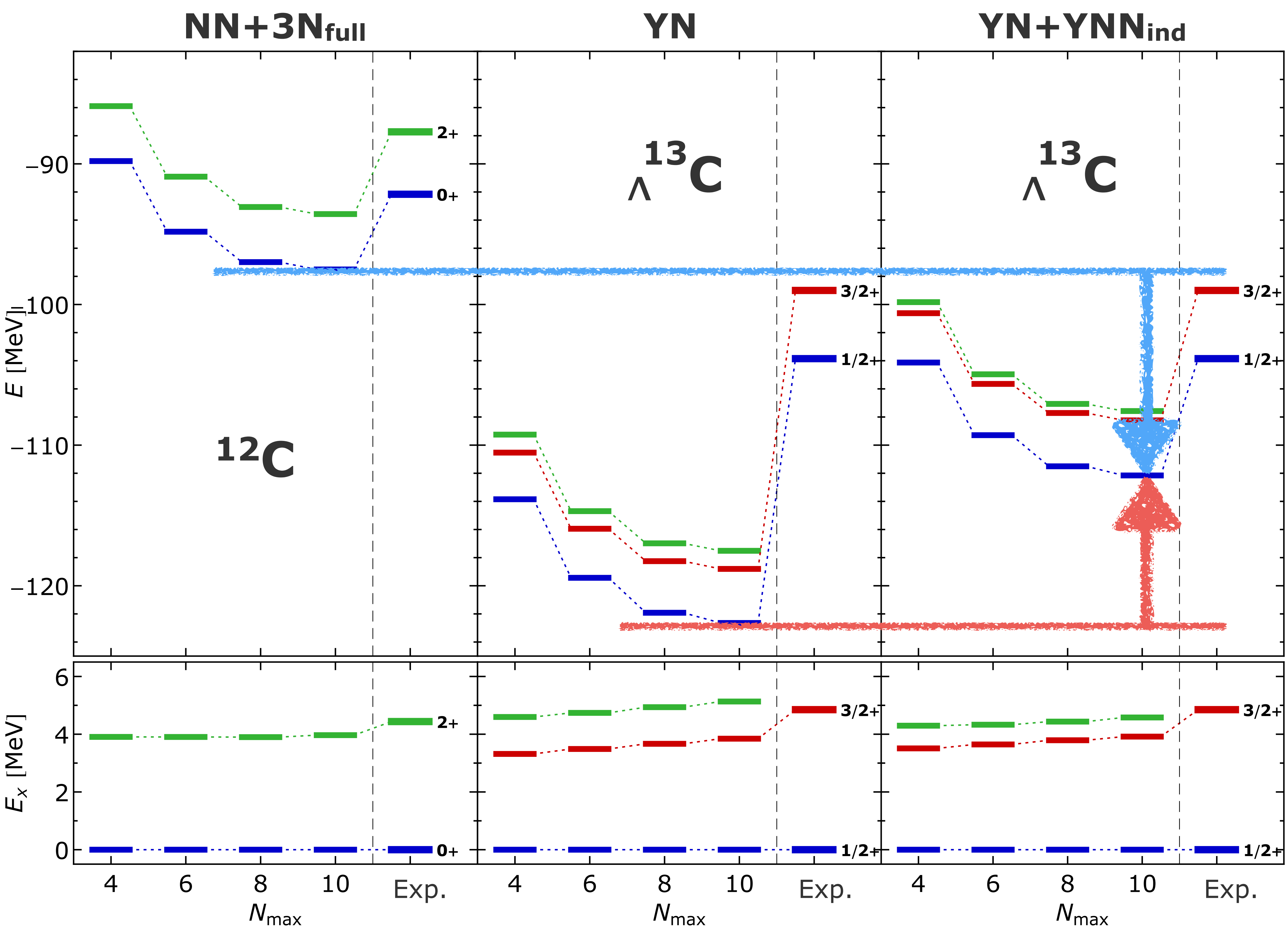
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm⁴

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm⁴

ħΩ=20 MeV

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

Wirth et al., in prep.



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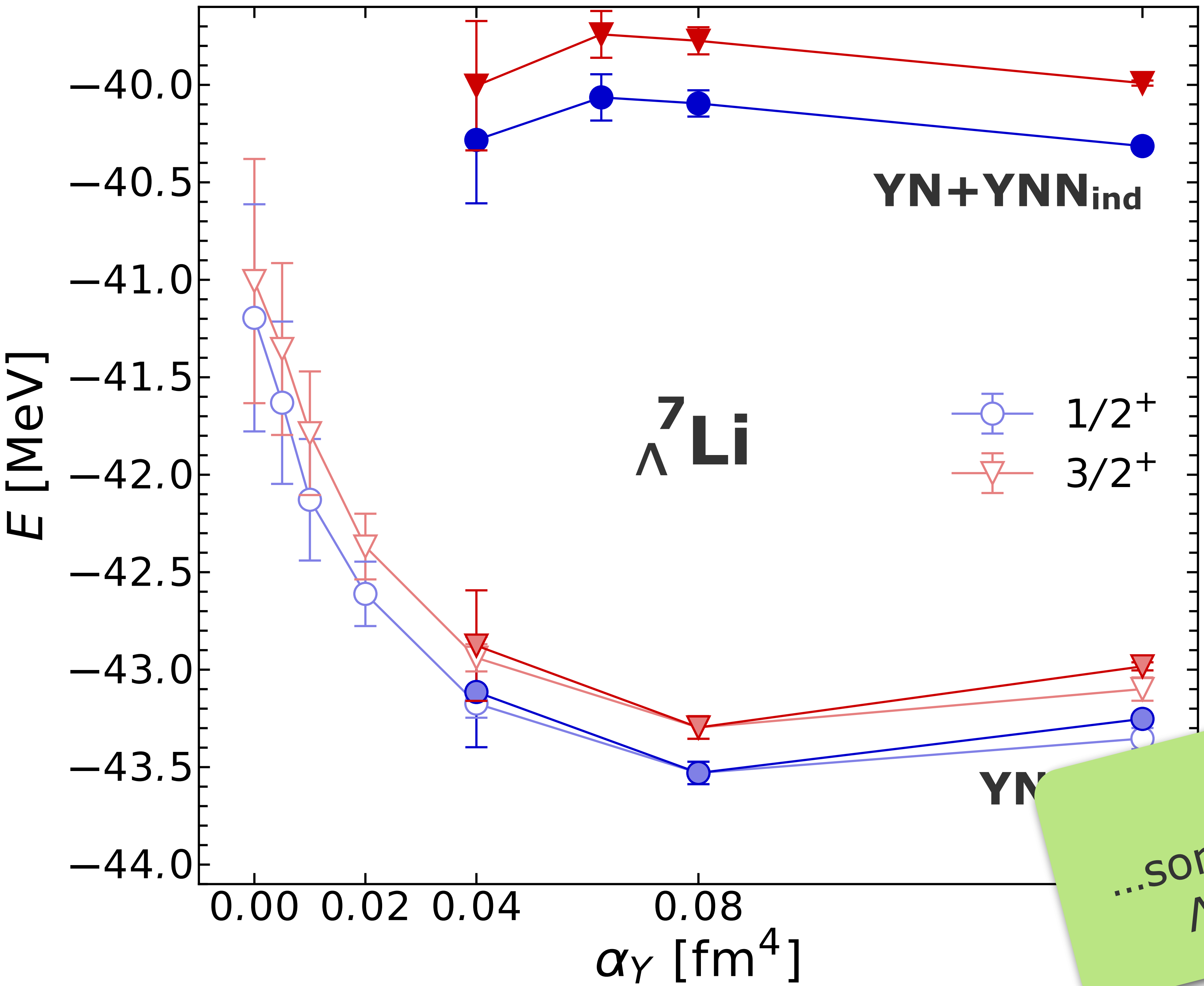
ħΩ=20 MeV

Induced YNN Interactions

Wirth et al., in prep.



- **induced YNN interactions** are surprisingly large in light hypernuclei

$V_{\mathrm{YNN_{ind}},\alpha} \sim 0.80\ |B_\Lambda|$

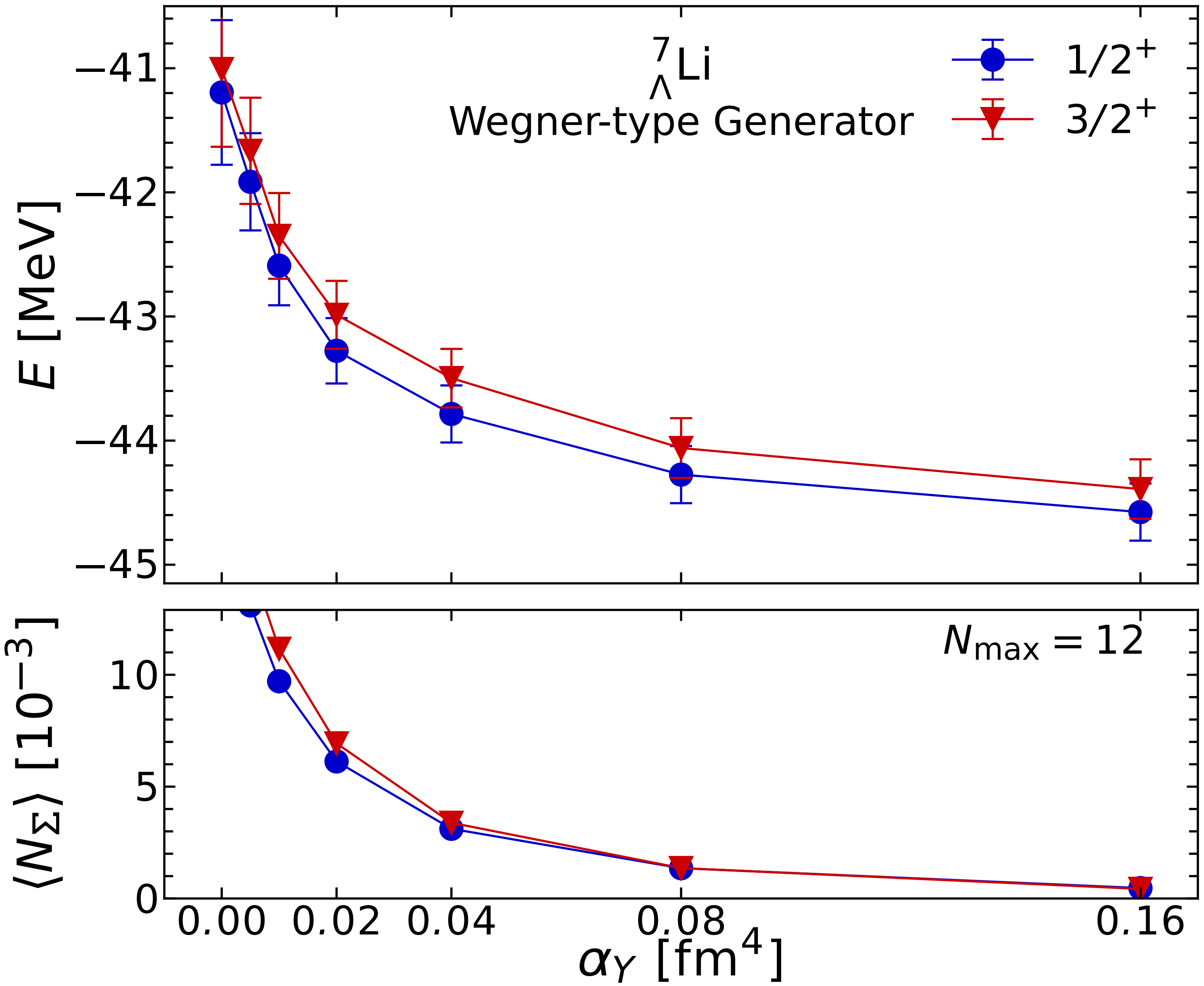
$V_{\mathrm{YNN_{ind}},\alpha} \sim 0.40\ |V_{\mathrm{YN},\alpha}|$

$V_{\mathrm{NNN_{ind}},\alpha} \sim 0.07\ |V_{\mathrm{NN},\alpha}|$

WHY ?
...something to do with
Λ-Σ conversion ?

Suppression of Λ-Σ Conversion

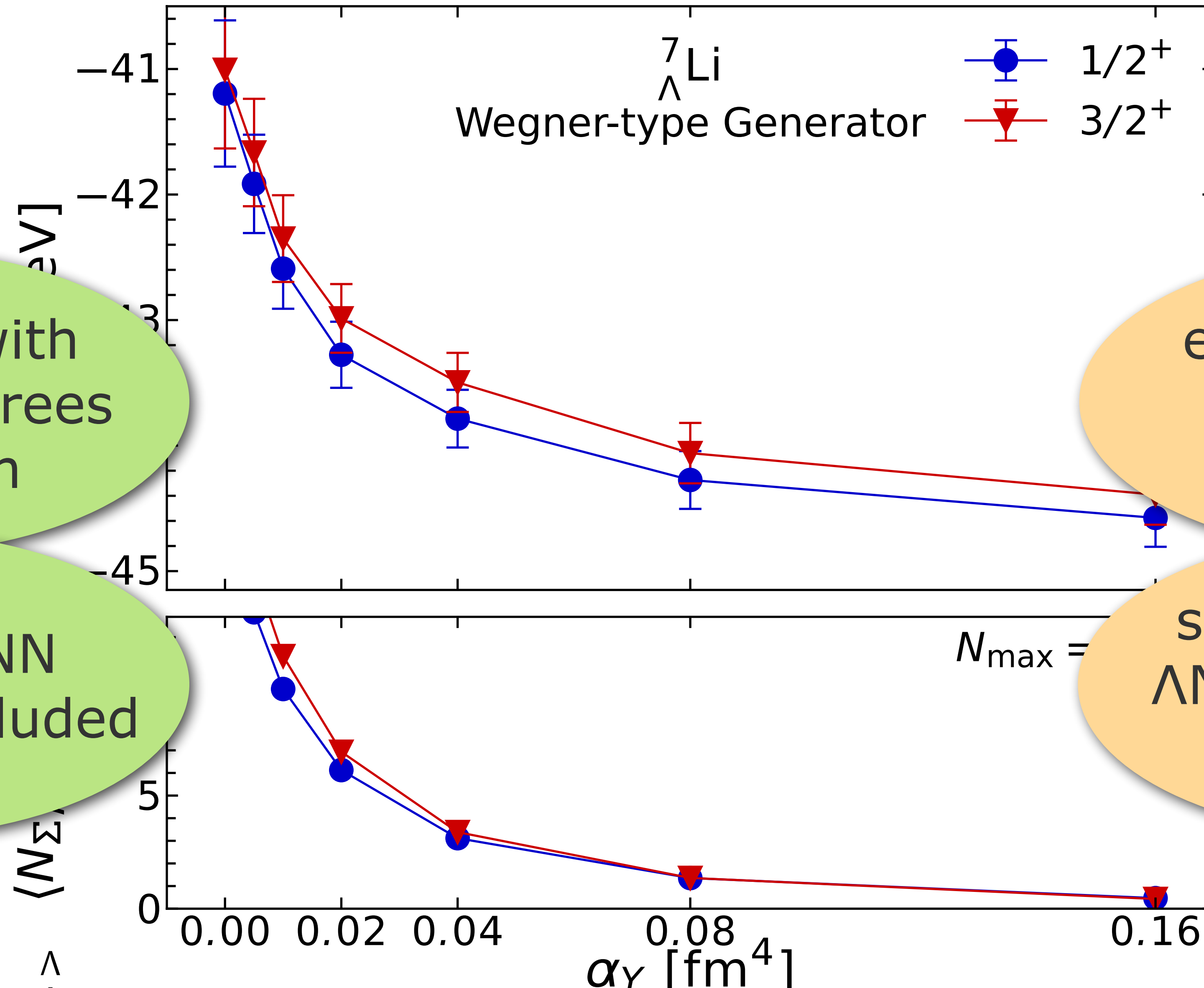
Wirth et al., in prep.



- design SRG-generator that **suppresses the Λ-Σ conversion** exclusively
- Σ admixture in the wave functions eliminated or "integrated out"
- same large induced YNN interactions as in standard SRG

Suppression of Λ-Σ Conversion

Wirth et al., in prep.

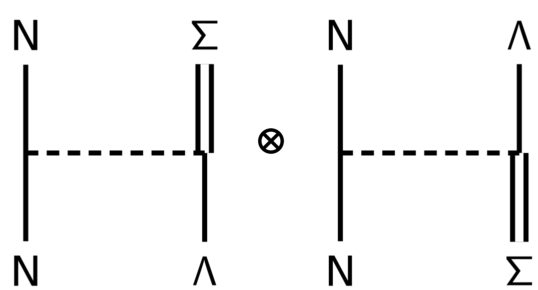


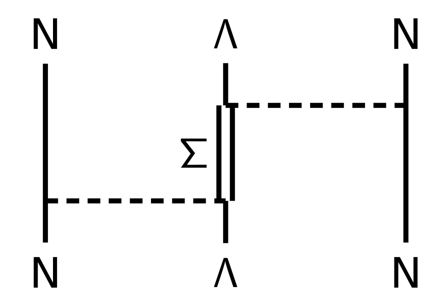
full theory with explicit Σ degrees of freedom

no initial YNN interaction included

effective Λ-only theory, Σ fully decoupled

strong repulsive ΛNN interaction is induced

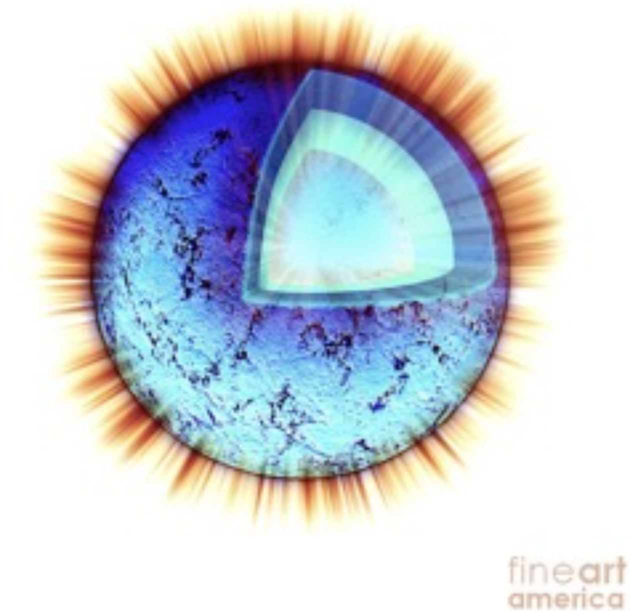


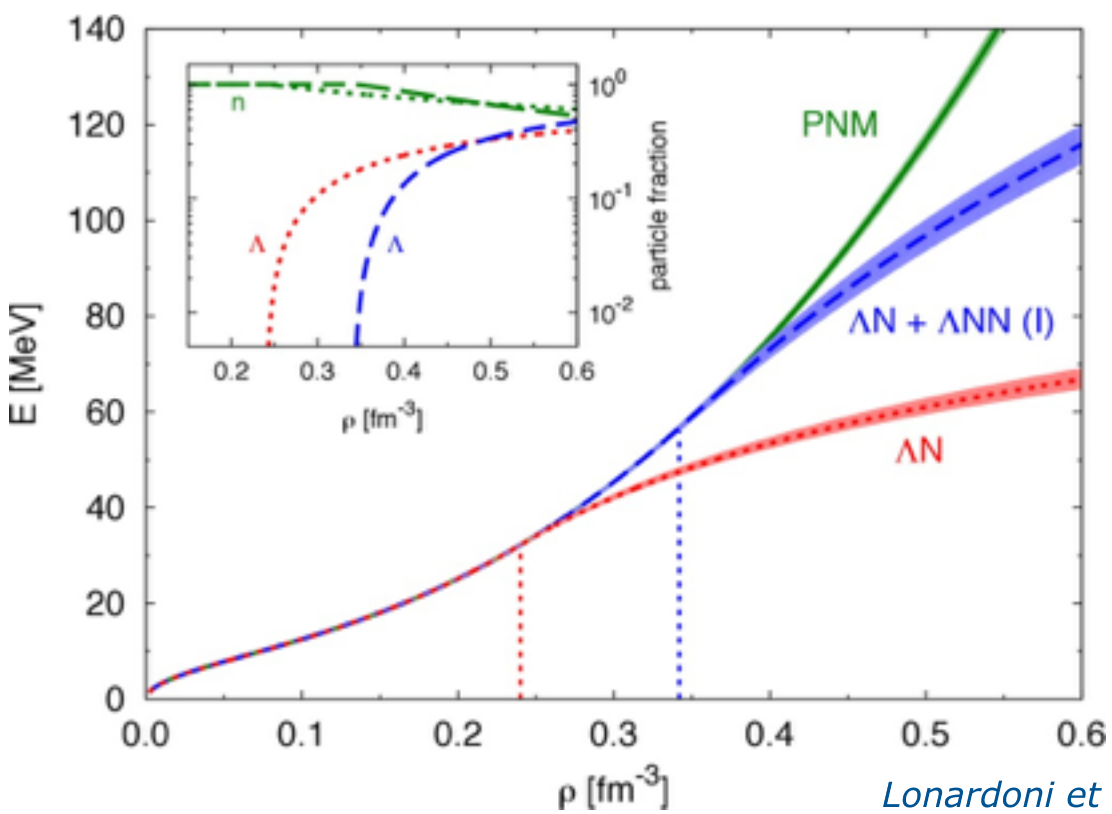


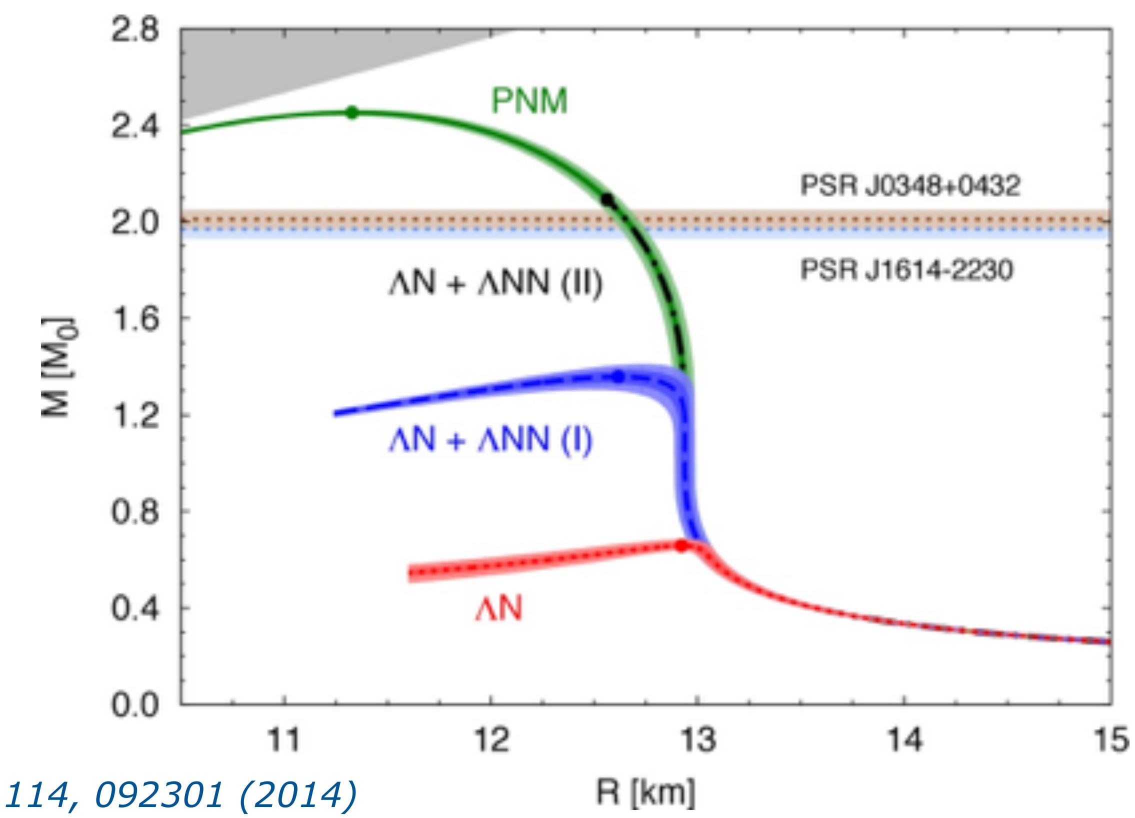
SRG evolves full coupled-channel theory to effective Λ-only theory

Implications for the Hyperon Puzzle

- neutron stars reach densities, where hyperon production should be energetically favorable
- including explicit Λs with ΛN interaction softens EOS - does not support $2M_\odot$ neutron star
- possible phenomenological fix: include strongly repulsive ΛNN interaction





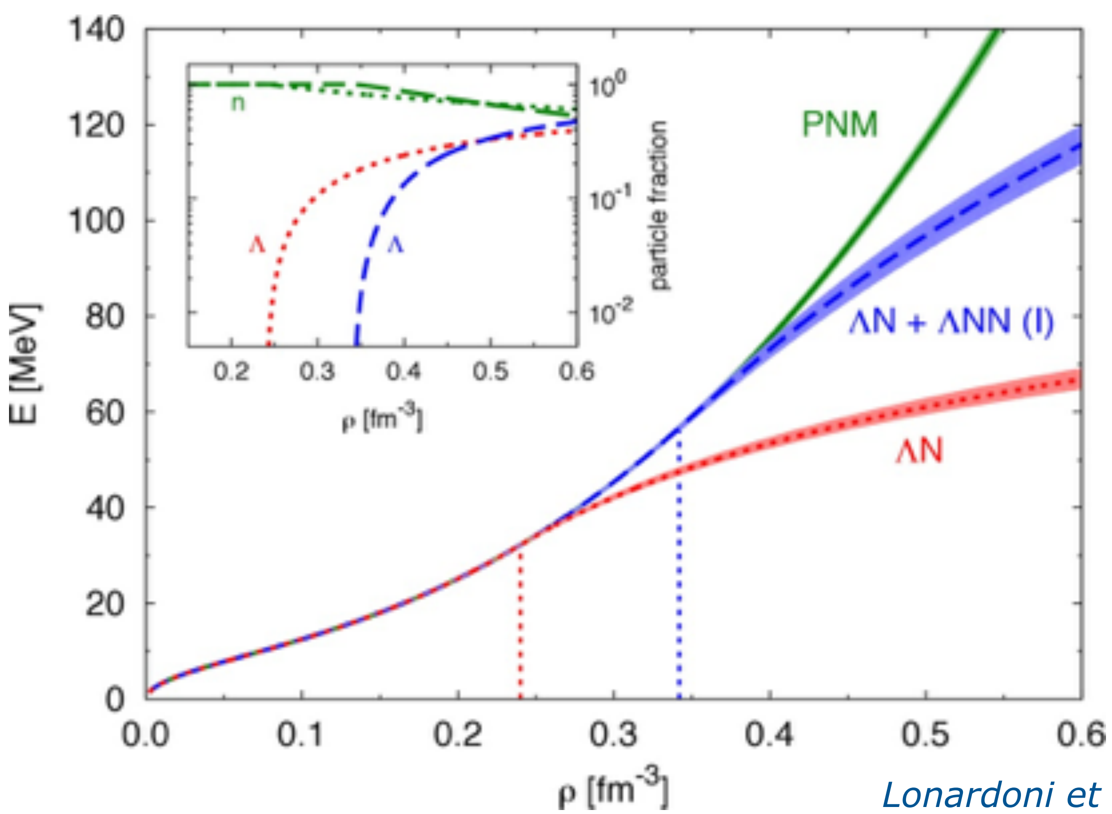


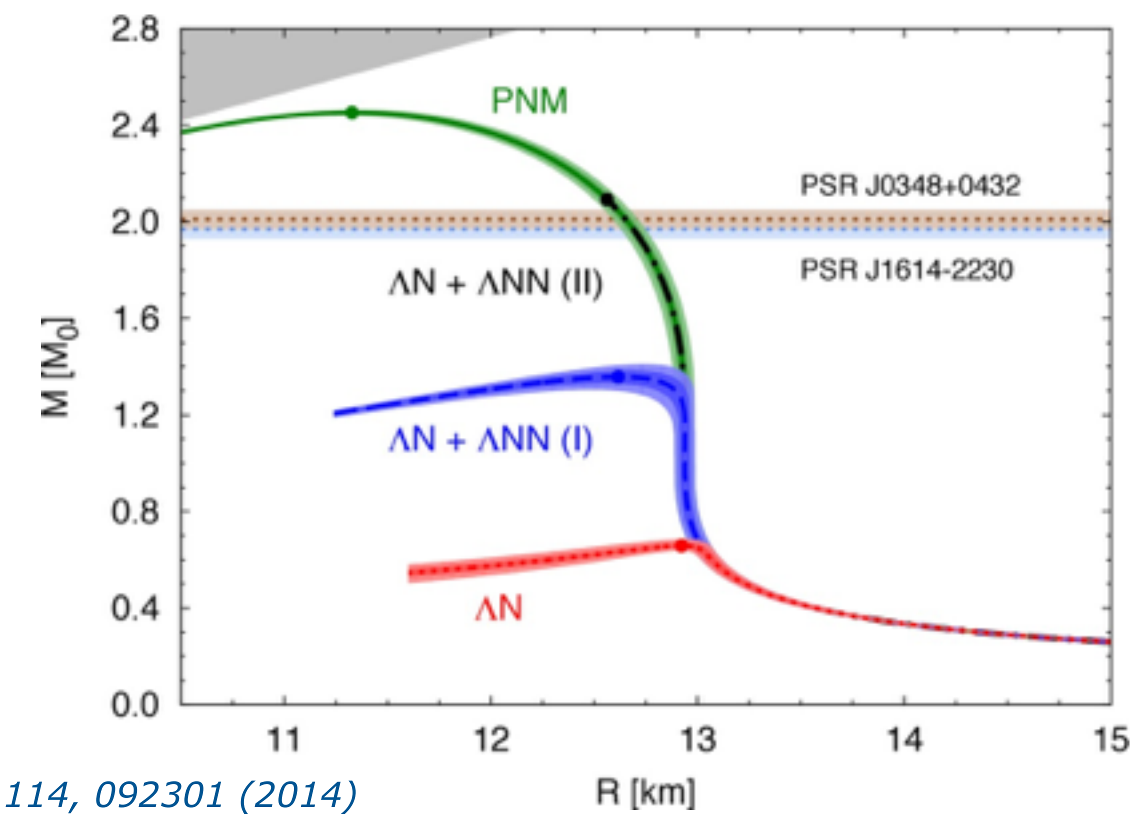
Lonardoni et al.; PRL 114, 092301 (2014)

Recent Example: AFDMC

Lonardoni et al.; PRL 114, 092301 (2014)

- **Auxiliary Field Diffusion Monte Carlo** calculations for hypernuclei and homogeneous matter
- **only include Λ degrees of freedom** explicitly with phenomenological ΛN and ΛNN interactions fitted to hypernuclei
- strongly repulsive ΛNN interaction shifts onset of Λ production to larger densities and **increases maximum neutron-star mass**



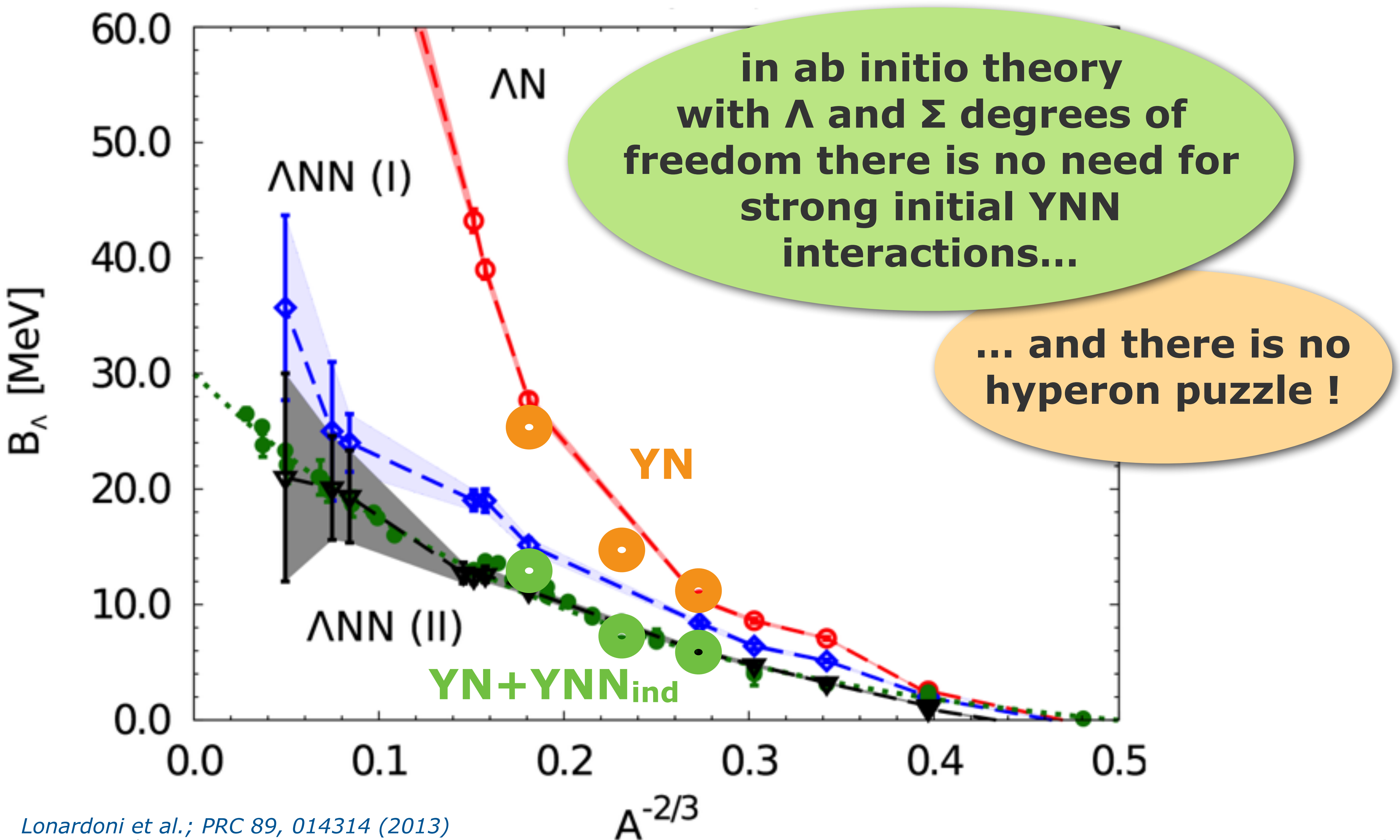


Lonardoni et al.; PRL 114, 092301 (2014)

Comparison to AFDMC

Lonardoni et al.; PRL 114, 092301 (2014); PRC 89, 014314 (2013)

- How do the binding energies of hypernuclei look like with AFDMC ?



Lonardoni et al.; PRC 89, 014314 (2013)

Epilogue

- **thanks to my group and my collaborators**
  - S. Alexa, E. Gebrerufael, T. Hüther, L. Mertes, S. Schulz, H. Spiess, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
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    TRIUMF, Vancouver
  - S. Binder
    Oak Ridge National Laboratory
  - H. Hergert
    NSCL / Michigan State University
  - J. Vary, P. Maris
    Iowa State University
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