Towards Accurate Calculations of Medium-Mass Nuclei
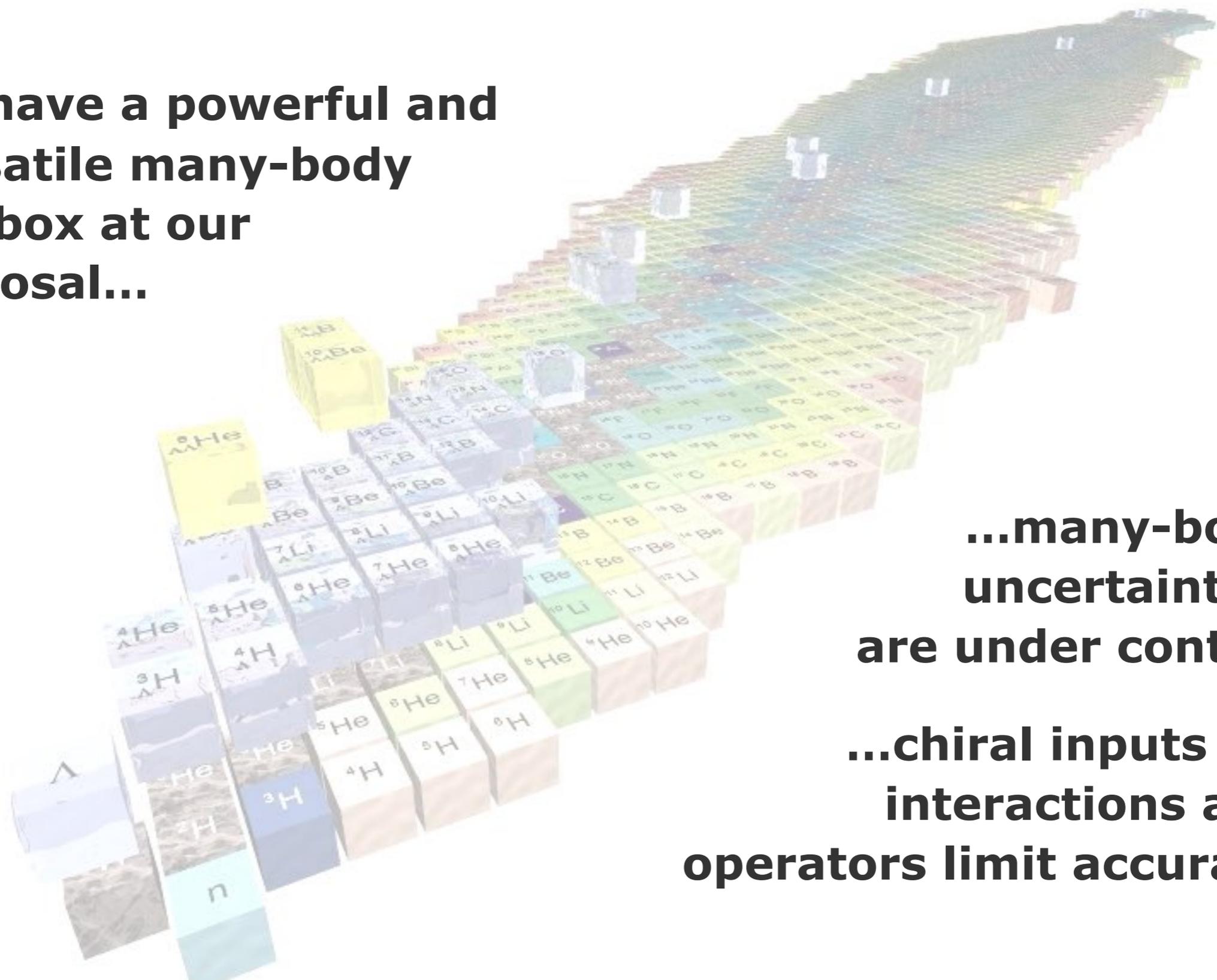
Robert Roth

TECHNISCHE
UNIVERSITÄT
DARMSTADT

we have a powerful and versatile many-body toolbox at our disposal...

...many-body uncertainties are under control

...chiral inputs for interactions and operators limit accuracy

Ab Initio Toolbox

light nuclei

NCSM

- solution of matrix eigenvalue problem in truncated many-body model space

- uncertainties: N_{max} convergence

In-Medium NCSM

- NCSM calculation with an in-medium SRG decoupled many-body Hamiltonian

- uncertainties: NO2B, E_{3max}, e_{max}, N_{max} convergence

In-Medium SRG

- decoupling ground-state from excitations through unitary transformation via flow equations

- uncertainties: NO2B initial and flow equation, E_{3max}, e_{max}

Coupled Cluster

- decoupling ground-state from excitations through similarity transformation via nonlinear amplitude equations

- uncertainties: triples correction, NO2B initial, E_{3max}, e_{max}

heavy nuclei

MBPT, SCGF,...

Ab Initio Toolbox - Add-Ons

Free-Space SRG

- momentum-space decoupling of initial Hamiltonian through unitary transformation
- consistent transformation of NN+3N interaction and all relevant operators
- uncertainties: induced many-body contributions

Basis Optimization

- Hartree-Fock basis
- natural orbitals from perturbatively improved density matrix
- uncertainties: NO2B, E_{3max}, e_{max}

multiple sources of uncertainties...

...quantification not trivial

Third Generation

Chiral Interactions

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)
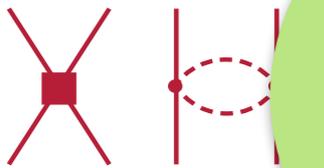*arXiv:1911.04955 (2019)*
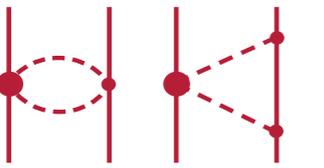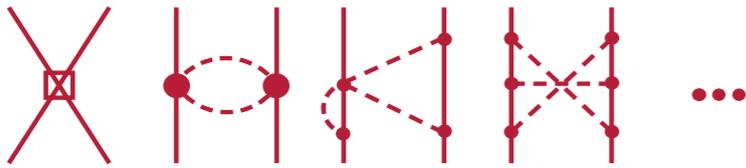
Nuclear Interactions from Chiral EFT

NN

LO

NLO

N2LO

N3LO

N4LO

3rd Generation

- NN+3N interactions with consistent chiral orders and cutoffs

- vary the chiral order and the cutoff systematically to assess uncertainties

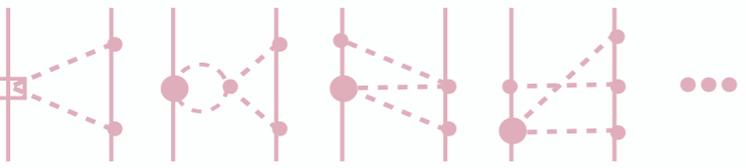- explore dependence on regulator scheme (local, non-local, semi-local)

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

LENPIC: analogous family with semi-local regulators

Strategy

■ **start from chiral NN interaction by Entem, Machleidt & Nosyk**

- LO to N3LO
- non-local regulator
- cutoff 450, 500, 550 MeV
- accurate reproduction of NN scattering data up to ~300 MeV

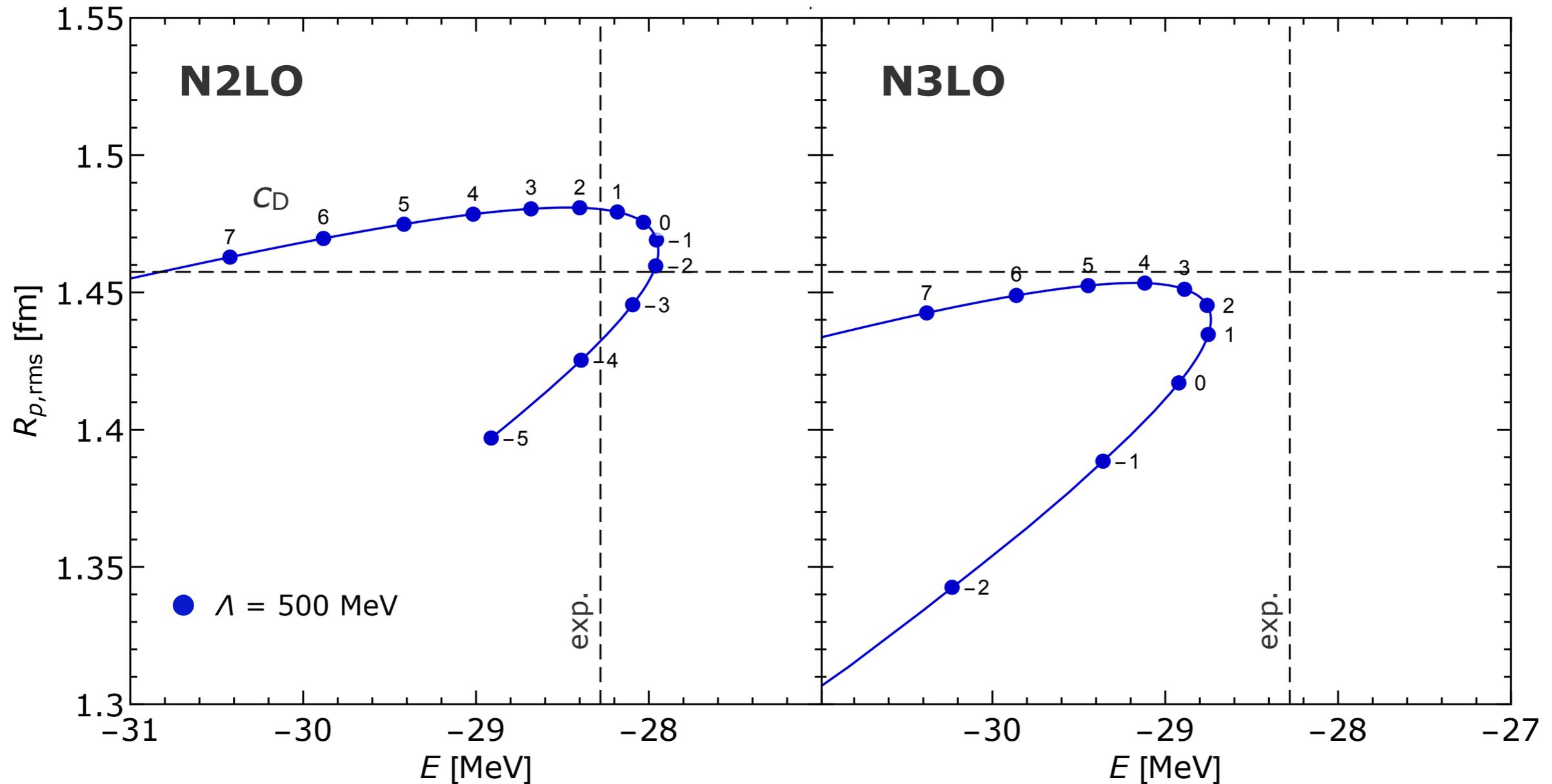■ **supplement non-local 3N interaction at N2LO and N3LO**

- 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 ^{3}H, ^{4}He energy and ^{4}He radius

^{4}He Ground State: c_D Scan

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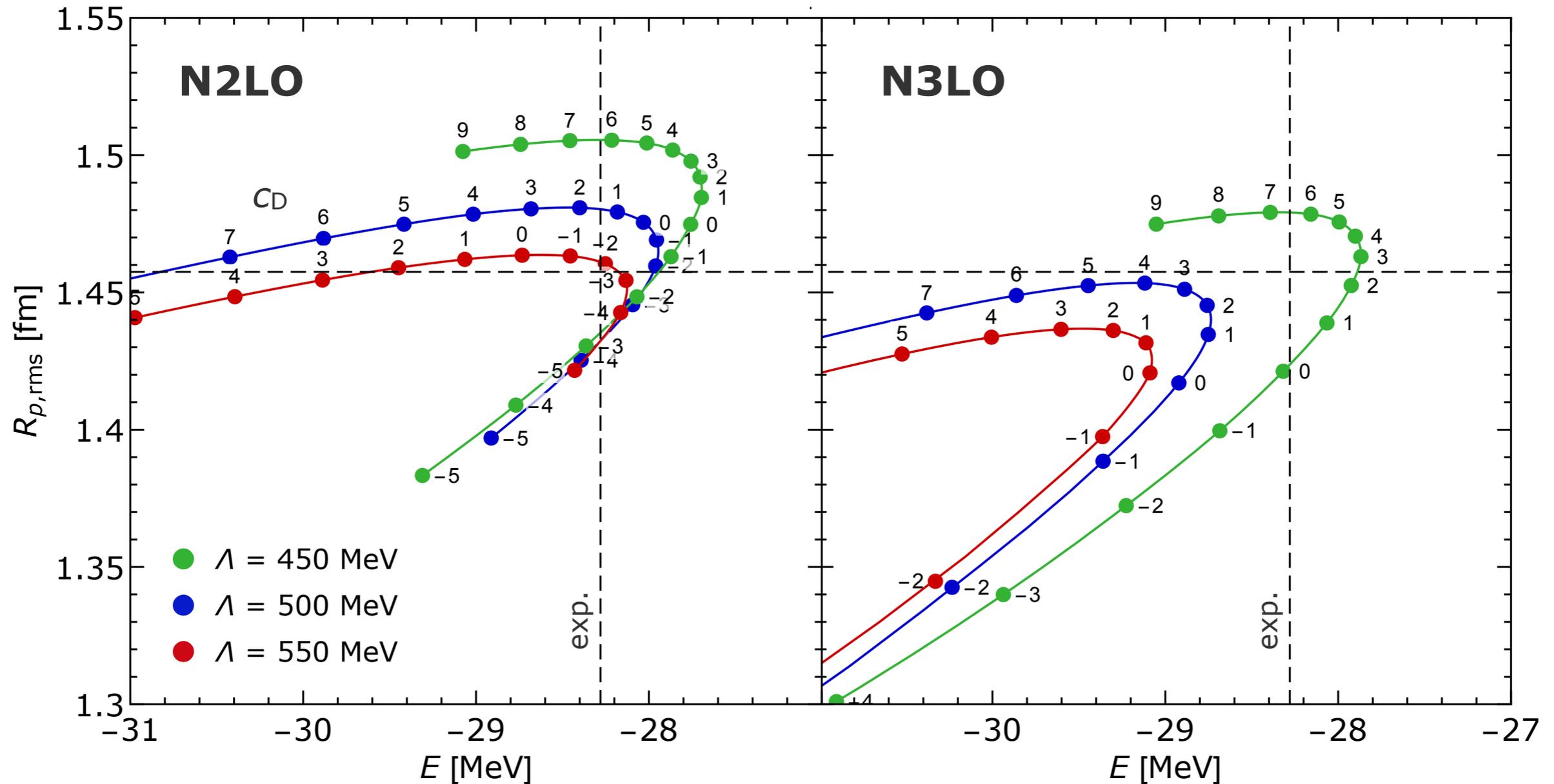
- Jacobi-NCSM calculations for ^{3}H and ^{4}He with bare interaction
- scanning c_D over large range, c_E always fit to ^{3}H binding energy

Medium-Mass Nuclei: c_D Scan
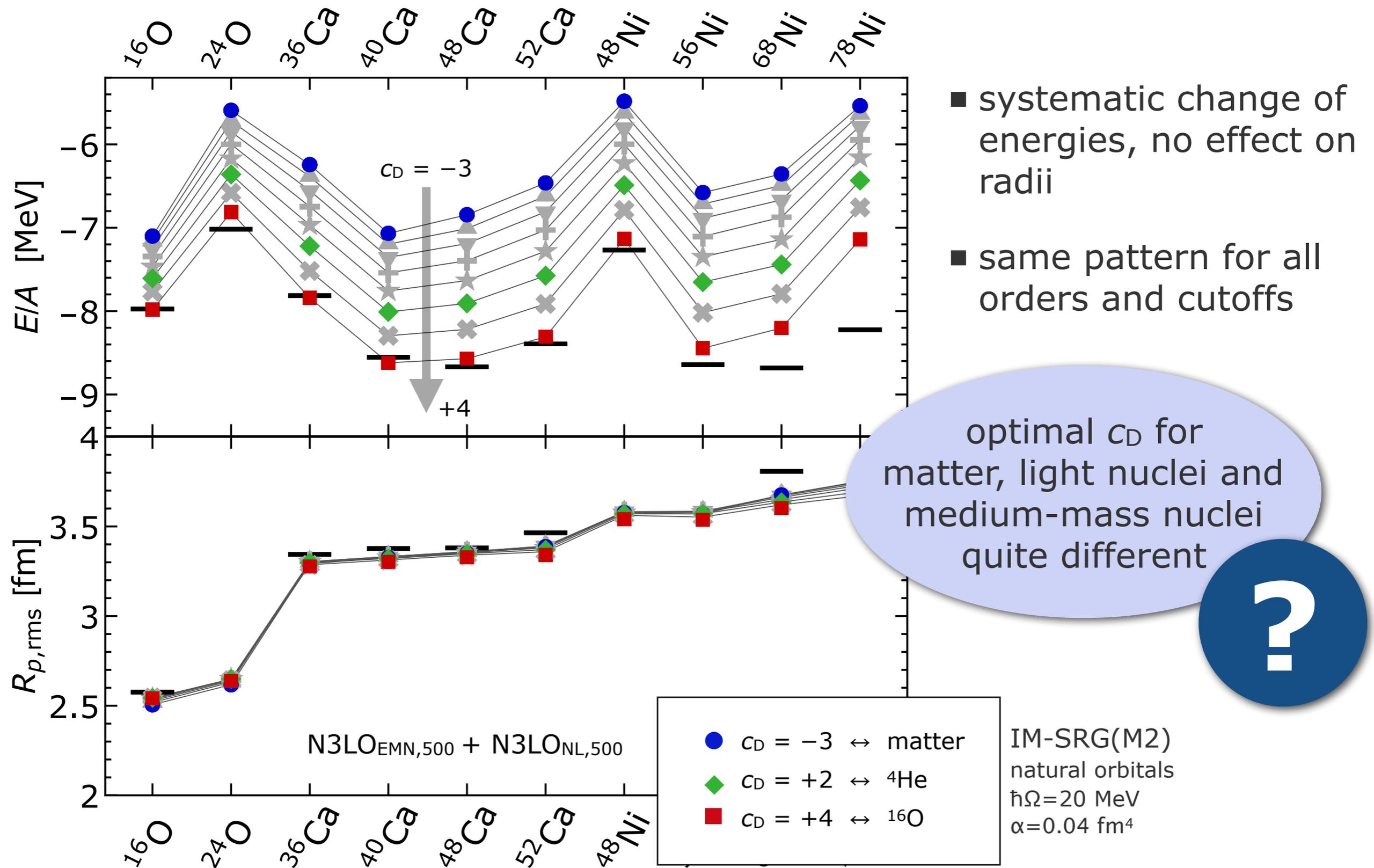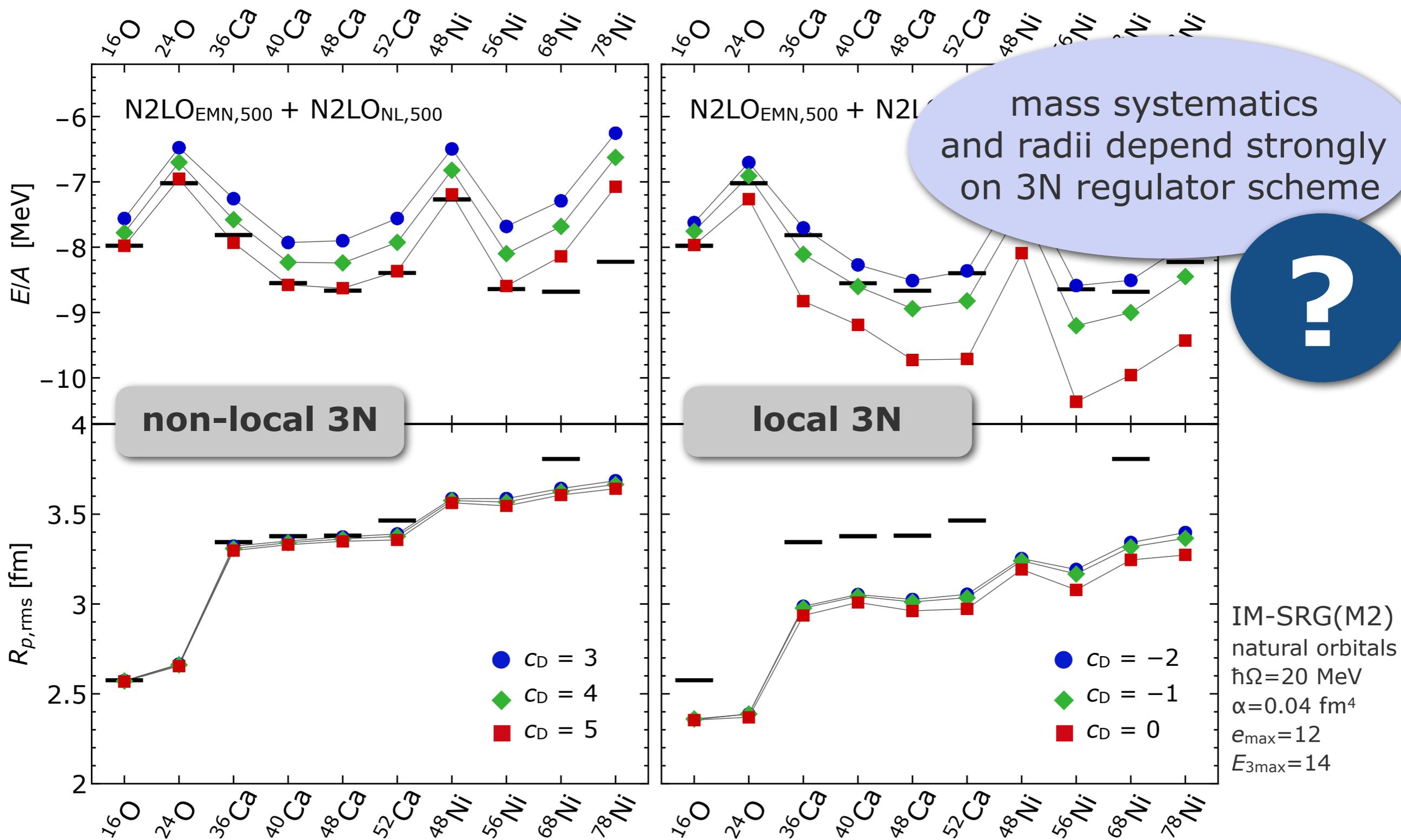
- systematic change of energies, no effect on radii

- same pattern for all orders and cutoffs

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

?

N3LO$_{EMN,500}$ + N3LO$_{NL,500}$

- $c_D = -3$ ↔ matter
- $c_D = +2$ ↔ ^{4}He
- $c_D = +4$ ↔ ^{16}O
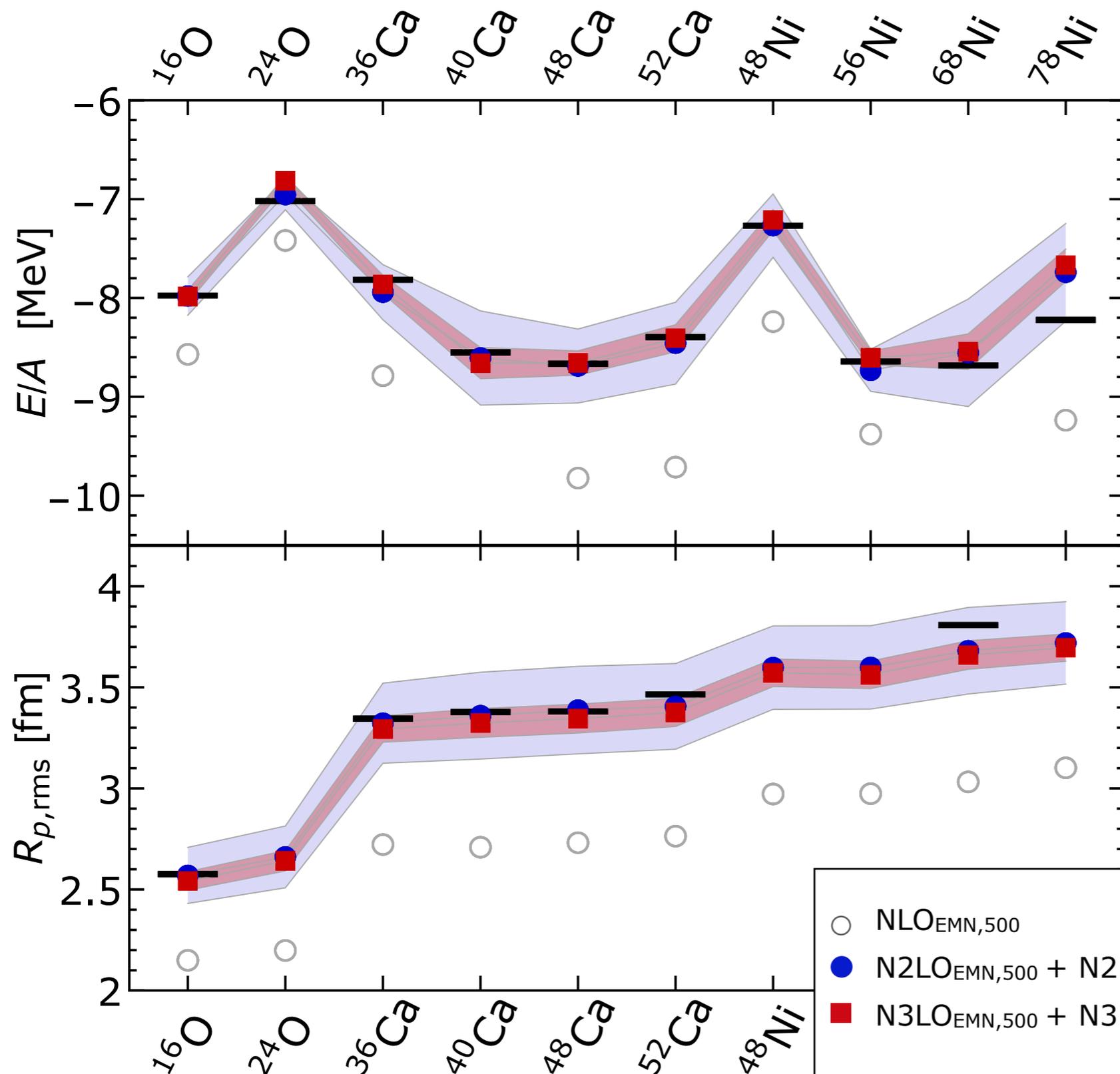
IM-SRG(M2)
natural orbitals
$\hbar\Omega = 20$ MeV
$\alpha = 0.04$ fm^4

Non-Local vs. Local 3N Regulator

Uncertainties

Interaction Uncertainties

- quantify uncertainties from order-by-order systematics

- simplified protocol based on expansion parameter $Q = q/\Lambda_B$

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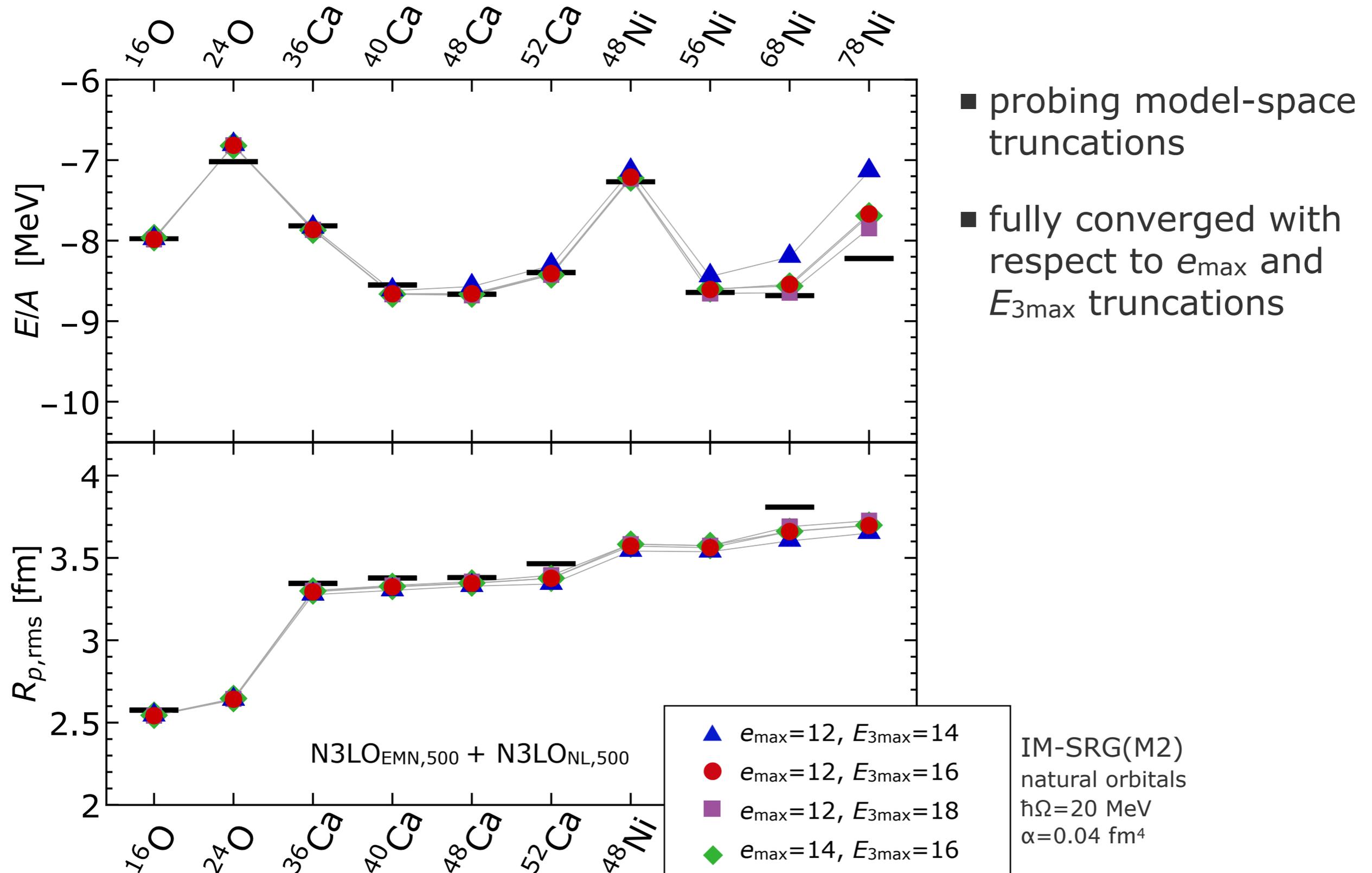$$\quad Q^4 |X_{NLO} - X_{LO}|,$$
$$\quad Q^5 |X_{LO}|)$$

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

Legend:
- ○ NLO$_{EMN,500}$
- ● N2LO$_{EMN,500}$ + N2LO$_{NL,500}$
- ■ N3LO$_{EMN,500}$ + N3LO$_{NL,500}$

Hüther et al.; arXiv:1911.04955

- probing model-space truncations

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

N3LO$_{EMN,500}$ + N3LO$_{NL,500}$

Legend:
- ▲ $e_{max}=12$, $E_{3max}=14$
- ● $e_{max}=12$, $E_{3max}=16$
- ■ $e_{max}=12$, $E_{3max}=18$
- ◆ $e_{max}=14$, $E_{3max}=16$

IM-SRG(M2)
natural orbitals
$\hbar\Omega=20$ MeV
$\alpha=0.04$ fm^4

Many-Body Uncertainties II

- 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%

$N3LO_{EMN,500} + N3LO_{NL,500}$

- α=0.04 fm⁴
- α=0.0625 fm⁴
- α=0.08 fm⁴

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

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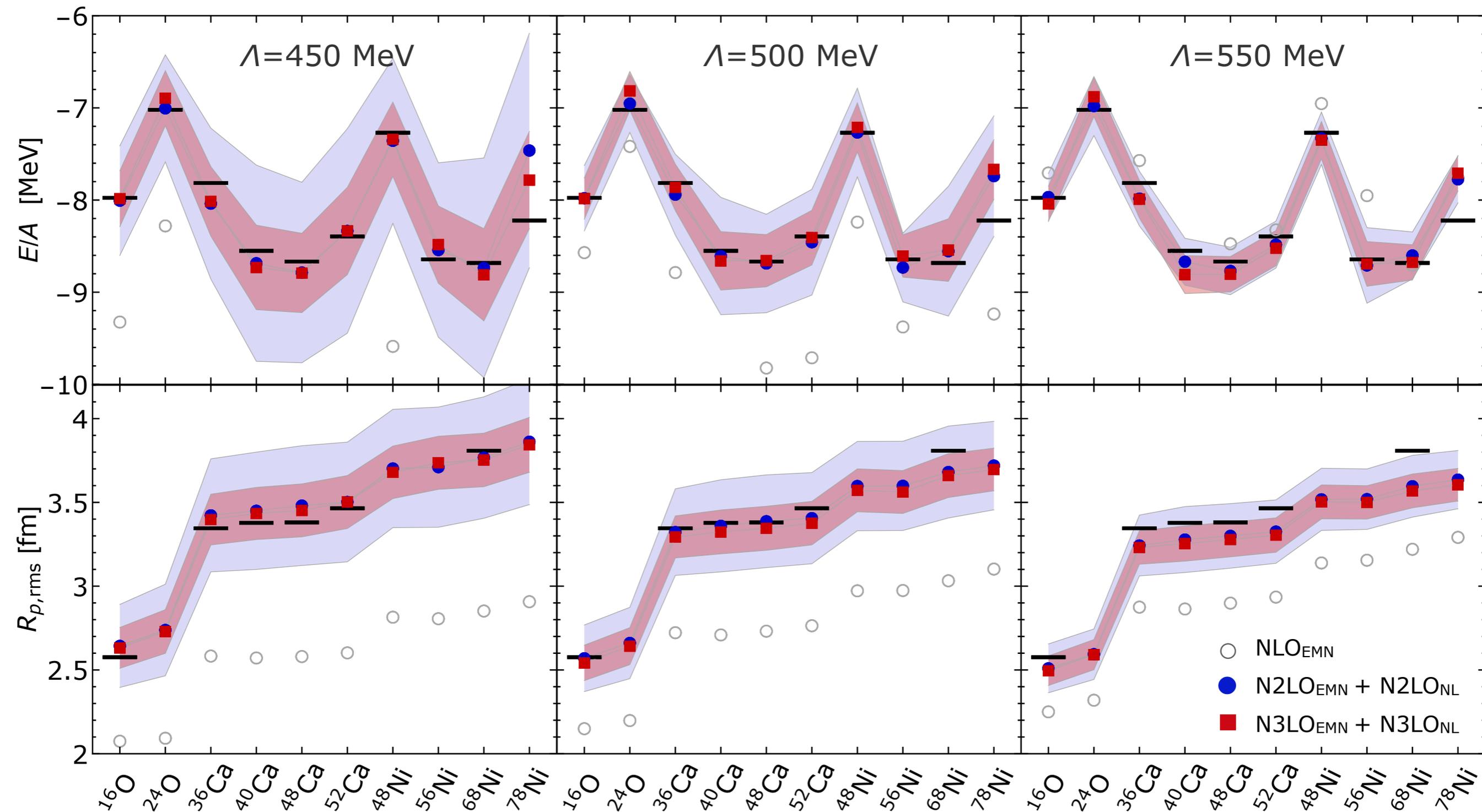
IM-SRG(M2), natural orbitals, $\hbar\Omega=20$ MeV, $\alpha=0.04$ fm^4, $e_{max}=12$, $E_{3max}=16$

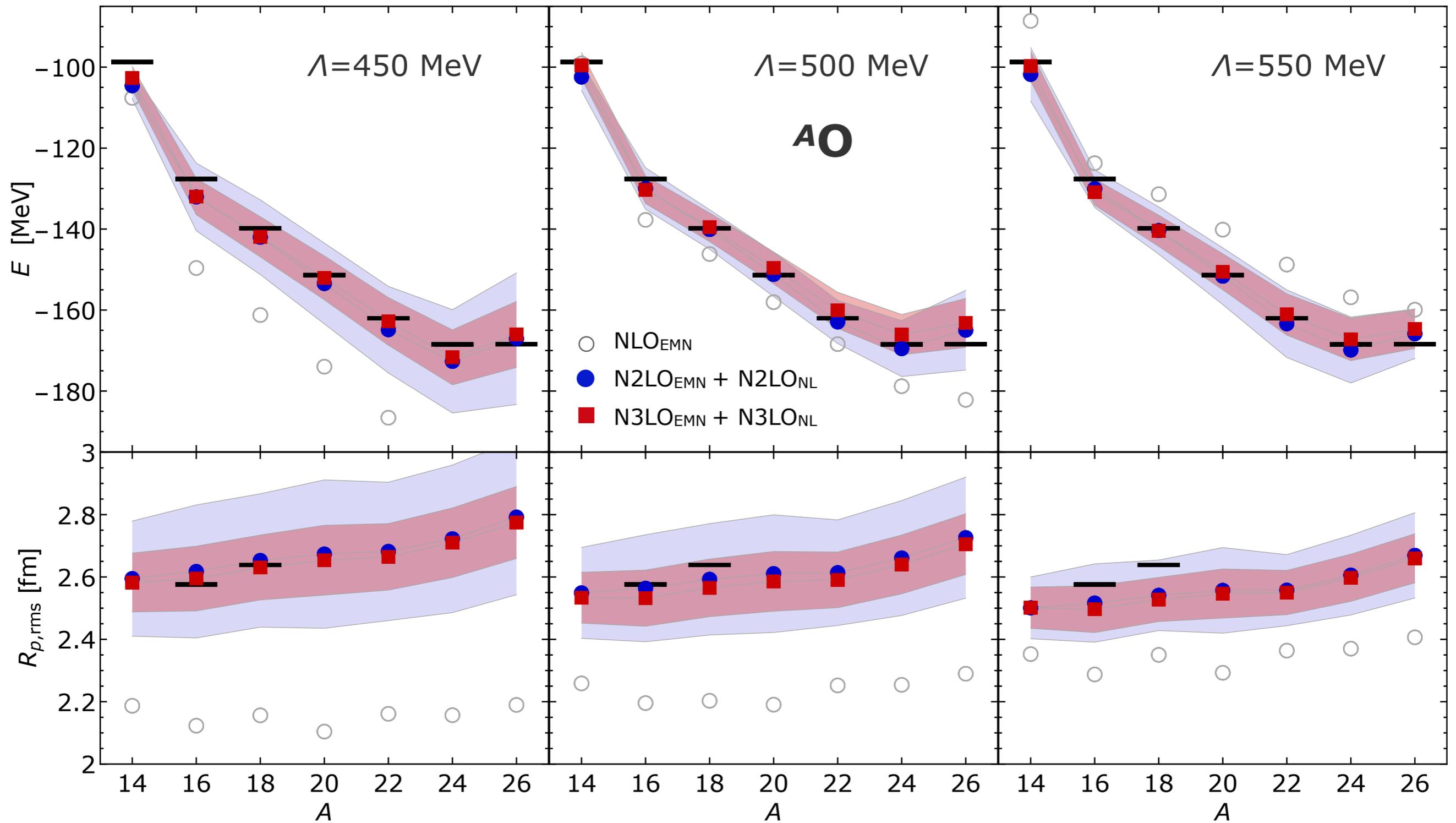error bands show interaction uncertainties

Medium-Mass Nuclei

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

Oxygen Isotopic Chain

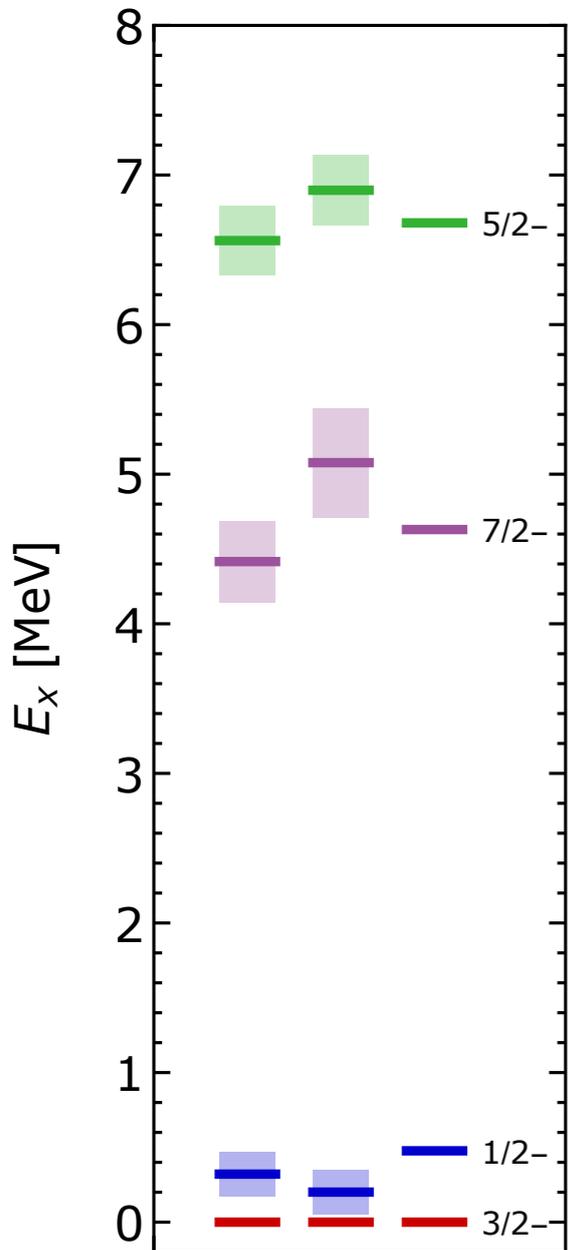IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV, α=0.04 fm⁴, e_{max}=12, E_{3max}=14, N_{ref}=2

error bands show interaction + many-body uncertainties

p-Shell Spectra
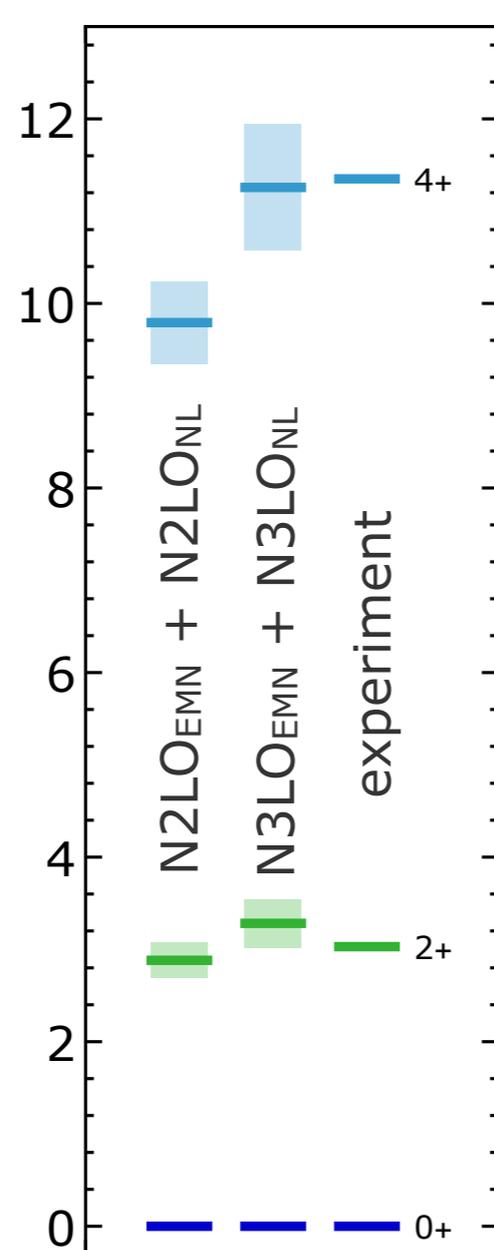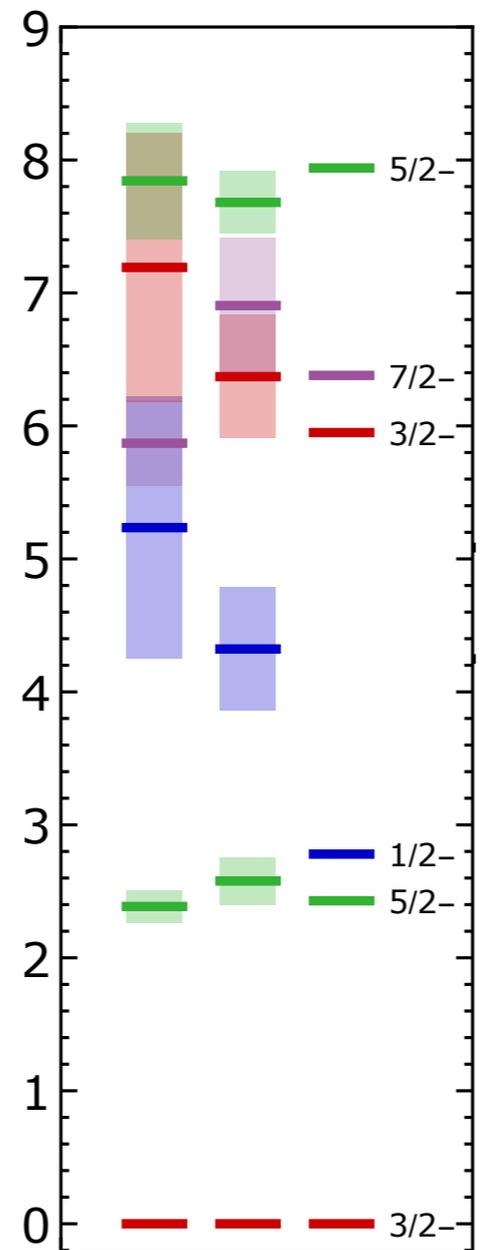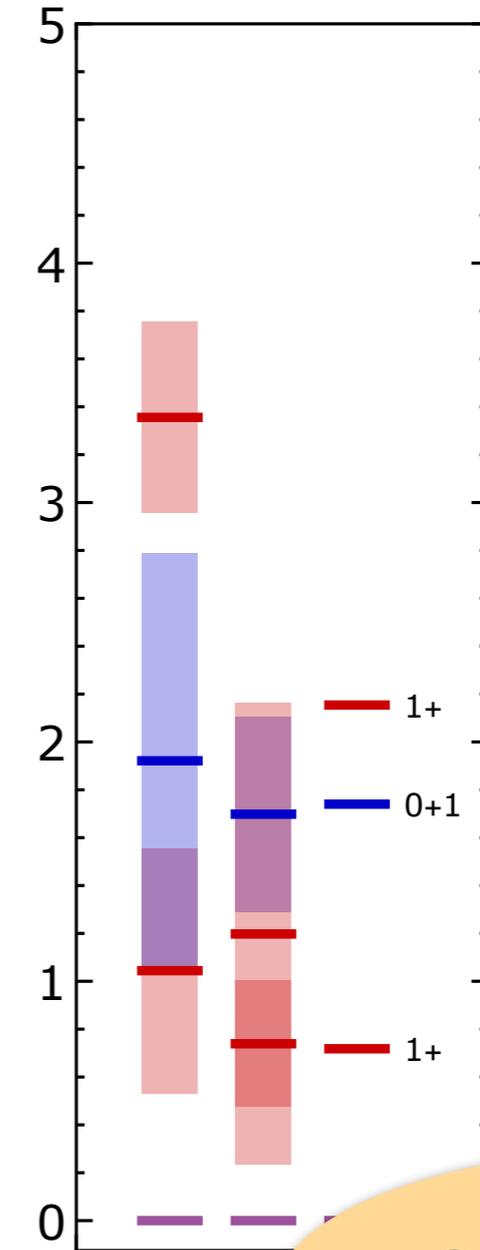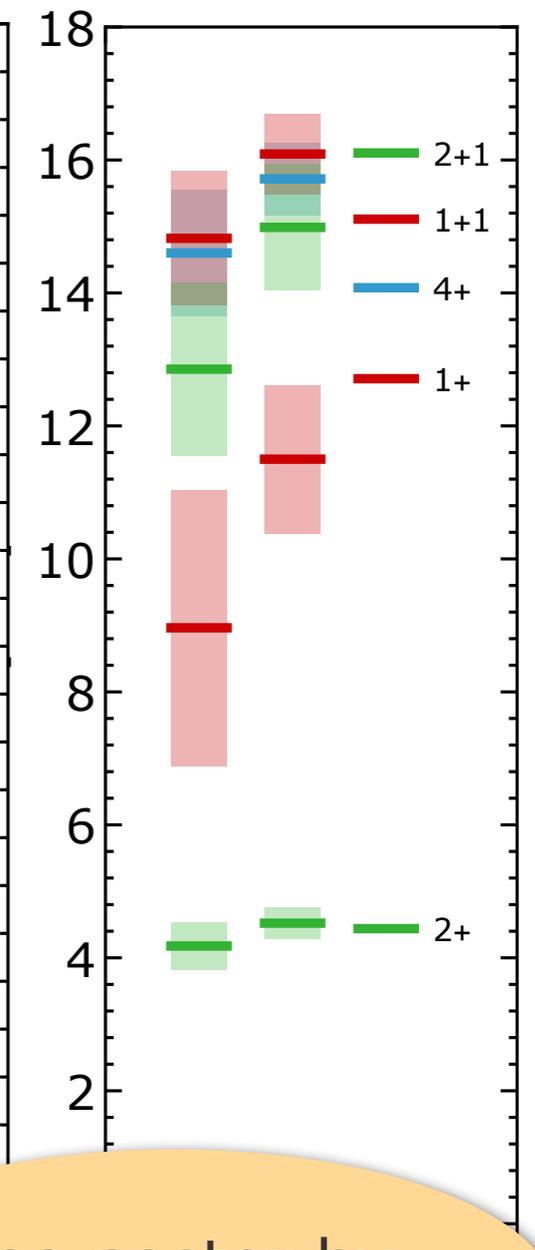
NCSM/IM-NCSM, Λ=500 MeV, ℏΩ=20 MeV
error bands show interaction uncertainties

see poster by
Tobias Mongelli

Uncertain Uncertainties

-or-

The "Expert Assessment"

2%... really?

Many-Body Uncertainties

~2% uncertainty due to NO2B truncations in IM-SRG

^{A}O

Legend:
- ▲ IM-NCSM attached
- ▼ IM-NCSM removed
- ◆ IM-NCSM
- ● NCSM, explicit 3N
- ● NCSM, NO2B

$N3LO_{EM}$ + $N2LO_{L,400}$
$\alpha = 0.08$ fm^4
natural orbitals / HF
$\hbar\Omega = 20$ MeV
$e_{max} = 12$
$N_{max} = 0$ reference
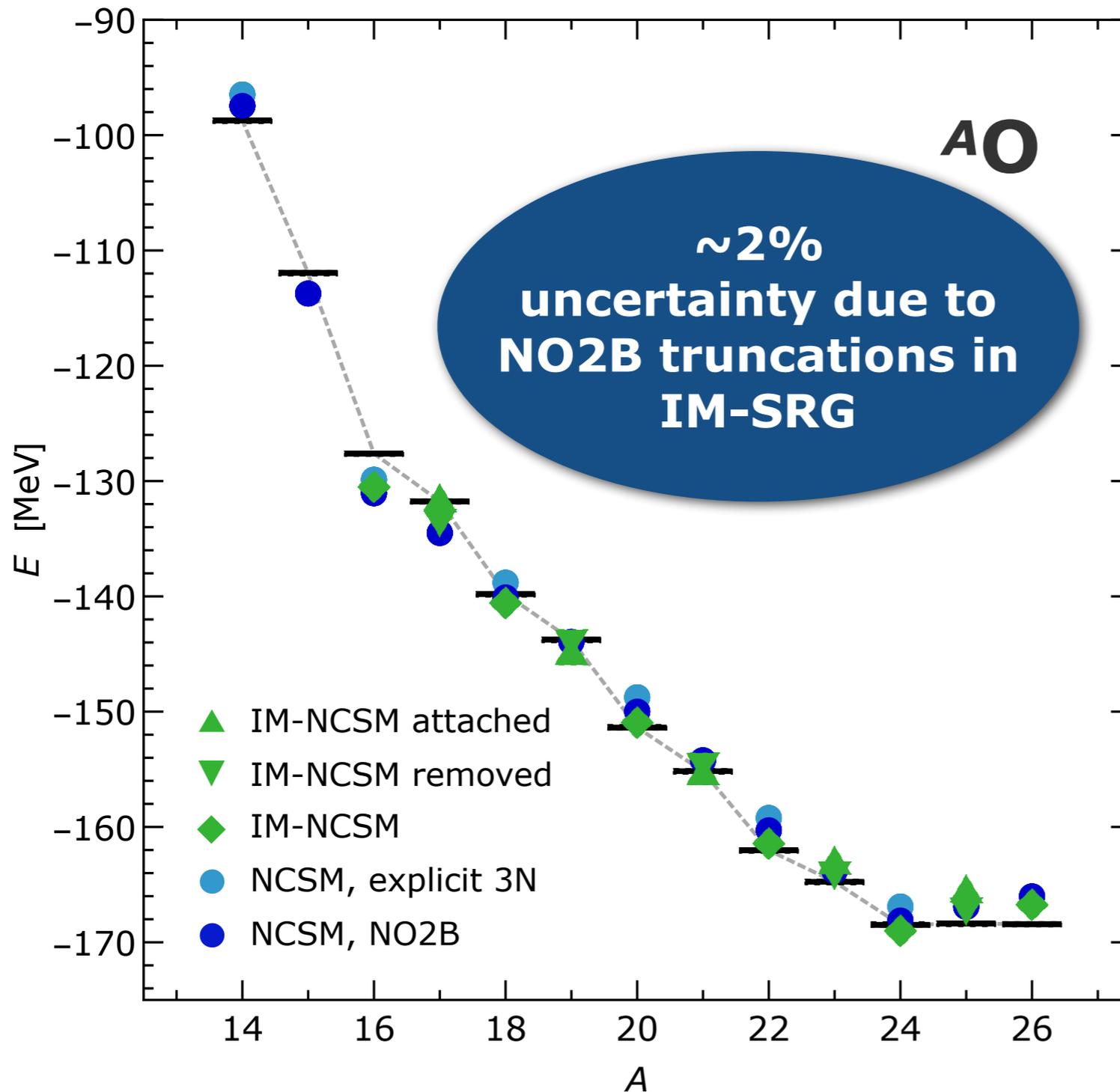
based on energies computed with a specific class of SRG-transformed Hamiltonians

does this hold for bare calculations, other interactions or other observables ???
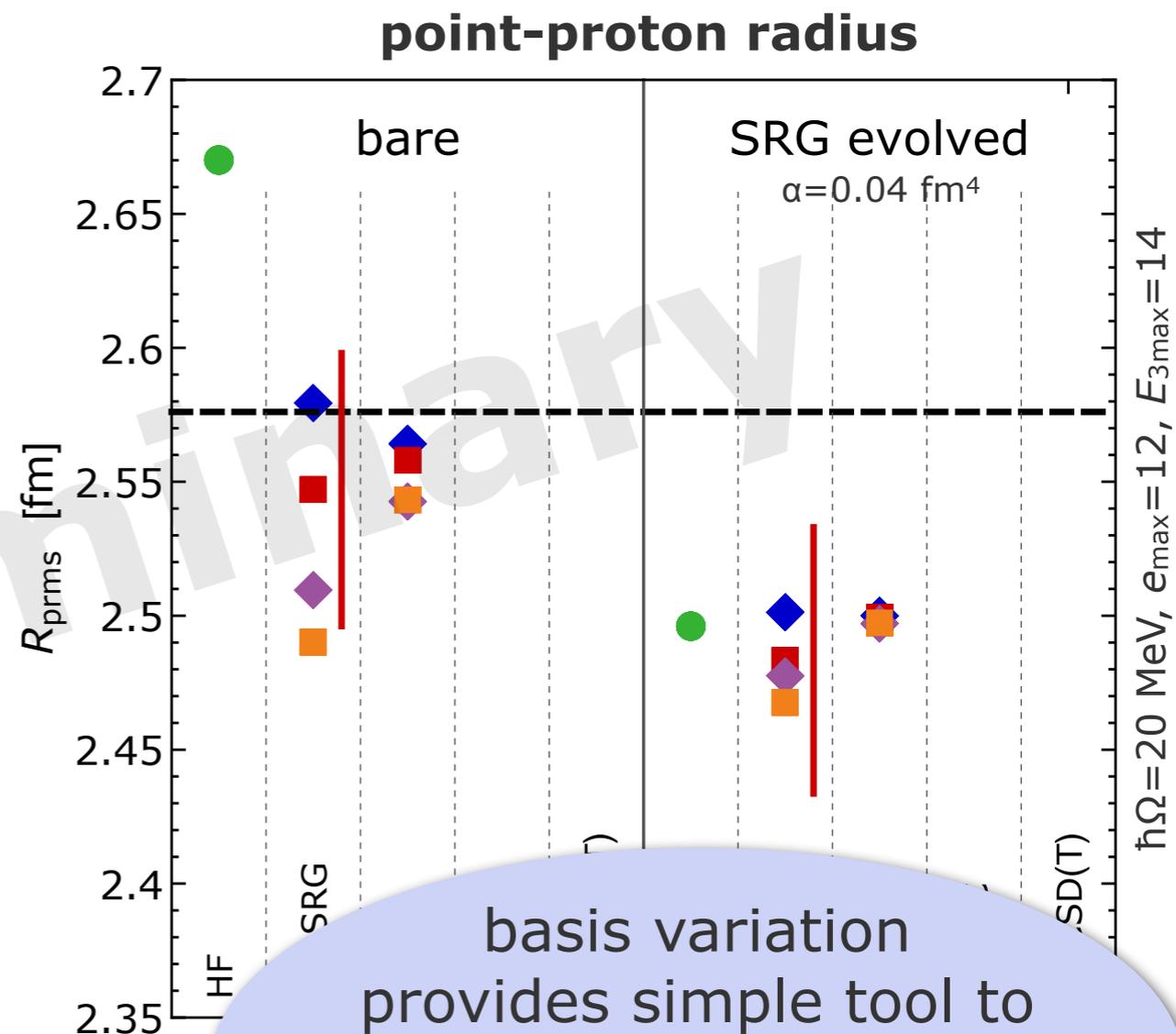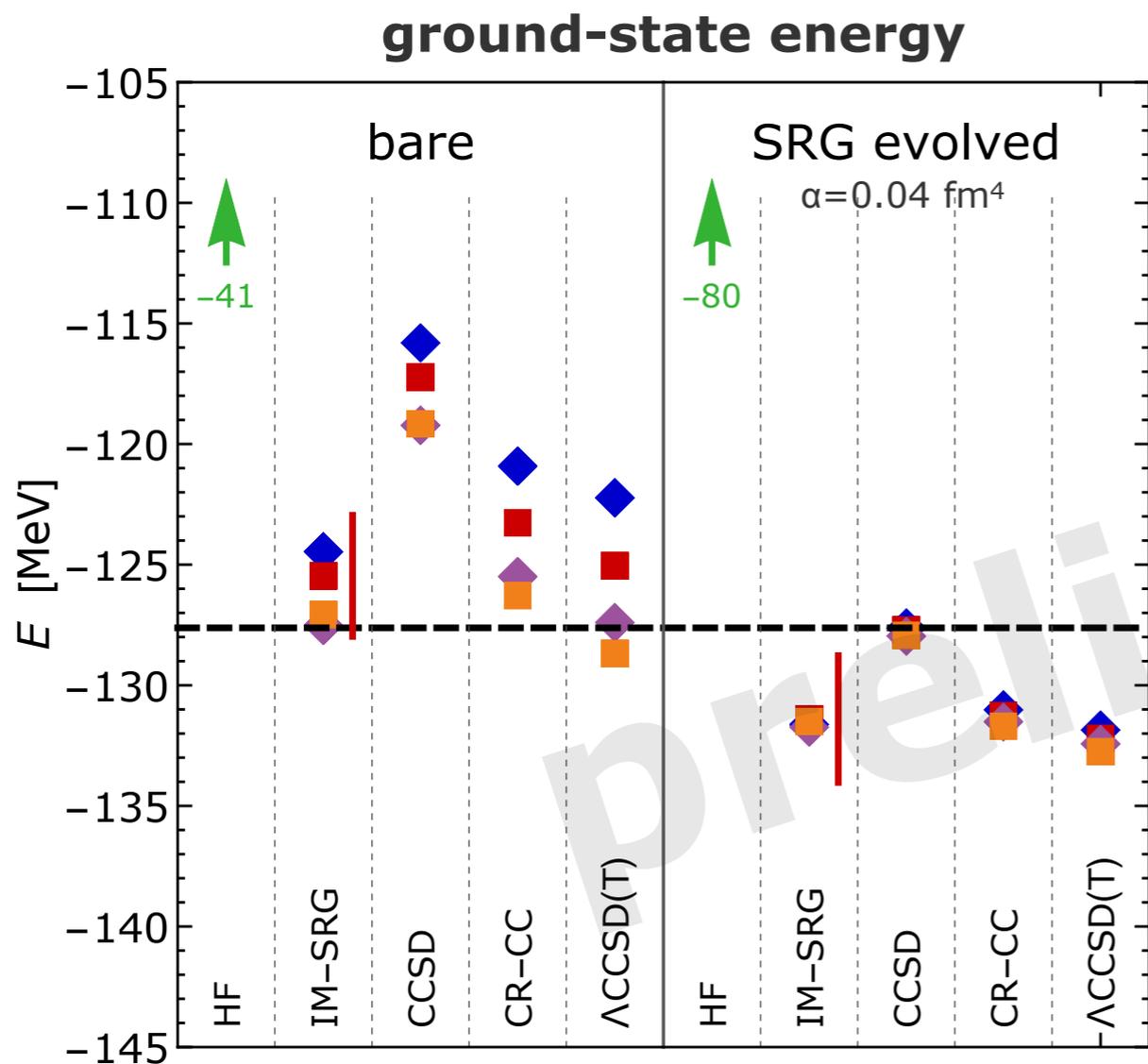
A Simple Exercise

revisit many-body uncertainties through a very simple exercise…

■ compare a few standard medium-mass calculations for ground-state energies and radii and compare results with…

- **bare and SRG-transformed Hamiltonians** starting from

$$N2LO_{SAT} \quad \text{and} \quad N3LO_{EMN,500} + N3LO_{NL,500}$$

- different **medium-mass methods**

$$\text{IM-SRG(M2), CCSD, CR-CC(2,3), } \Lambda\text{-CCSD(T)}$$

- different **single-particle bases**
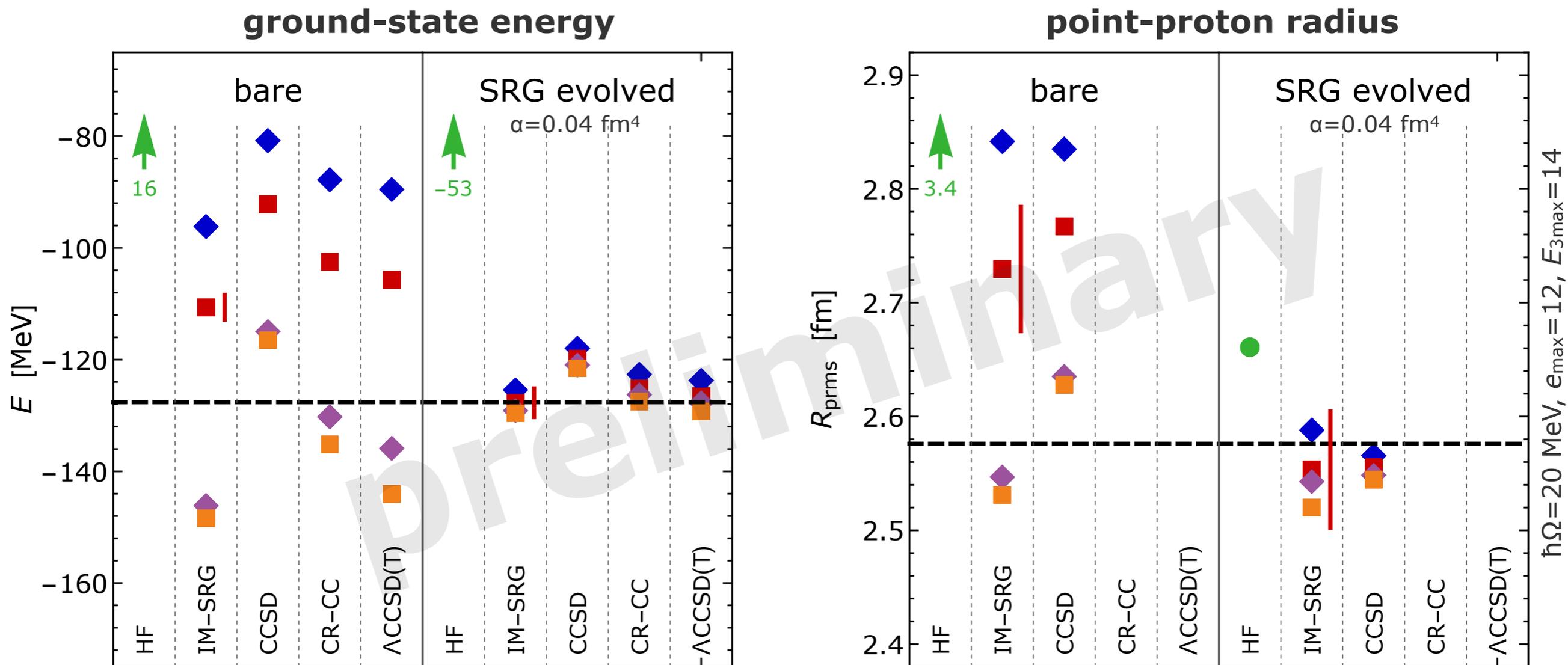
Hartree-Fock, natural orbitals, more creative

^{16}O with N2LO$_{SAT}$

ground-state energy

bare | SRG evolved ($\alpha=0.04$ fm^4)

E [MeV]

HF · IM–SRG · CCSD · CR–CC · ΛCCSD(T) | HF · IM–SRG · CCSD · CR–CC · ΛCCSD(T)

point-proton radius

bare | SRG evolved ($\alpha=0.04$ fm^4)

R_{prms} [fm]

$\hbar\Omega=20$ MeV, $e_{max}=12$, $E_{3max}=14$

basis variation provides simple tool to probe uncertainties due to reference state, NO2B, E_{3max},...

♦ standard HF basis for actual Hamiltonian

■ standard NAT basis for actual Hamiltonian

♦ HF basis for SRG-evolved Hamiltonian with $\alpha=0.08$ fm^4

■ NAT basis for SRG-evolved Hamiltonian with $\alpha=0.08$ fm^4

^{16}O with N3LO$_{EMN,500}$+N3LO$_{NL,500}$

ground-state energy

point-proton radius

standard HF basis for actual Hamiltonian

standard NAT basis for actual Hamiltonian

HF basis for SRG-evolved Hamiltonian with α=0.08 fm⁴

NAT basis for SRG-evolved Hamiltonian with α=0.08 fm⁴

Summary

some solutions

...new family of NN+3N interactions up to N3LO with non-local regulators for different cutoffs

...quantification of interaction and many-body uncertainties

...excellent description of ground-state energies, radii, spectra

more questions

...why the drastic differences between local and non-local 3N regulators ?

...why the different optimal c_D values in few-body/many-body/matter ?

...are we sometimes overly optimistic with our many-body uncertainties ?

Epilogue

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

  - S. Alexa, **T. Hüther**, M. Knöll, L. Mertes, T. Mongelli, J. Müller, K. Vobig, T. Wolfgruber &
    K. Hebeler, A. Tichai
    Technische Universität Darmstadt

  - T. Duguet
    CEA Saclay

  - P. Navrátil
    TRIUMF, Vancouver

  - H. Hergert, R. Wirth
    NSCL / Michigan State University

  - J. Vary, P. Maris
    Iowa State University

  - R. Machleidt
    University of Idaho

  - E. Epelbaum, H. Krebs, P. Reinhard &
    the LENPIC Collaboration
    Universität Bochum, …