Ab Initio Calculations of Nuclear Structure

Lecture 4: Precision, Uncertainties,...

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Overview

- **Lecture 1: Hamiltonian**

  Prelude • Many-Body Quantum Mechanics • Nuclear Hamiltonian • Matrix Elements • Two-Body Problem • Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**

  Similarity Renormalization Group • Many-Body Problem • Configuration Interaction • No-Core Shell Model • Basis Optimization

- **Lecture 3: Medium-Mass Nuclei**

  Normal Ordering • Coupled-Cluster Theory • In-Medium Similarity Renormalization Group • Many-Body Perturbation Theory

- **Project: Do-It-Yourself NCSM**

  Three-Body Problem • Numerical SRG Evolution • NCSM Eigenvalue Problem • Lanczos Algorithm

- **Lecture 4: Precision, Uncertainties, and Applications**

  Chiral Interactions for Precision Calculations • Uncertainty Quantification • Applications to Nuclei and Hypernuclei

Chiral Interactions for Precision Calculations

A Brief History… Incomplete and Totally Biased

1st Generation

2007: first ab initio calculation of mid-p-shell nuclei with local chiral 3N interaction: $N3LO_{EM}$ + $N2LO_{L,500}$ *PRL 99, 042501 (2007)*

2012: SRG transformed NN+3N interactions and reduced 3N cutoffs for oxygen & calcium isotopes *PRL 109, 052501 (2012)*

2014: overbinding beyond oxygen and catastrophic radii *PLB 736, 119 (2014)*

2nd Generation

2015: combined fit of few and many-body observables to improve radii, sacrificing phase-shifts: $N2LO_{SAT}$ *PRC 91, 051301(R) (2015)*

2016: magic interactions constructed from a SRG evolved NN interaction plus bare 3N parametrization *PRC 83, 031301(R) (2011)* *PRC 93, 011302 (2016)*

3rd Generation

2016: systematic order-by-order calculations up to N3LO of neutron and nuclear matter *PRC 94, 054307 (2016)* *PRL 122, 042501 (2019)*

2019: systematic order-by-order calculations up to N3LO in light and medium-mass nuclei… *PRC 96, 024004 (2017)* *arXiv:1911.04955 (2019)*

A Brief History… Incomplete and Totally Biased

Antiquity

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Middle Ages

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Renaissance

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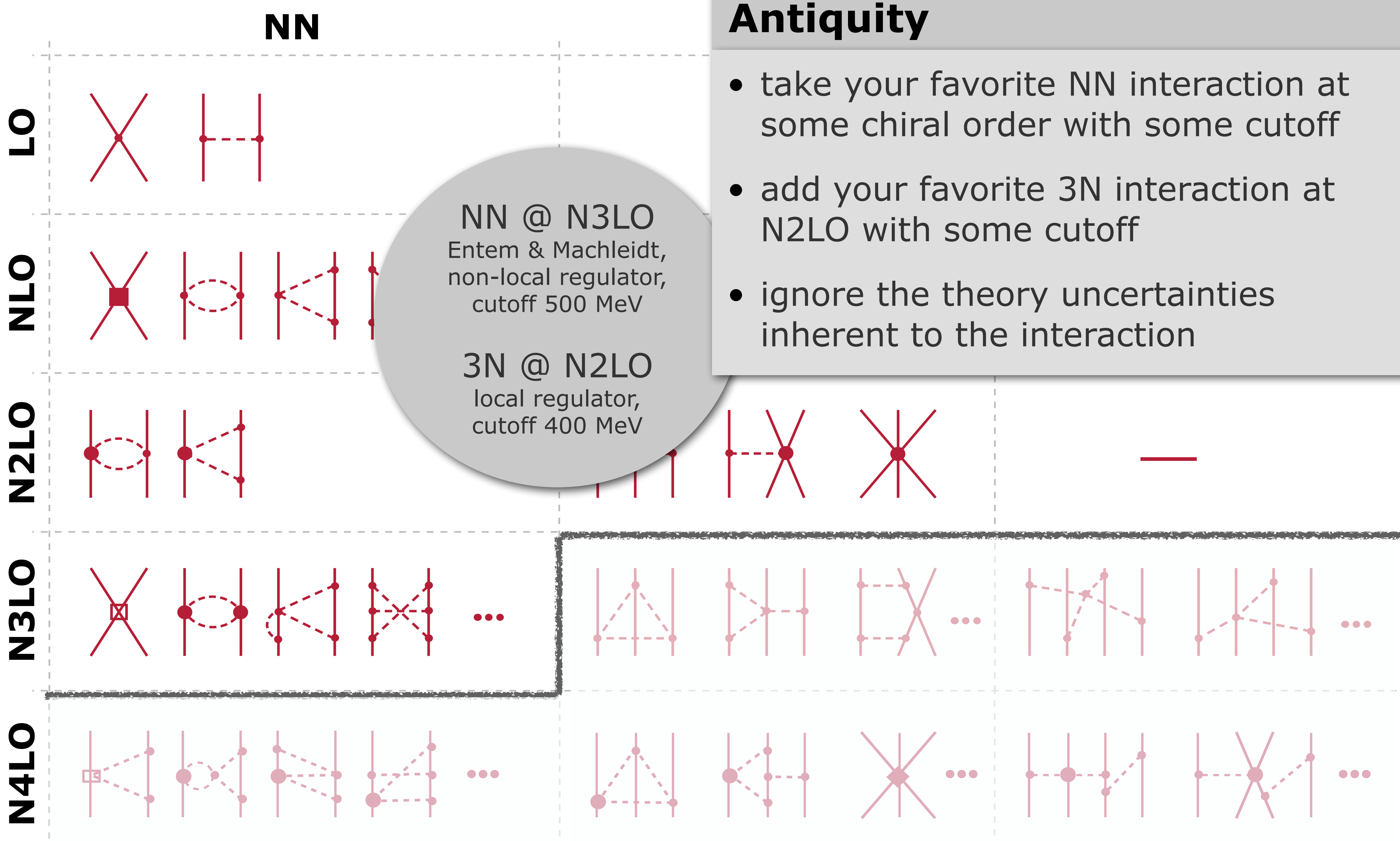
Nuclear Interactions from Chiral EFT



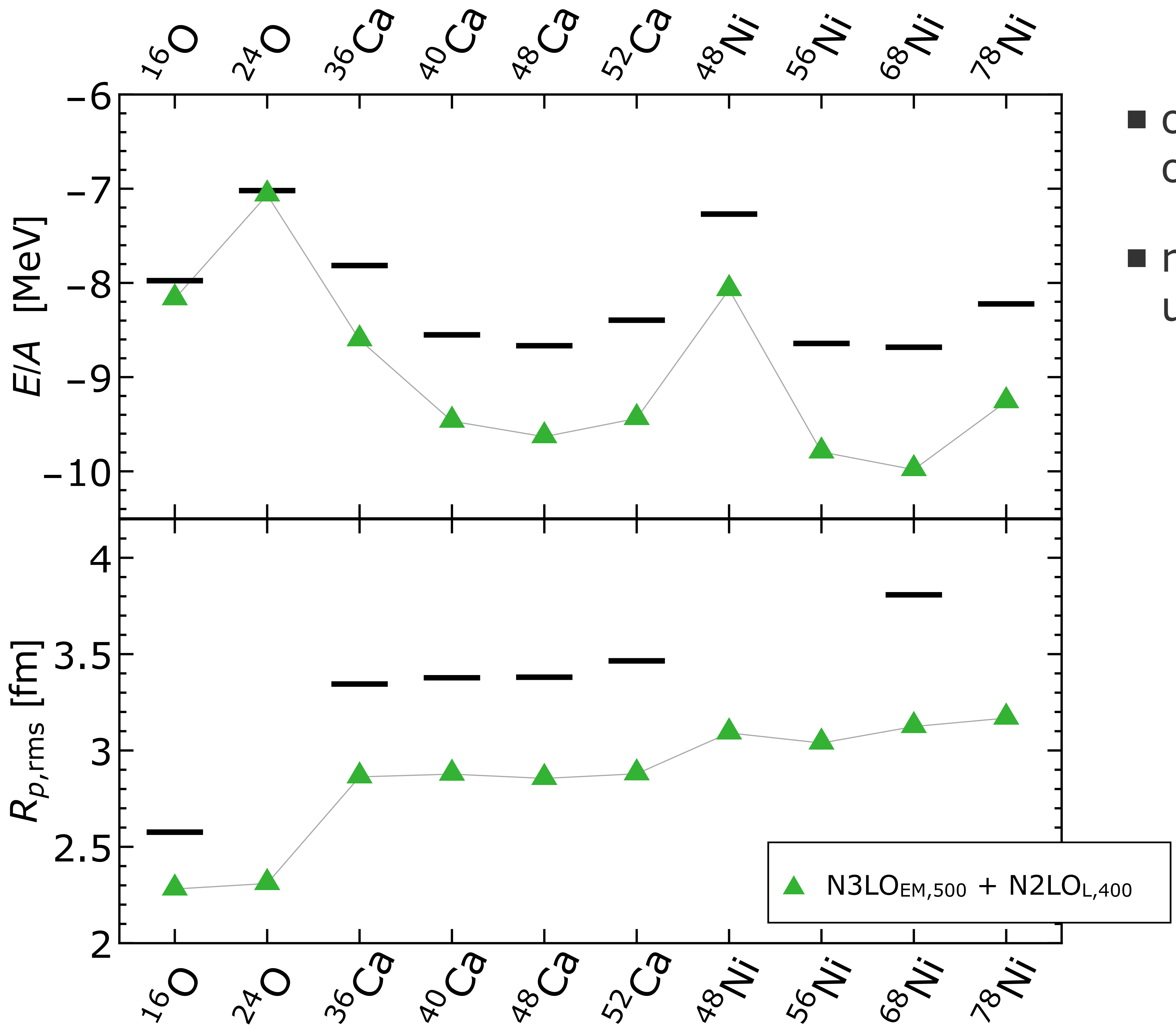
NN @ N3LO
Entem & Machleidt, non-local regulator, cutoff 500 MeV

3N @ N2LO
local regulator, cutoff 400 MeV

Antiquity

- take your favorite NN interaction at some chiral order with some cutoff
- add your favorite 3N interaction at N2LO with some cutoff
- ignore the theory uncertainties inherent to the interaction

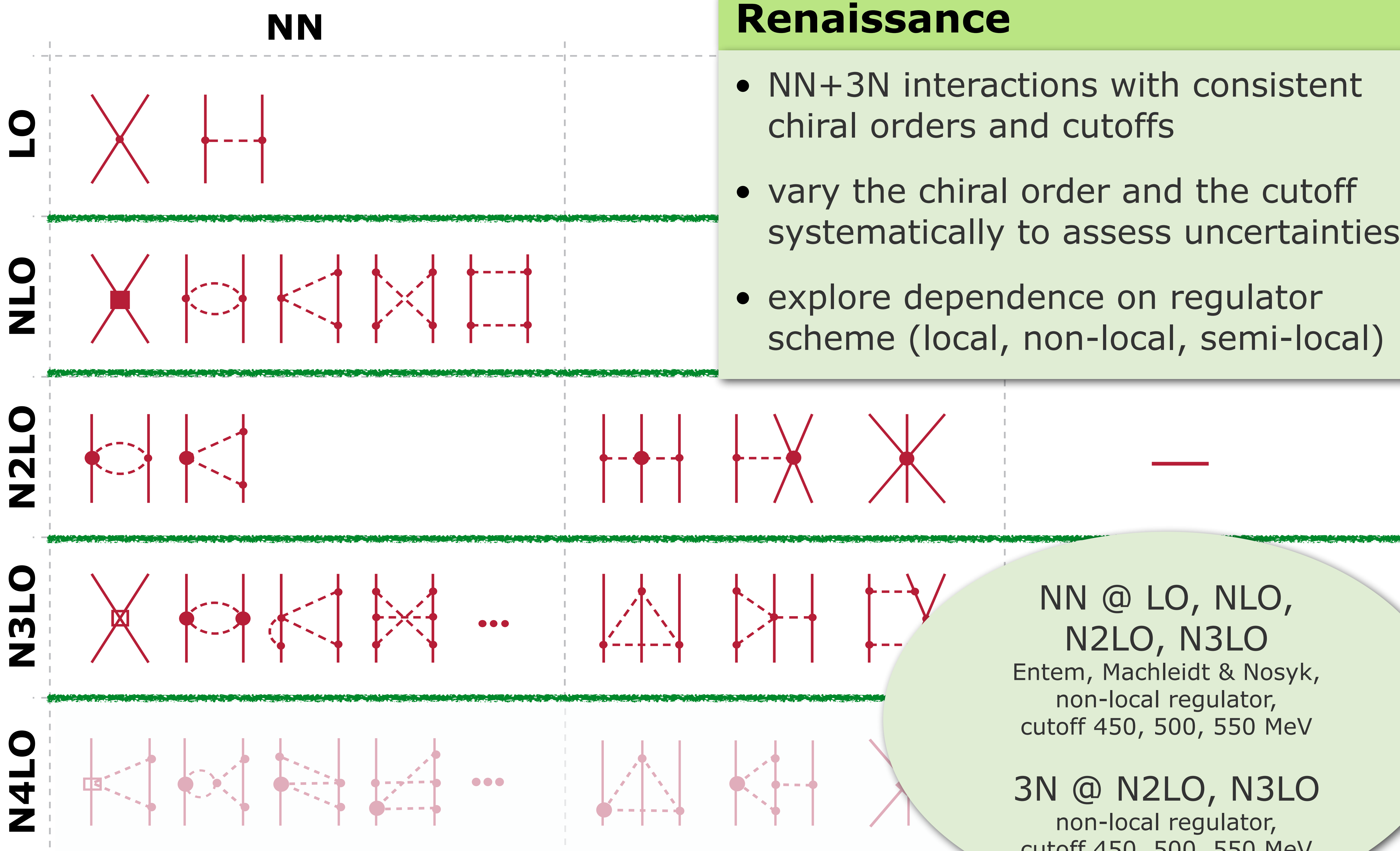
Medium-Mass Nuclei: Antiquity



- overbinding beyond oxygen isotopes
- radii significantly underestimated

IM-SRG(M2)
natural orbitals
$\hbar\Omega$=20 MeV
e_{max}=12, E_{3max}=16
α=0.04 fm^4

Nuclear Interactions from Chiral EFT



Renaissance

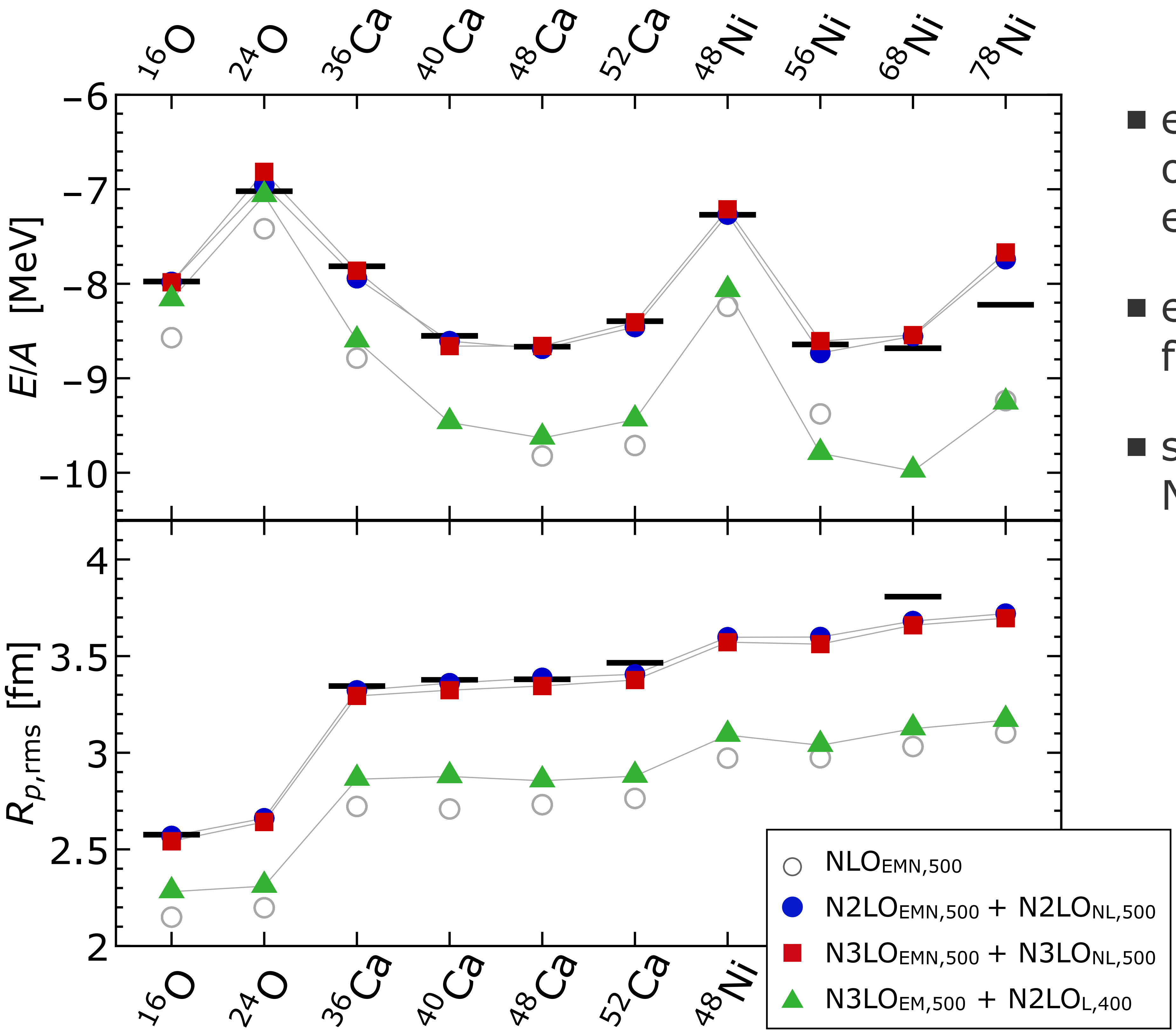
- NN+3N interactions with consistent chiral orders and cutoffs
- vary the chiral order and the cutoff systematically to assess uncertainties
- explore dependence on regulator scheme (local, non-local, semi-local)

NN @ LO, NLO, N2LO, N3LO
Entem, Machleidt & Nosyk,
non-local regulator,
cutoff 450, 500, 550 MeV

3N @ N2LO, N3LO
non-local regulator,
cutoff 450, 500, 550 MeV

Medium-Mass Nuclei: Renaissance

Hüther et al.; PLB 808, 135651 (2020)



- excellent reproduction of ground-state energies
- excellent agreement for radii
- stable results for N2LO and N3LO

IM-SRG(M2)
natural orbitals
ħΩ=20 MeV
e_{max}=12, E_{3max}=16
α=0.04 fm⁴

Let's Go Slowly…

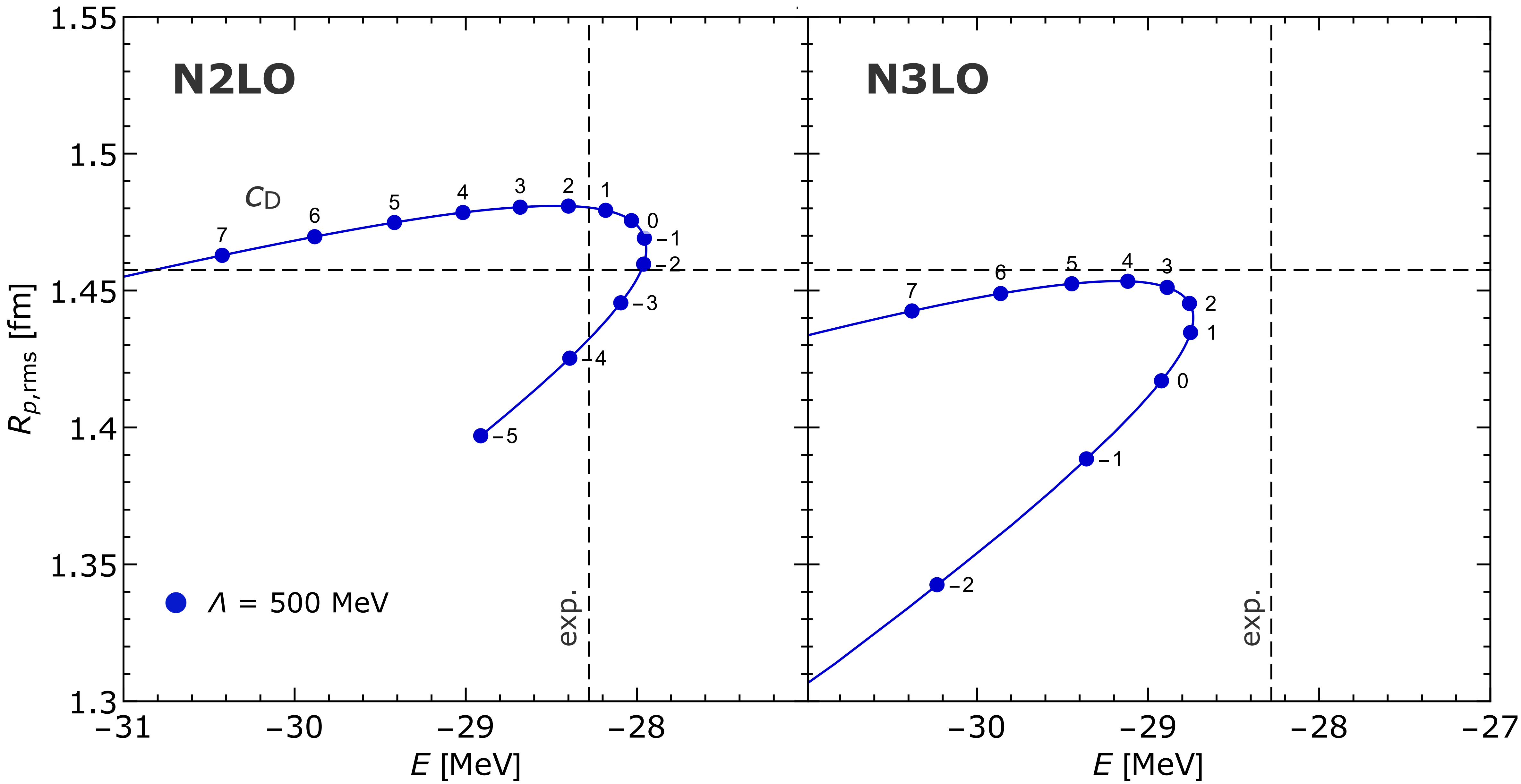
Strategy

Hüther et al.; PLB 808, 135651 (2020)

- **start from chiral NN interaction by Entem, Machleidt & Nosyk**
  PRC 96, 024004 (2017)
  - LO to N3LO
  - non-local regulator
  - cutoff 450, 500, 550 MeV
  - accurate reproduction of NN scattering data up to ~300 MeV
- **supplement non-local 3N interaction at N2LO and N3LO**
  - N2LO or N3LO, consistent with NN interaction
  - non-local regulator, as in NN interaction
  - cutoff 450, 500, 550 MeV, consistent with NN interaction
- **fix c_E in few-body sector, keep c_D as a parameter**
  - c_E fit to triton binding energy
  - alternative: c_E from combined fit to ^3H, ^4He energy and ^4He radius

^{4}He Ground State: c_D Scan

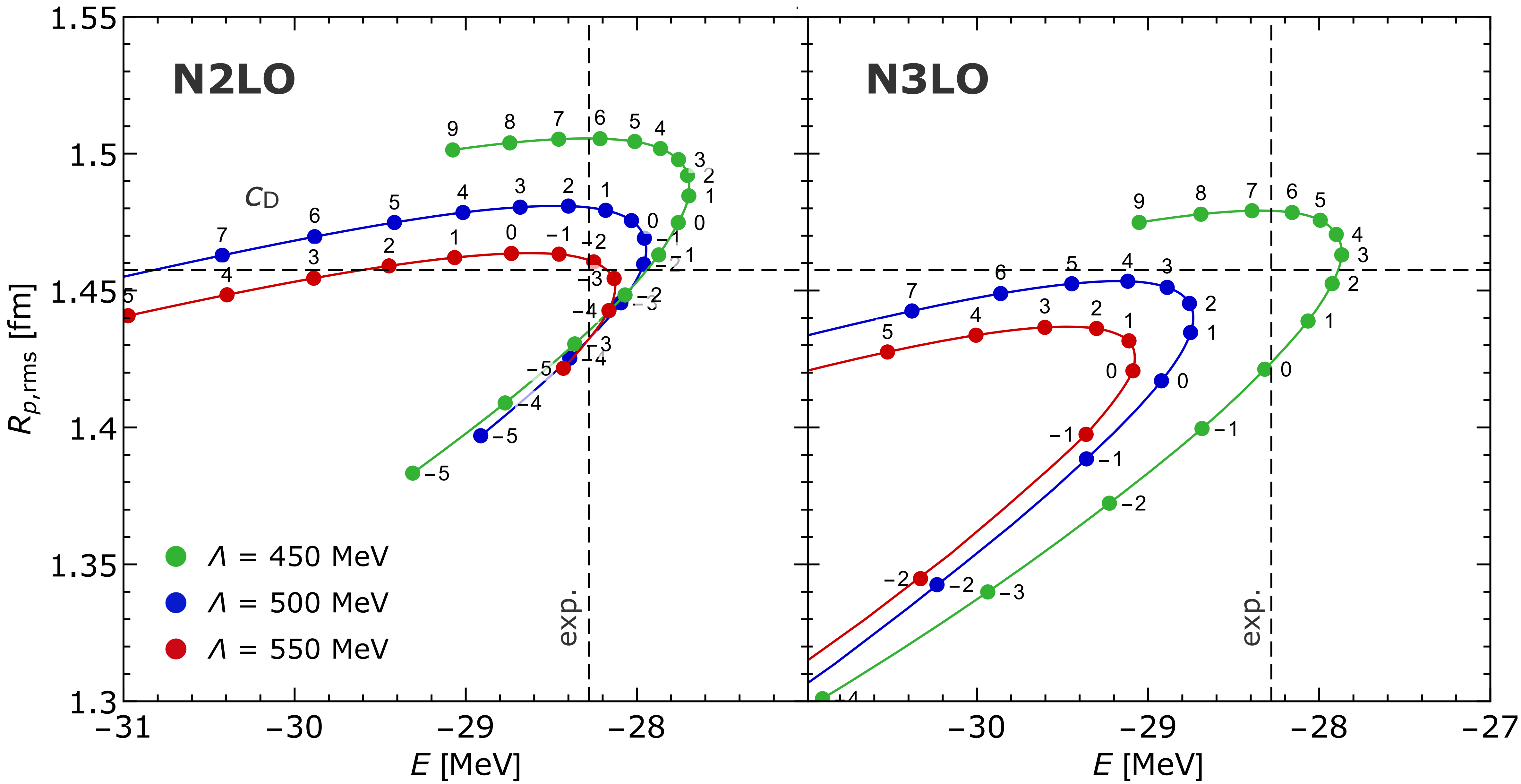
Hüther et al.; PLB 808, 135651 (2020)



- Jacobi-NCSM calculations for ^{3}H and ^{4}He with bare interaction
- scanning c_D over large range, c_E always fit to ^{3}H binding energy

^{4}He Ground State: c_D Scan

Hüther et al.; PLB 808, 135651 (2020)



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Medium-Mass Nuclei: c_D Scan

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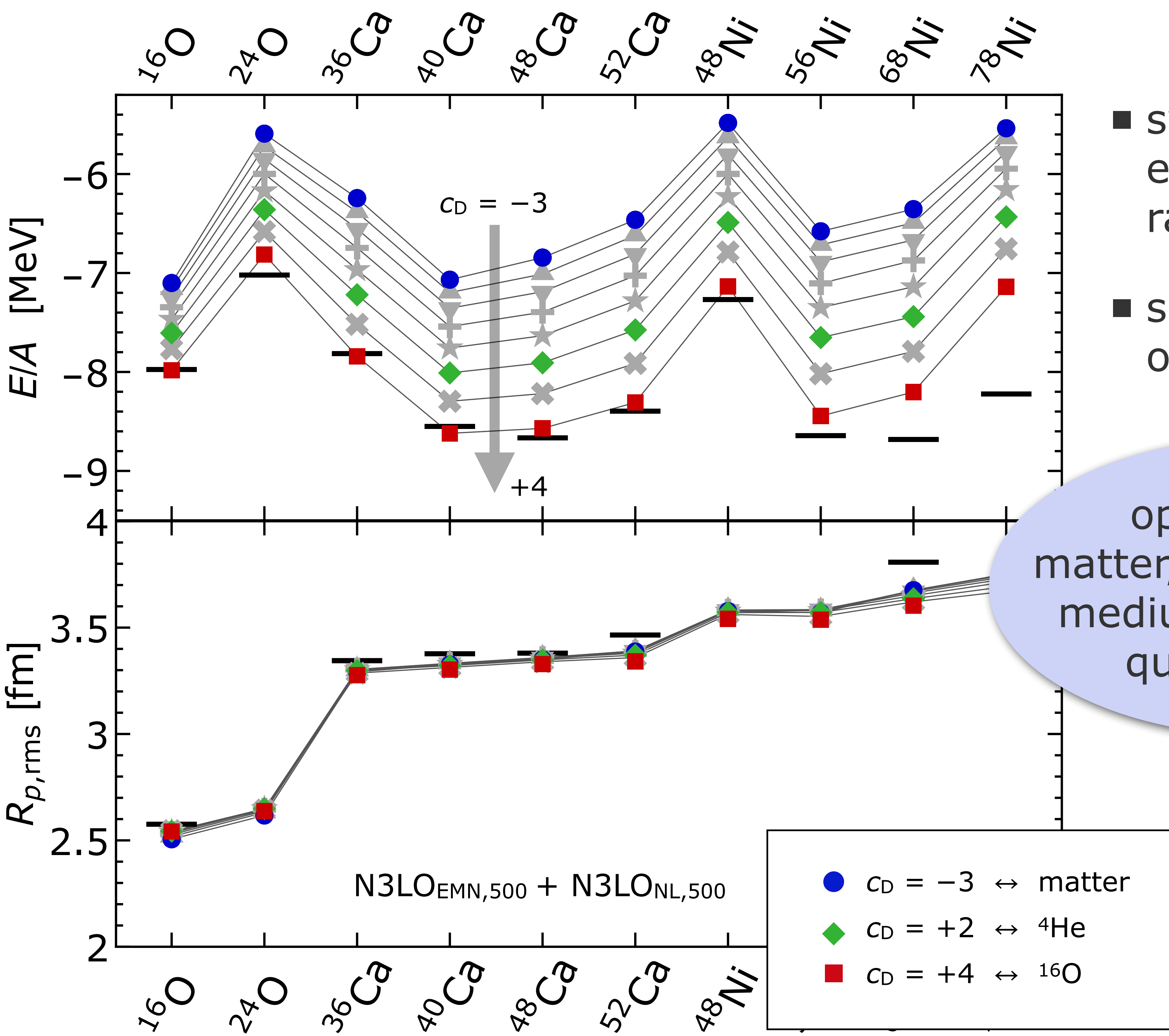


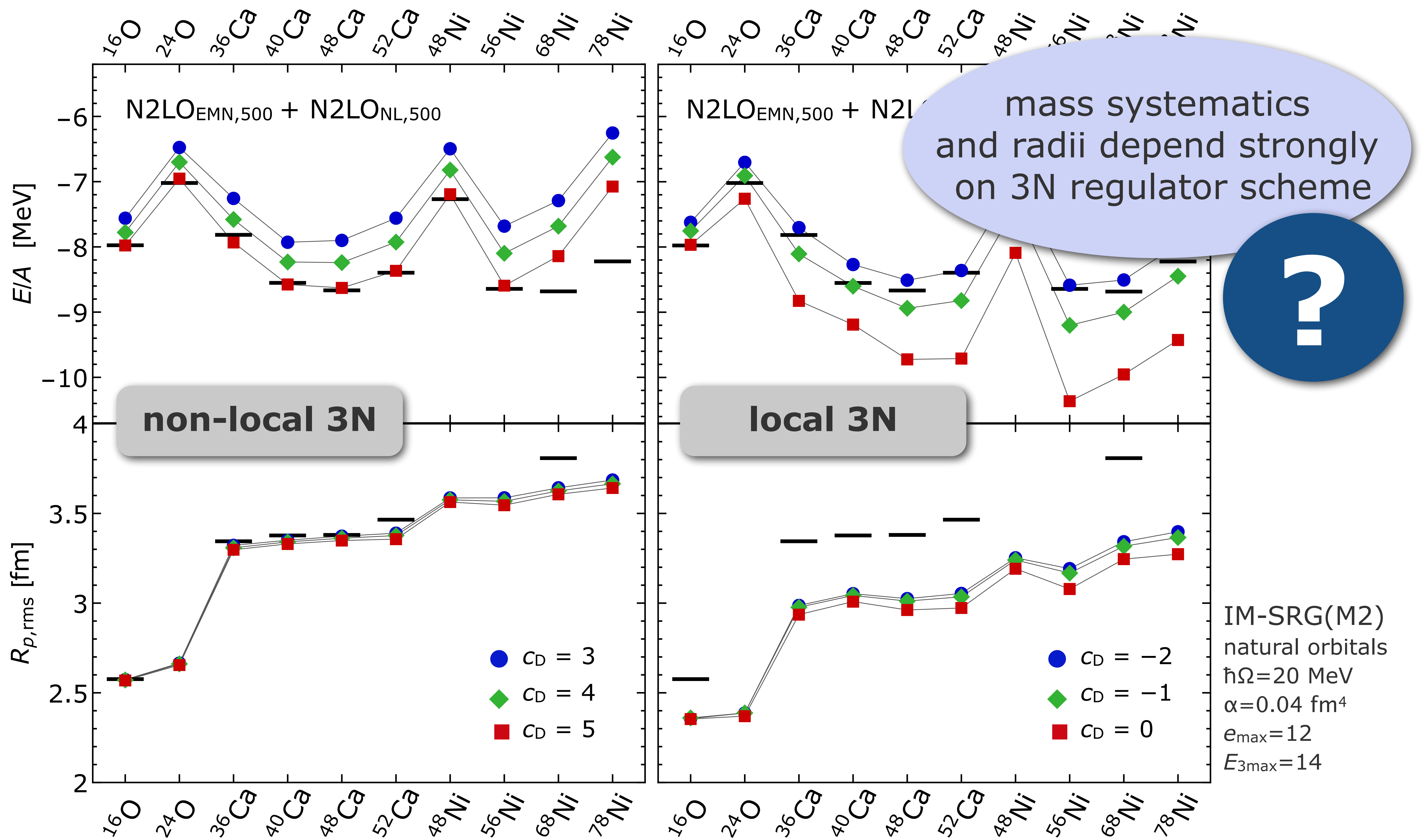
- systematic change of energies, no effect on radii
- same pattern for all orders and cutoffs

optimal c_D for matter, light nuclei and medium-mass nuclei quite different

?

IM-SRG(M2)
natural orbitals
ħΩ=20 MeV
α=0.04 fm⁴

Non-Local vs. Local 3N Regulator



IM-SRG(M2)
natural orbitals
$\hbar\Omega$=20 MeV
α=0.04 fm^4
e_{max}=12
E_{3max}=14

Uncertainties

Ab Initio Nuclear Structure Theory

$$H\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

Hamiltonian

Chiral Effective Field Theory

Pre-Conditioning

Similarity Renormalization Group

Many-Body Solution

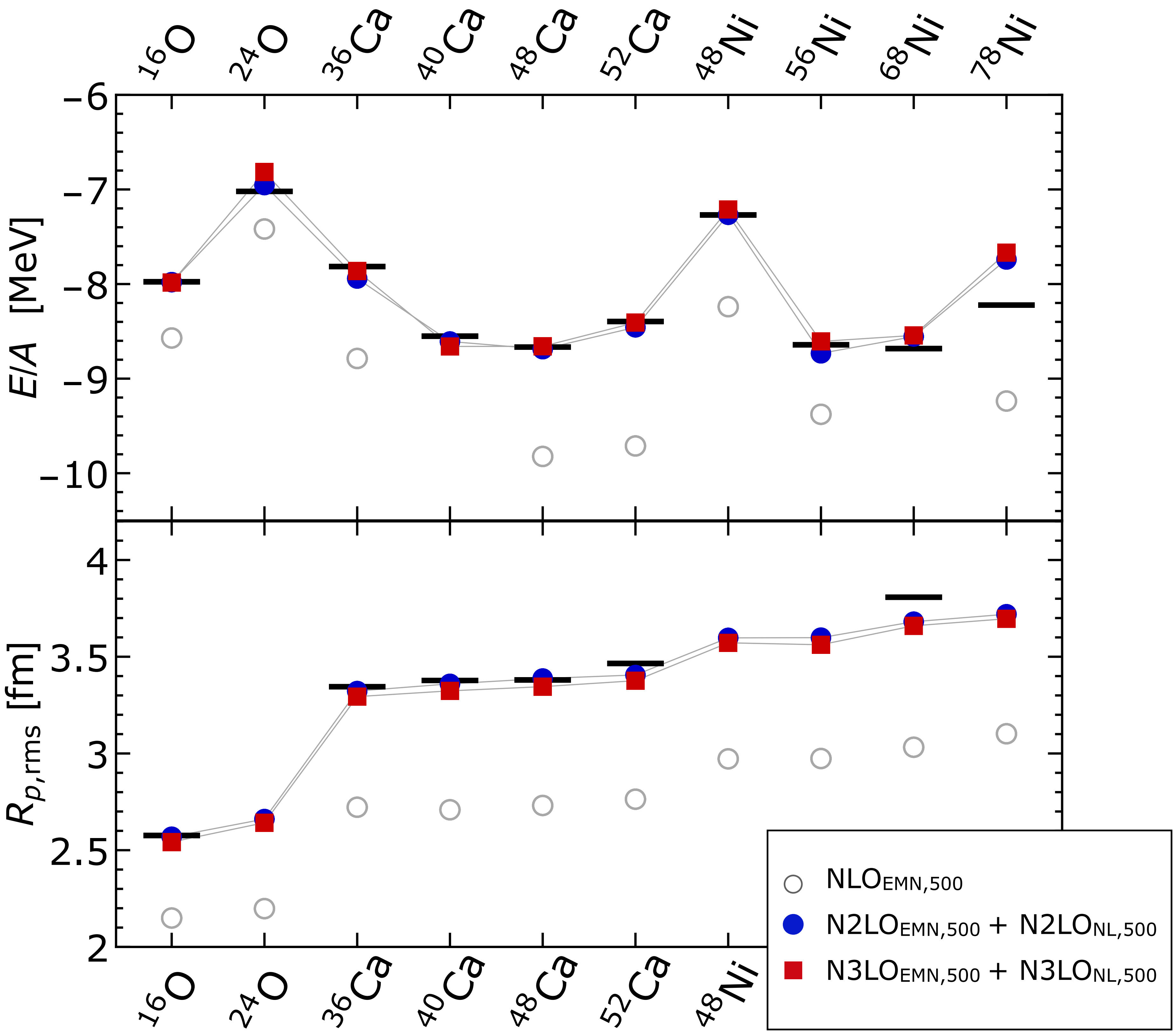
CI, NCSM, IM-SRG, CC, SCGF, MBPT...

each step involves truncations and induces uncertainties that have to be quantified...

...in order to claim the 'ab initio' label

Interaction Uncertainties

Hüther et al.; PLB 808, 135651 (2020)



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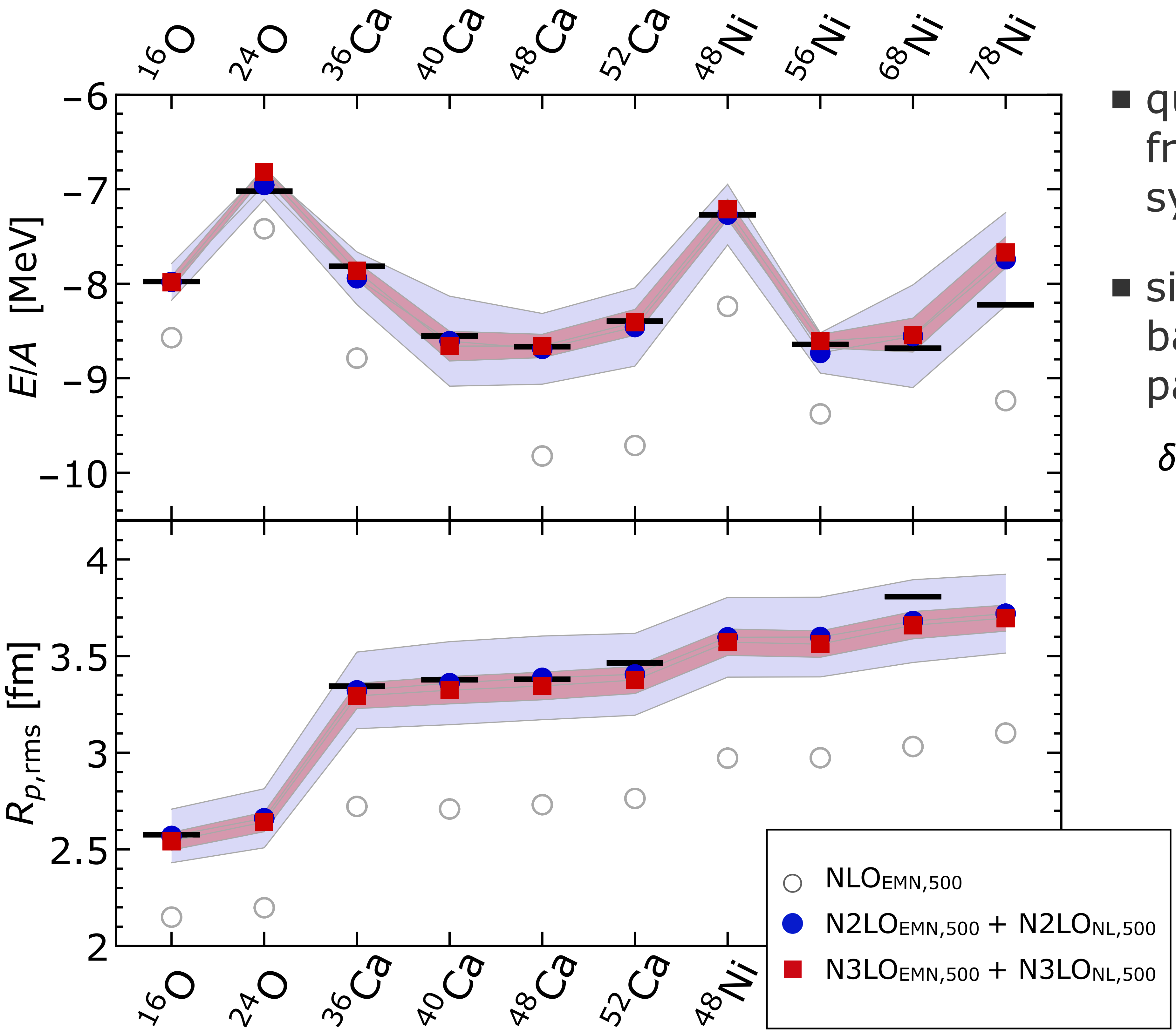
Interaction Uncertainties

Hüther et al.; PLB 808, 135651 (2020)



- quantify uncertainties from order-by-order systematics
- simplified protocol based on expansion parameter $Q=q/\Lambda_B$

$$\delta X_{N3LO} = \max(Q\,|X_{N3LO} - X_{N2LO}|,\; Q^2|X_{N2LO} - X_{NLO}|,\; Q^4|X_{NLO} - X_{LO}|,\; Q^5|X_{LO}|)$$

PRC 98, 014002 (2018)
PRC 93, 044002 (2016)

IM-SRG(M2)
natural orbitals
$\hbar\Omega$=20 MeV
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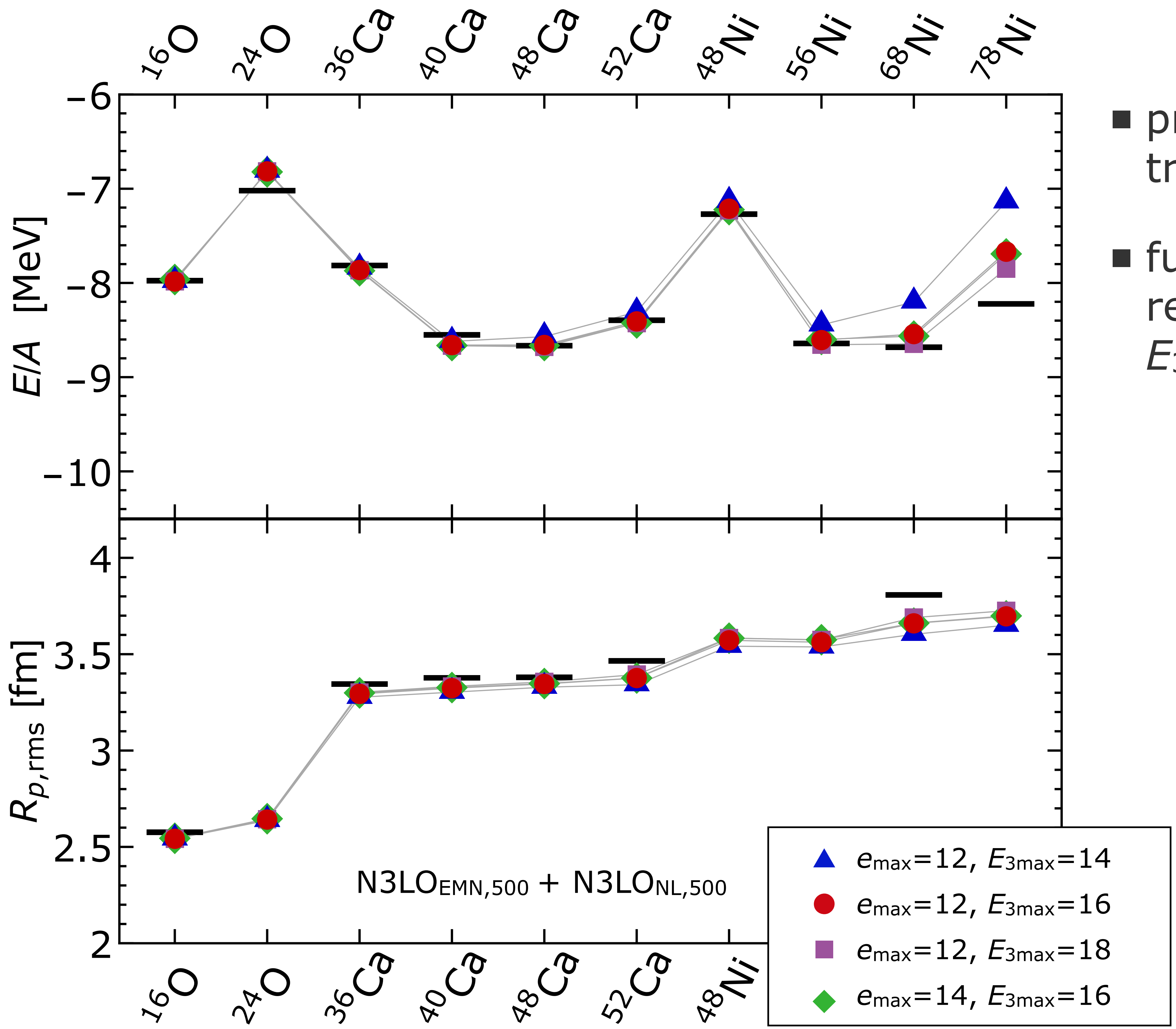
LENPIC

Many-Body Uncertainties I

Hüther et al.; PLB 808, 135651 (2020)

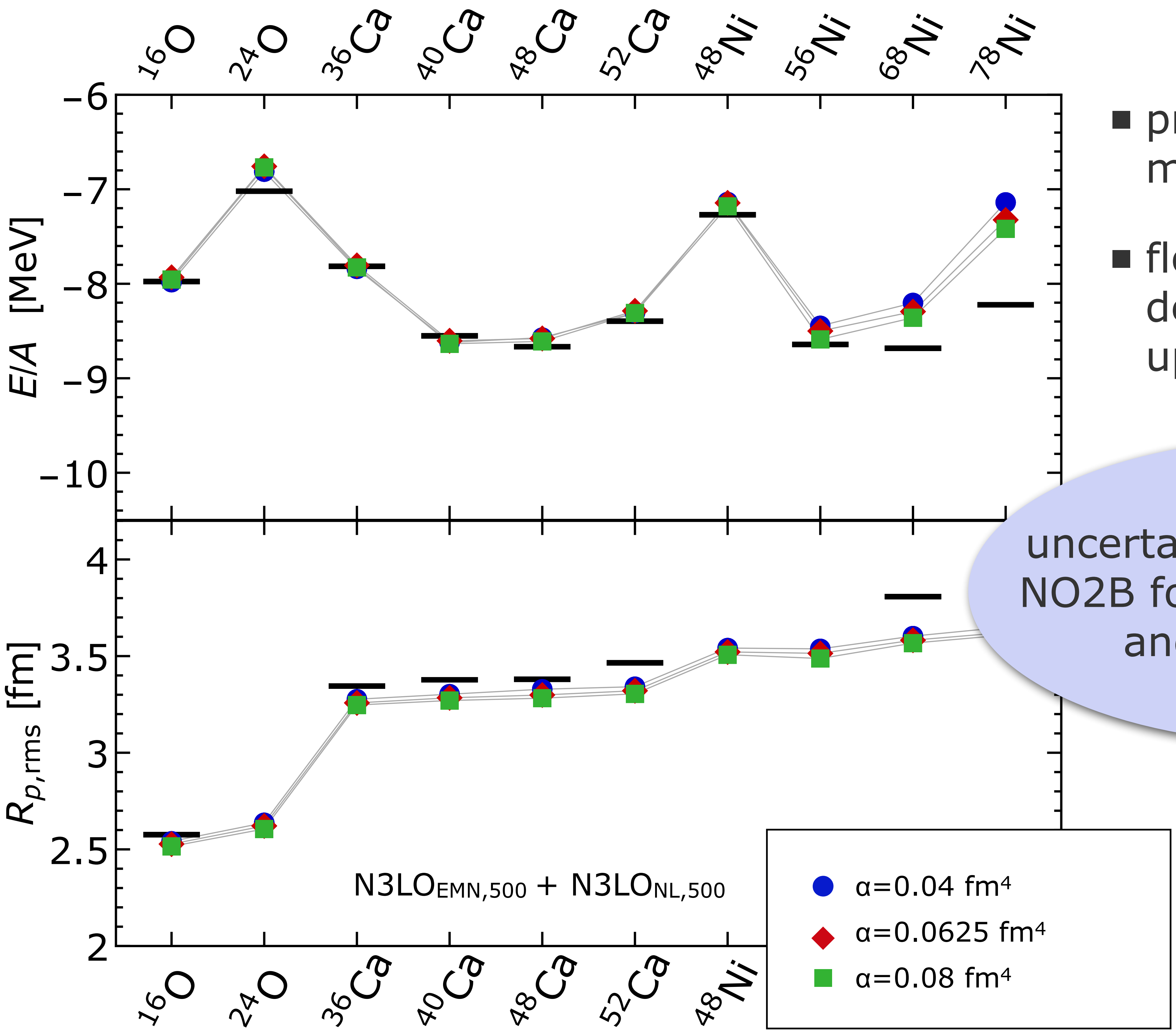


- probing model-space truncations
- fully converged with respect to e_{max} and E_{3max} truncations

IM-SRG(M2)
natural orbitals
ħΩ=20 MeV
α=0.04 fm⁴

Many-Body Uncertainties II

Hüther et al.; PLB 808, 135651 (2020)



- probing SRG induced many-body terms
- flow-parameter dependence negligible up into nickel isotopes

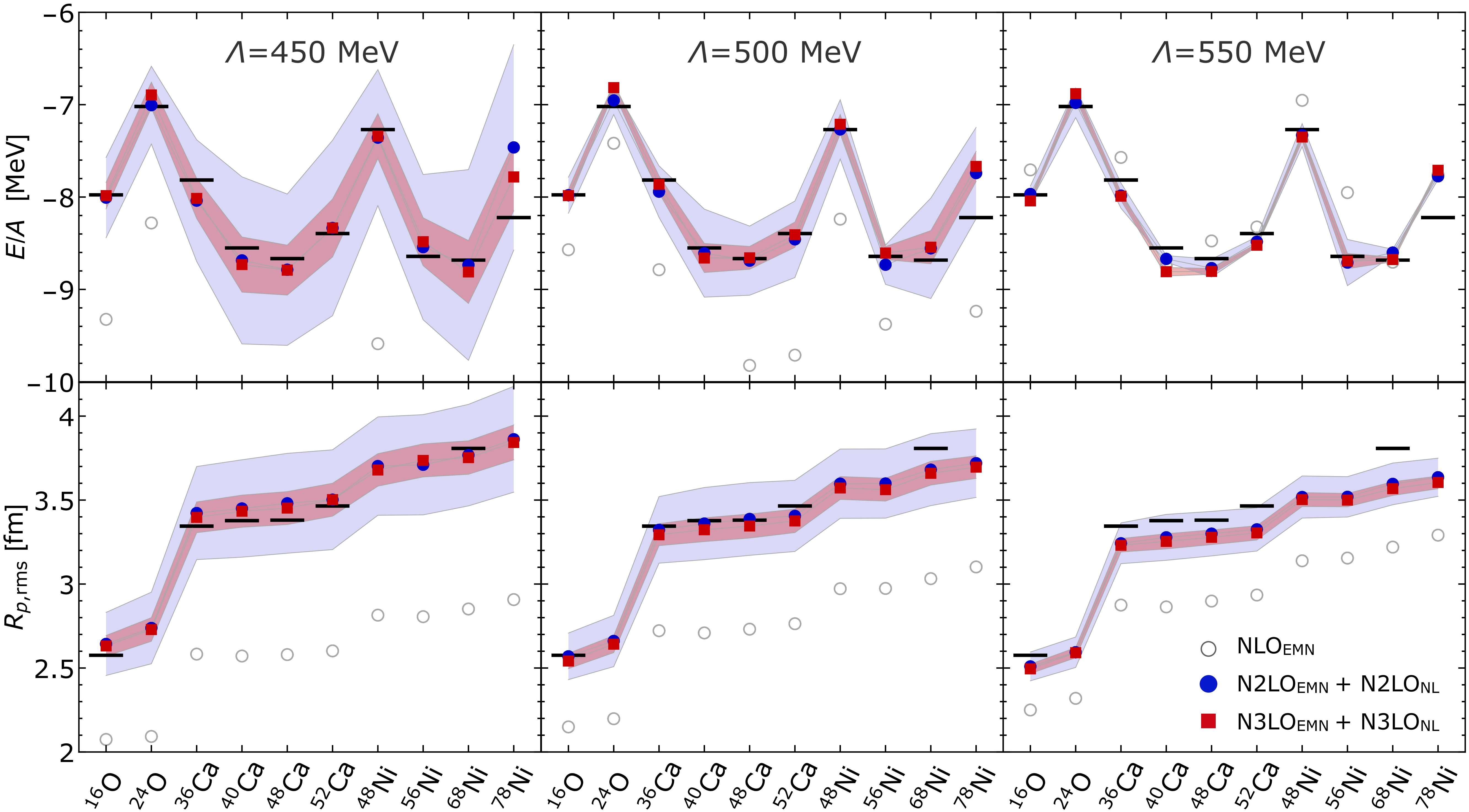
many-body uncertainties dominated by NO2B for initial Hamiltonian and IM-SRG flow-equations

~2%

IM-SRG(M2)
natural orbitals
ħΩ=20 MeV
e_{max}=12, E_{3max}=14

Medium-Mass Nuclei

Hüther et al.; PLB 808, 135651 (2020)

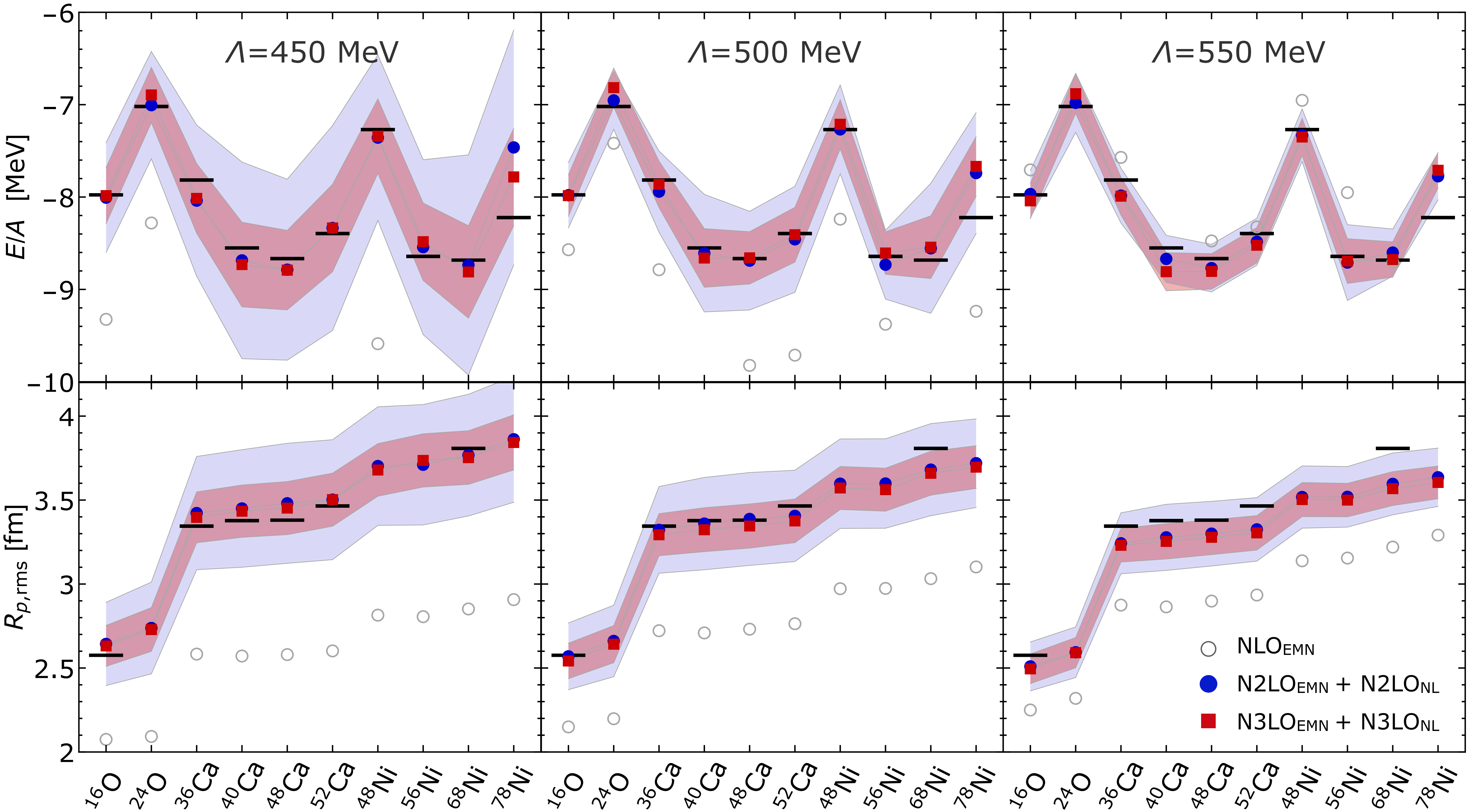


IM-SRG(M2), natural orbitals, ħΩ=20 MeV, α=0.04 fm^4, e_{max}=12, E_{3max}=16

error bands show interaction uncertainties

Medium-Mass Nuclei

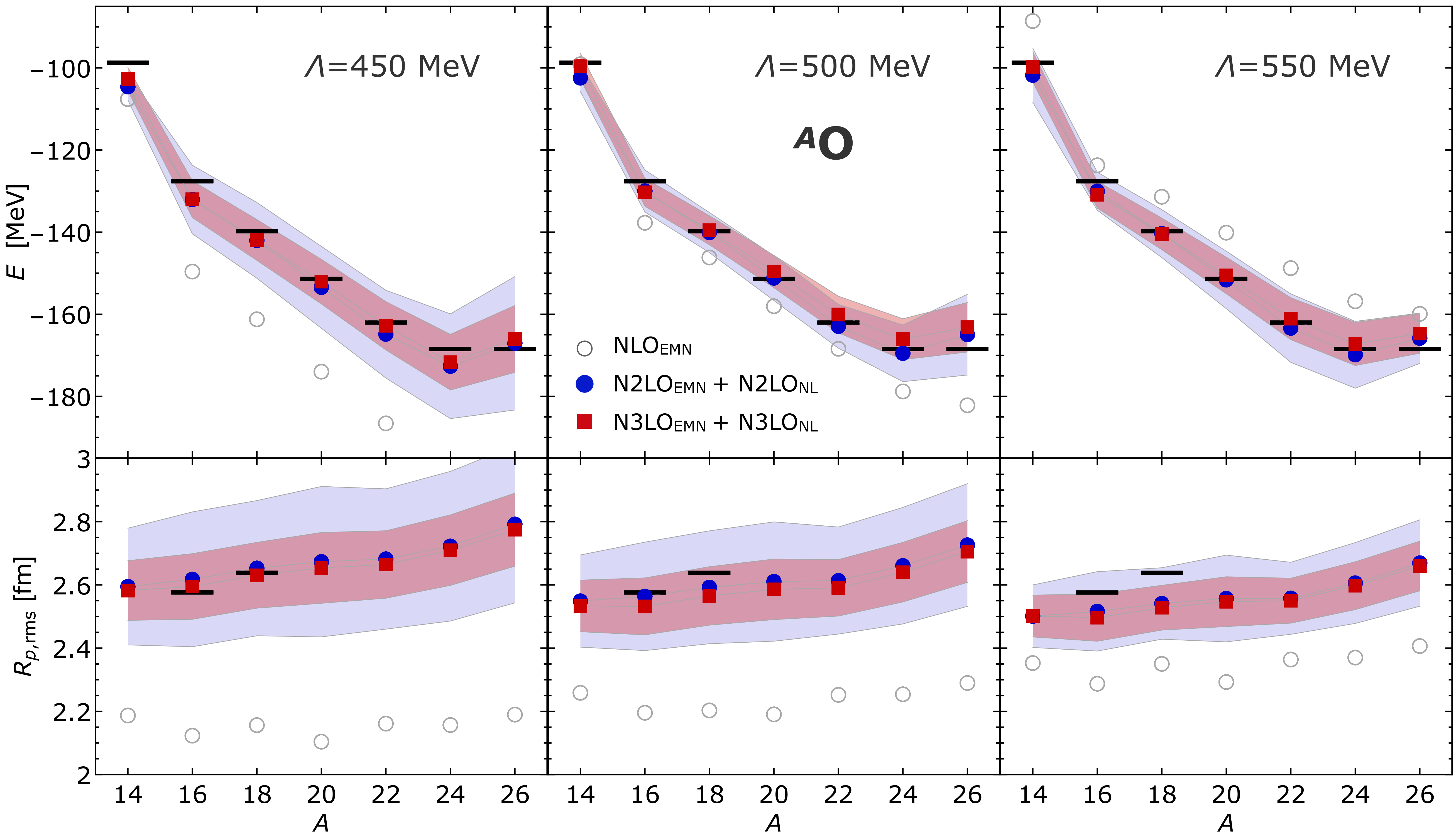
Hüther et al.; PLB 808, 135651 (2020)



IM-SRG(M2), natural orbitals, ħΩ=20 MeV, α=0.04 fm^4, e_{max}=12, E_{3max}=16
error bands show interaction + many-body uncertainties

Oxygen Isotopic Chain

Hüther et al.; PLB 808, 135651 (2020)

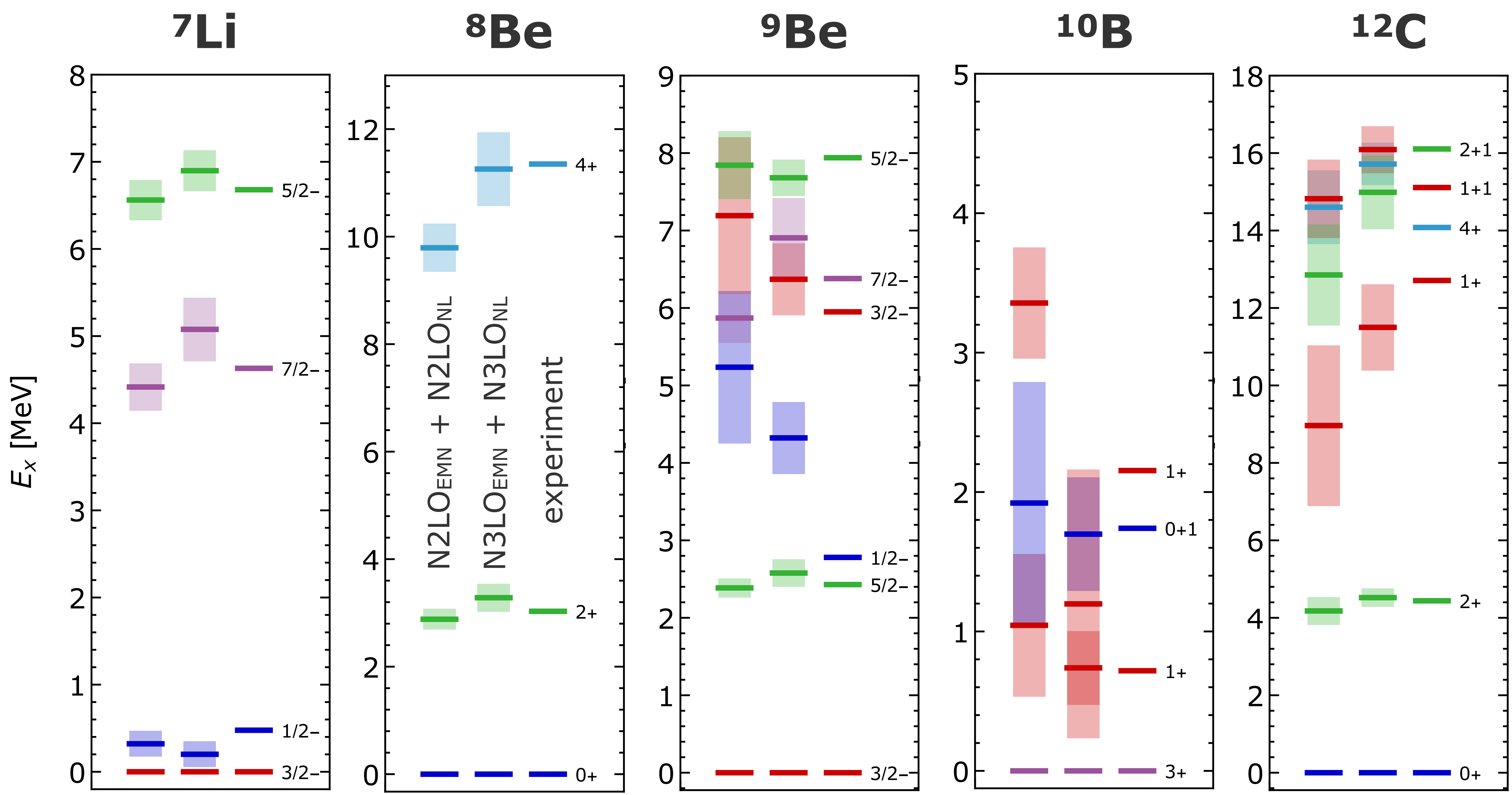


IM-NCSM, natural orbitals, ħΩ=20 MeV, α=0.04 fm⁴, e_{max}=12, E_{3max}=14, N_{ref}=2

error bands show interaction + many-body uncertainties

p-Shell Spectra

Hüther et al.; PLB 808, 135651 (2020)

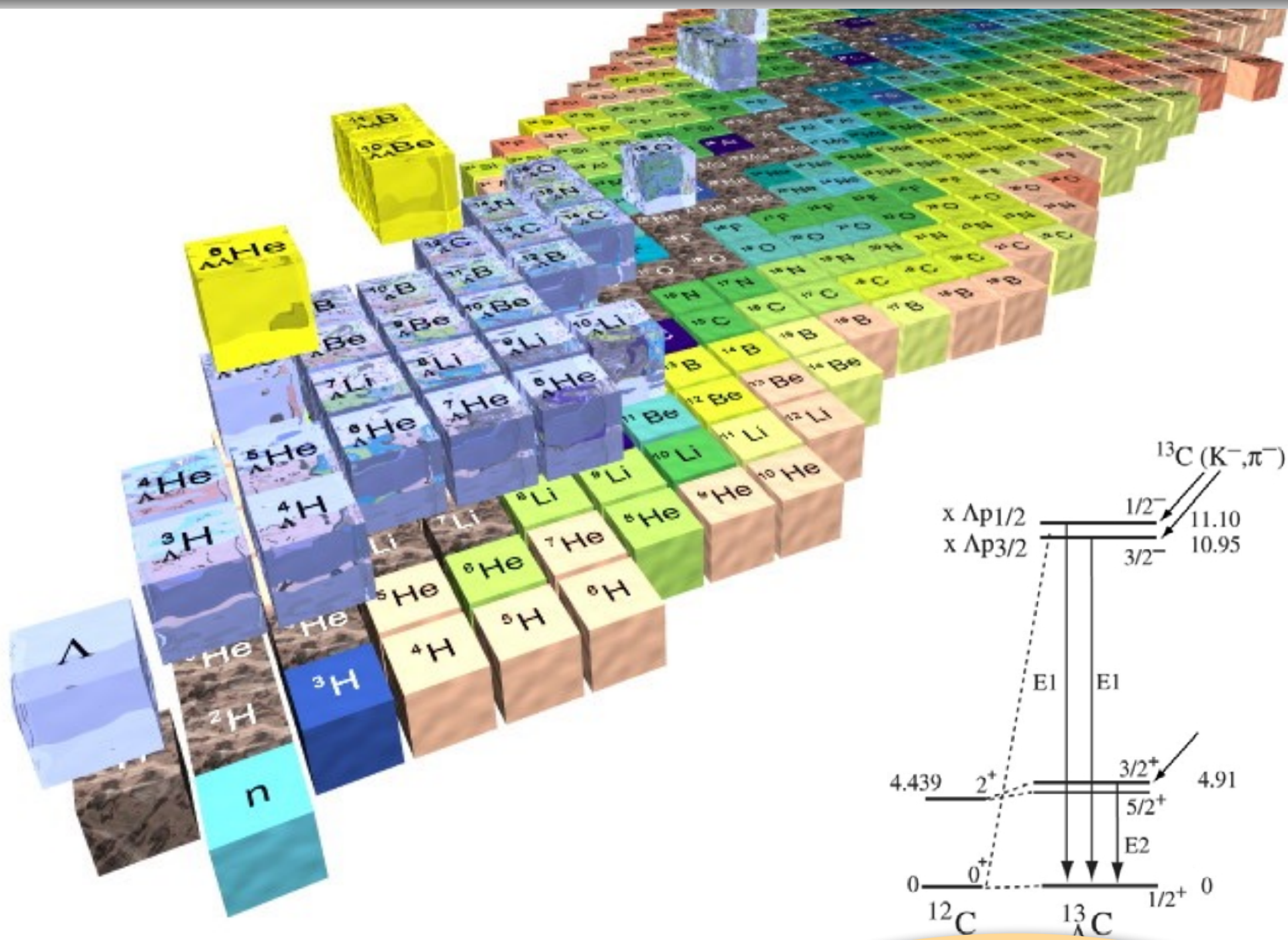


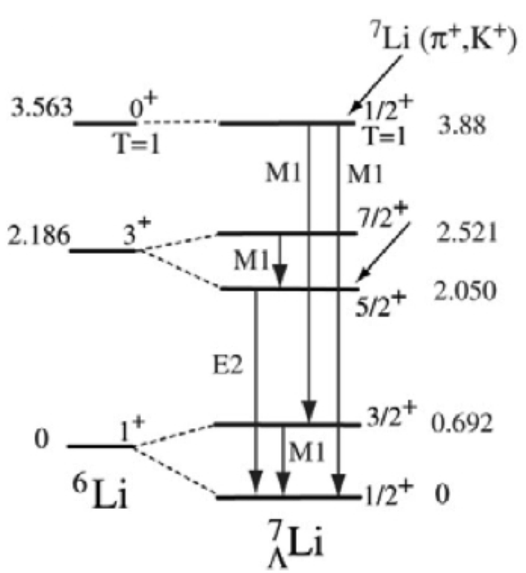
NCSM/IM-NCSM, Λ=500 MeV, $\hbar\Omega$=20 MeV
error bands show interaction uncertainties

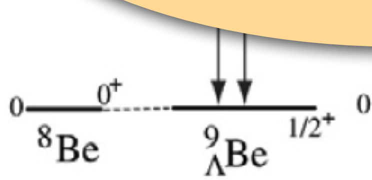
Hypernuclei

$$N_f = 2 \quad \rightarrow \quad N_f = 3$$

Ab Initio Hypernuclear Structure





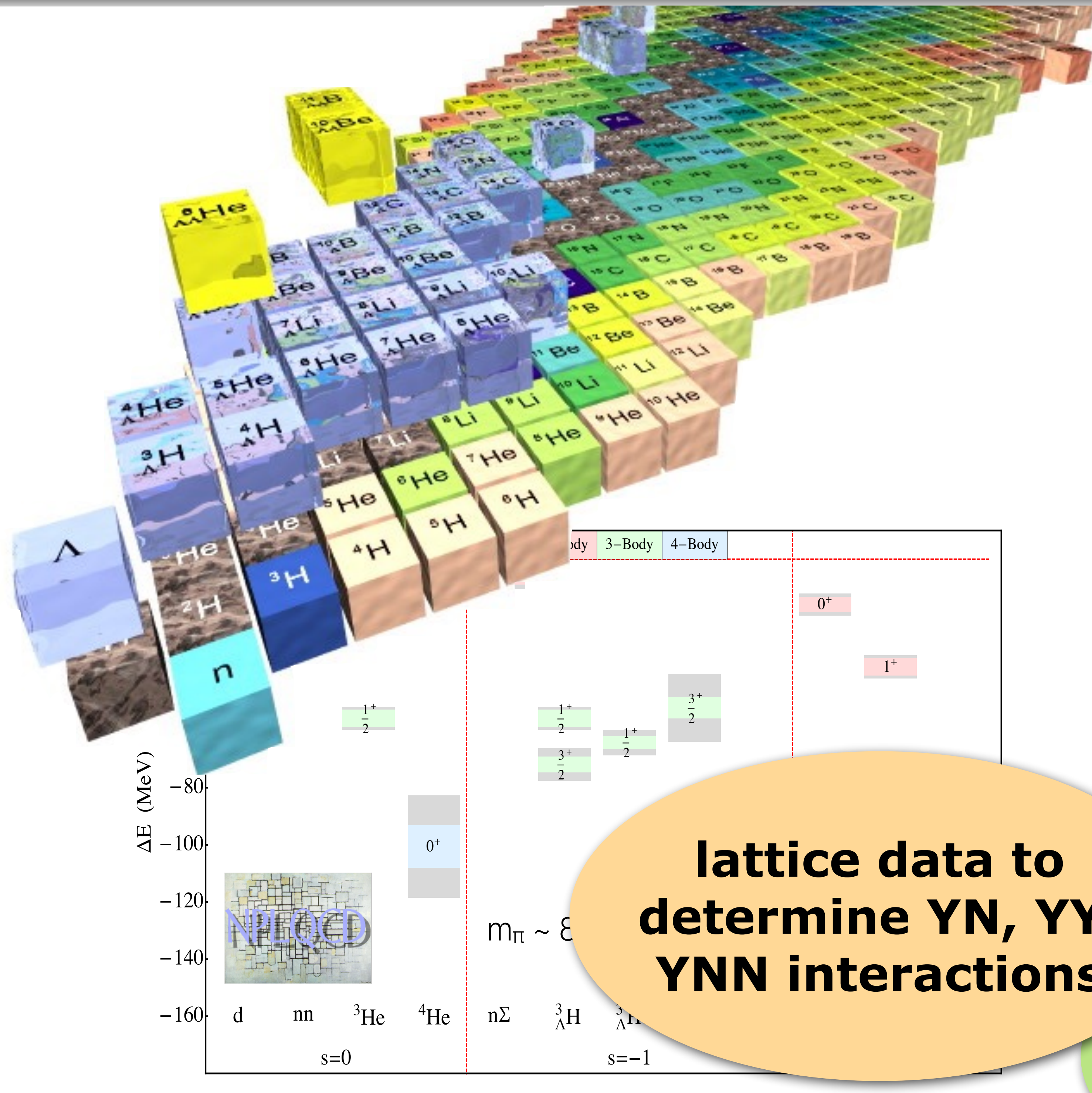


- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body and phenomen. shell-model, mean-field or cluster-model calculations done so far
- chiral YN & YY interactions at (N)LO are available

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

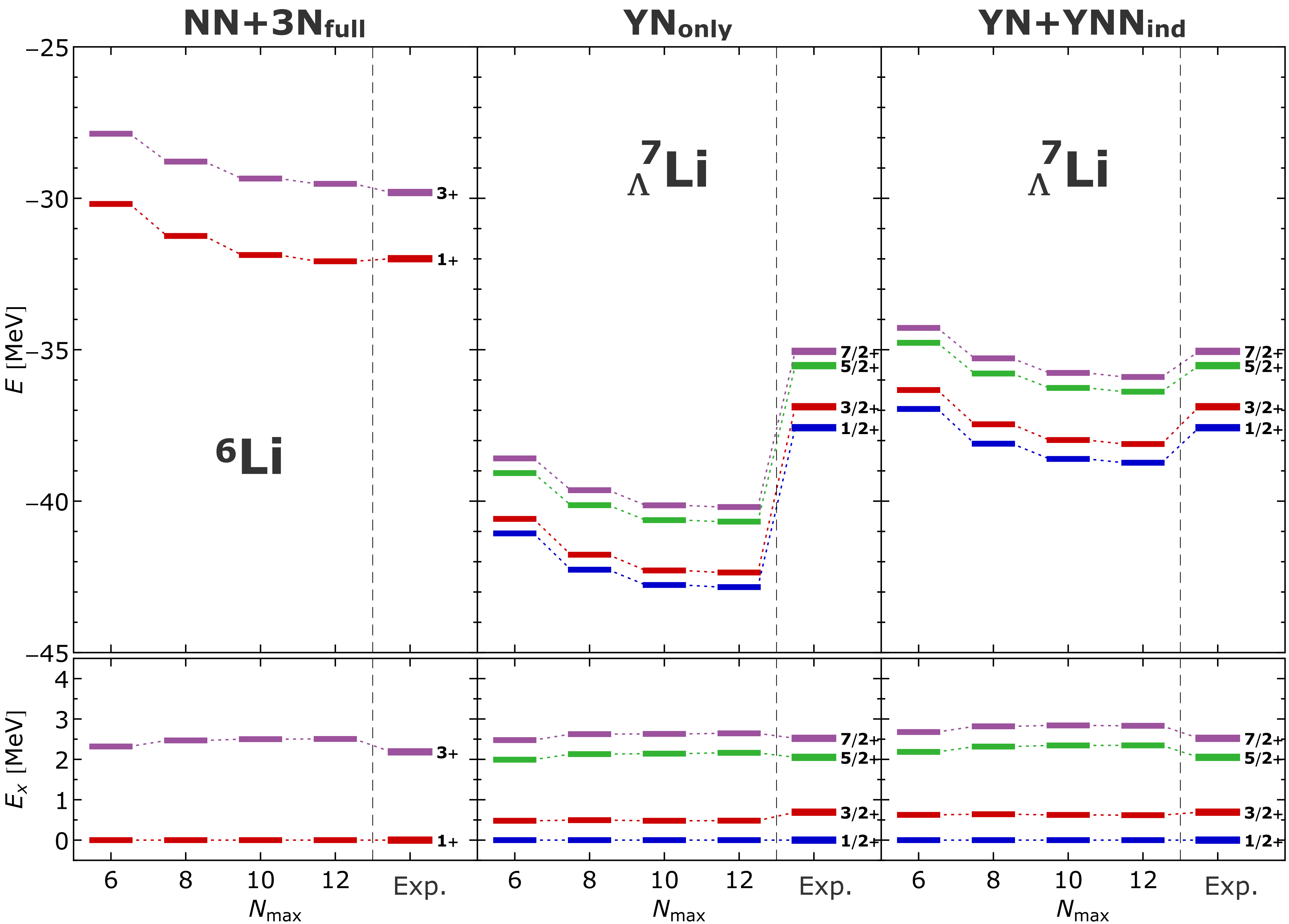
Ab Initio Toolbox for Hypernuclei

Wirth et al.; PRL 113, 192502 (2014); PRL 117, 182501 (2016)

- **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 $\Lambda\Sigma$-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.; PRL 113, 192502 (2014); PRL 117, 182501 (2016)



NCSM

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

chiral YN
LO
Λ_{YN}=700 MeV
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ħΩ=20 MeV

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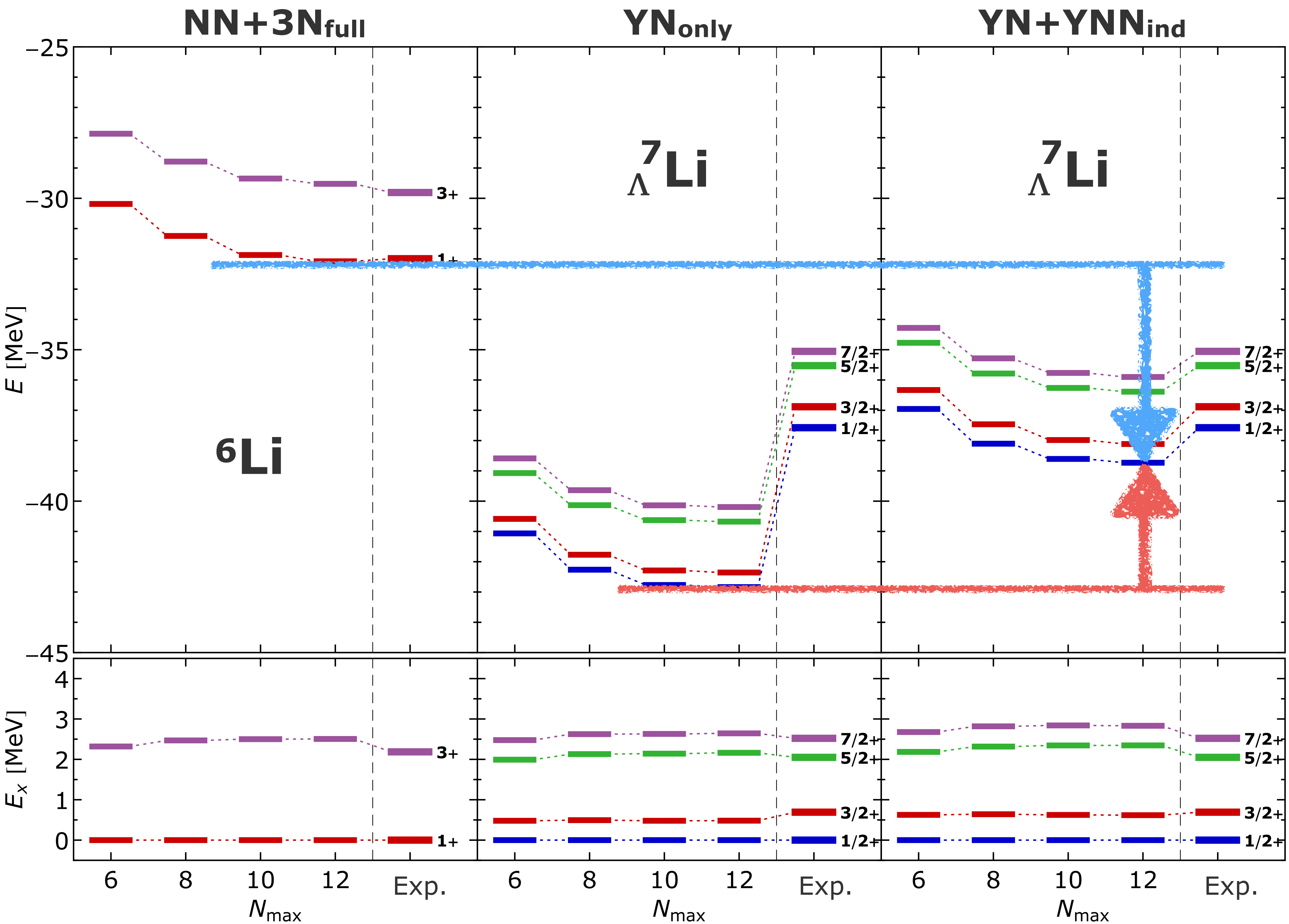

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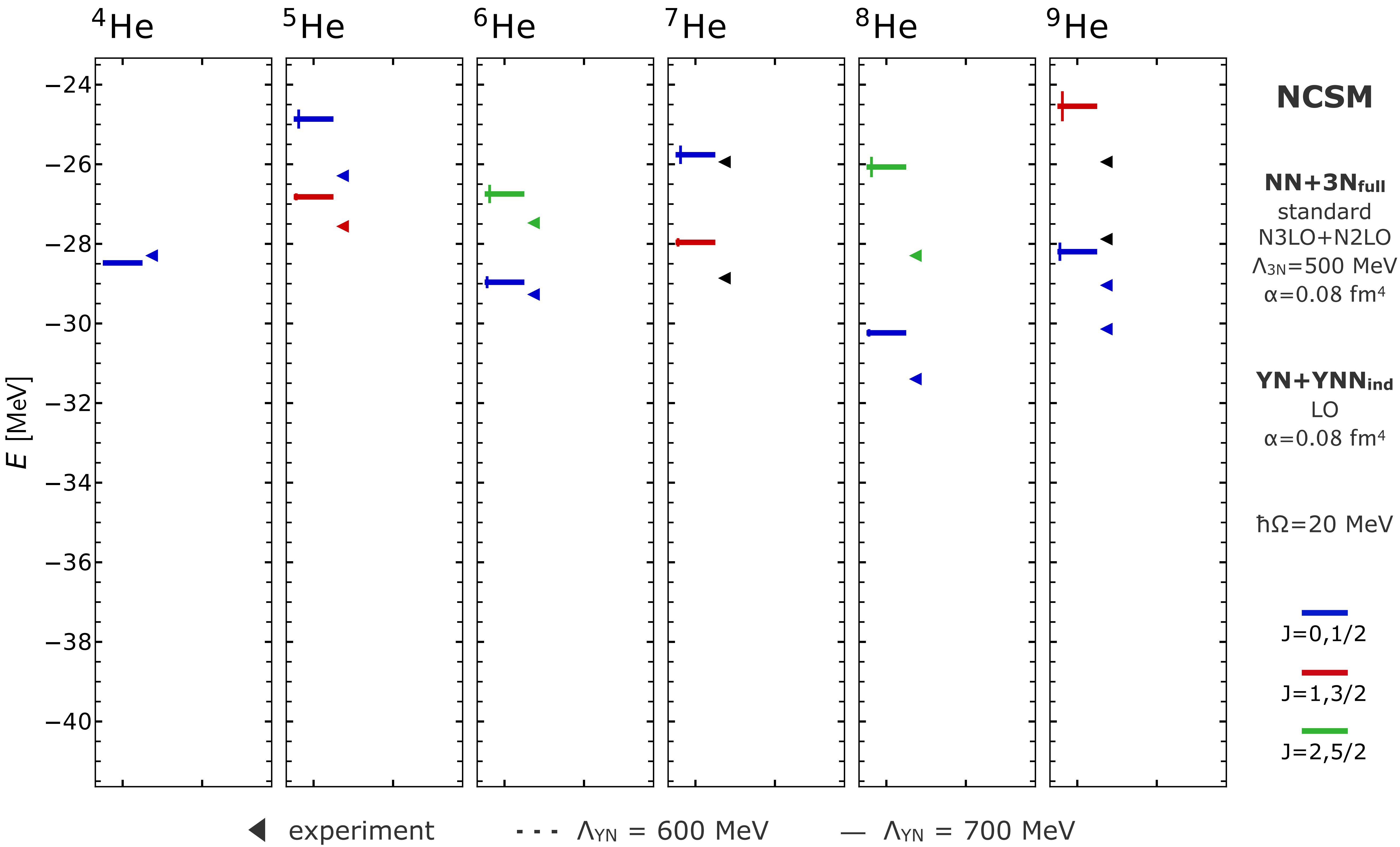
Light Neutron-Rich Hypernuclei

Wirth et al.; PLB 779, 336 (2018)



Light Neutron-Rich Hypernuclei

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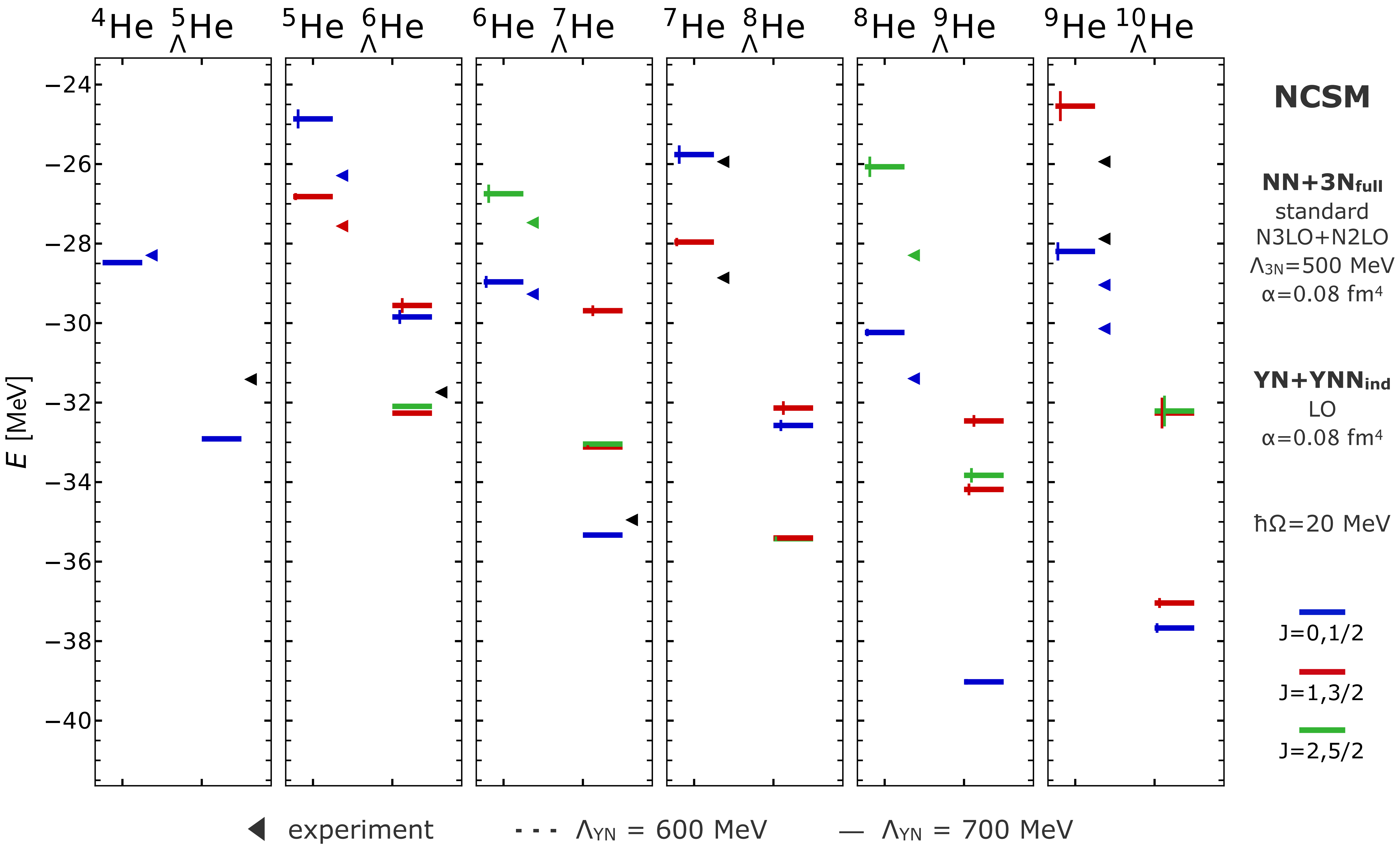
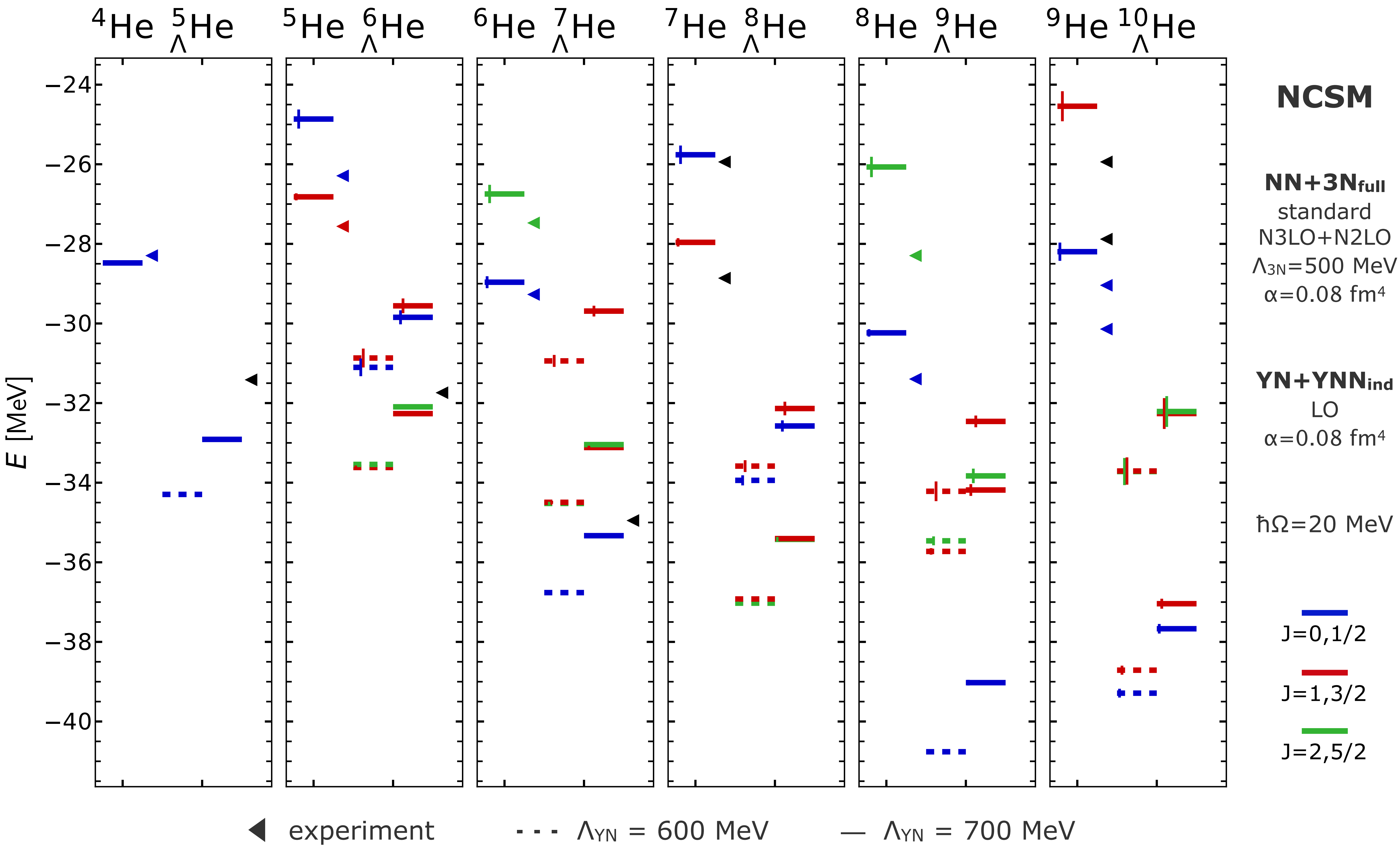


Light Neutron-Rich Hypernuclei

Wirth et al.; PLB 779, 336 (2018)



More Ab Initio...

- **Quantum Monte-Carlo Approches**
  - Variational Monte Carlo
  - Green's Function Monte Carlo, Diffusion / Auxiliary Field Monte Carlo
- **Nuclear Lattice EFT**
  - chiral EFT meets Lattice QCD technology
- **Propagator Methods**
  - Self-Consistent (Gorkov) Green's Function
- **Nuclear and Neutron Matter**
  - Quantum Monte Carlo
  - Many-Body Perturbation Theory
- **Coupling to Continuum**
  - Gamow basis and resonating group method
  - bridge to reaction theory

Ab Initio Frontiers

- **ab initio theory is entering new territory...**
  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT
  - **precision frontier**
    precision spectroscopy of light nuclei, including current contributions
  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum frontier**
    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 and my collaborators**
  - S. Alexa, T. Hüther, M. Knöll, D. Kromm, L. Mertes, T. Mongelli, J. Müller, M. Müller, K. Schröder, K. Vobig, C. Walde, L. Wagner, C. Wenz, T. Wolfgruber & K. Hebeler, A. Tichai
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  - J. Vary, P. Maris
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