A Practitioner's View of Next-Generation Chiral Interactions

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Last Year at TRIUMF…

$$c_D = -0.2 \rightarrow 0.8$$

Eur. Phys. J. A (2018) **54**: 76
DOI 10.1140/epja/i2018-12530-6

Erratum

**Erratum to: Uncertain
from ^{3}H β decay**

P. Klos[1,2,a], A. Carbone[1,2,b], K. Hebeler[1,2,c],
[1] Institut für Kernphysik, Technische Universitä
ExtreMe Matter Institute EMMI
Department of Physi
Max-Planck-Insti

ginal article: Eur

Received: 2
Published o

our article the
is consistent wit

lt the c_D

PHYSICAL REVIEW LETTERS **121,** 049901(E) (2018)

Erratum: Chiral Effective Field Theory Predictions for Muon Capture on Deuteron and ^{3}He [Phys. Rev. Lett. 108, 052502 (2012)]

L. E. Marcucci, A. Kievsky, S. Rosati, R. Schiavilla, and M. Viviani

(Received 29 June 2018; published 25 July 2018)

121.049901

the three-nucleon contact inte
lation reads [2]

he Letter should be re
nchanged). (2) Tables

lly very small, and th
of the proton-proton w
clusions of those stud
me observables as in th
tritium Gamow-Telle

PHYSICAL REVIEW LETTERS **122,** 029901(E) (2019)

Erratum: Three-Nucleon Low-Energy Constants from the Consistency of Interactions and Currents in Chiral Effective Field Theory [Phys. Rev. Lett. 103, 102502 (2009)]

Doron Gazit, Sofia Quaglioni, and Petr Navrátil

(Received 27 November 2018; published 15 January 2019)

Consequences

- revise ‘standard’ interactions we use in many-body calculations

- reexamine ad-hoc choices made in the 3N sector
  - regulator scheme: local vs. non-local vs. semi-local
  - regulator scale
  - determination and sensitivity to c_D

- address deficiencies observed in previous-generation interactions
  - radii beyond the lightest isotopes
  - overbinding in medium-mass nuclei

- use ‘fast’ many-body methods to explore a large set of interactions

Practitioner’s Toolbox

No-Core Shell Model & Friends

No-Core Shell Model

- solution of matrix eigenvalue problem in truncated many-body model space
- **universality:** all nuclei and all bound-state observables on the same footing
- **but:** limited by model-space convergence

In-Medium Similarity Renormalization Group

- decoupling ground-state from excitations through unitary transformation via flow equation
- **efficiency:** favorable scaling gives access to medium-mass nuclei
- **but:** limited to ground-state observables

Many-Body Perturbation Theory

- power-series expansion of energies and states
- **simplicity:** low-order contributions can be evaluated very easily and efficiently
- **but:** order-by-order convergence problematic

Natural-Orbital NCSM

J. Müller, A. Tichai, K. Vobig, R. Roth, PRC (2019) in print

MBPT
basis optimization

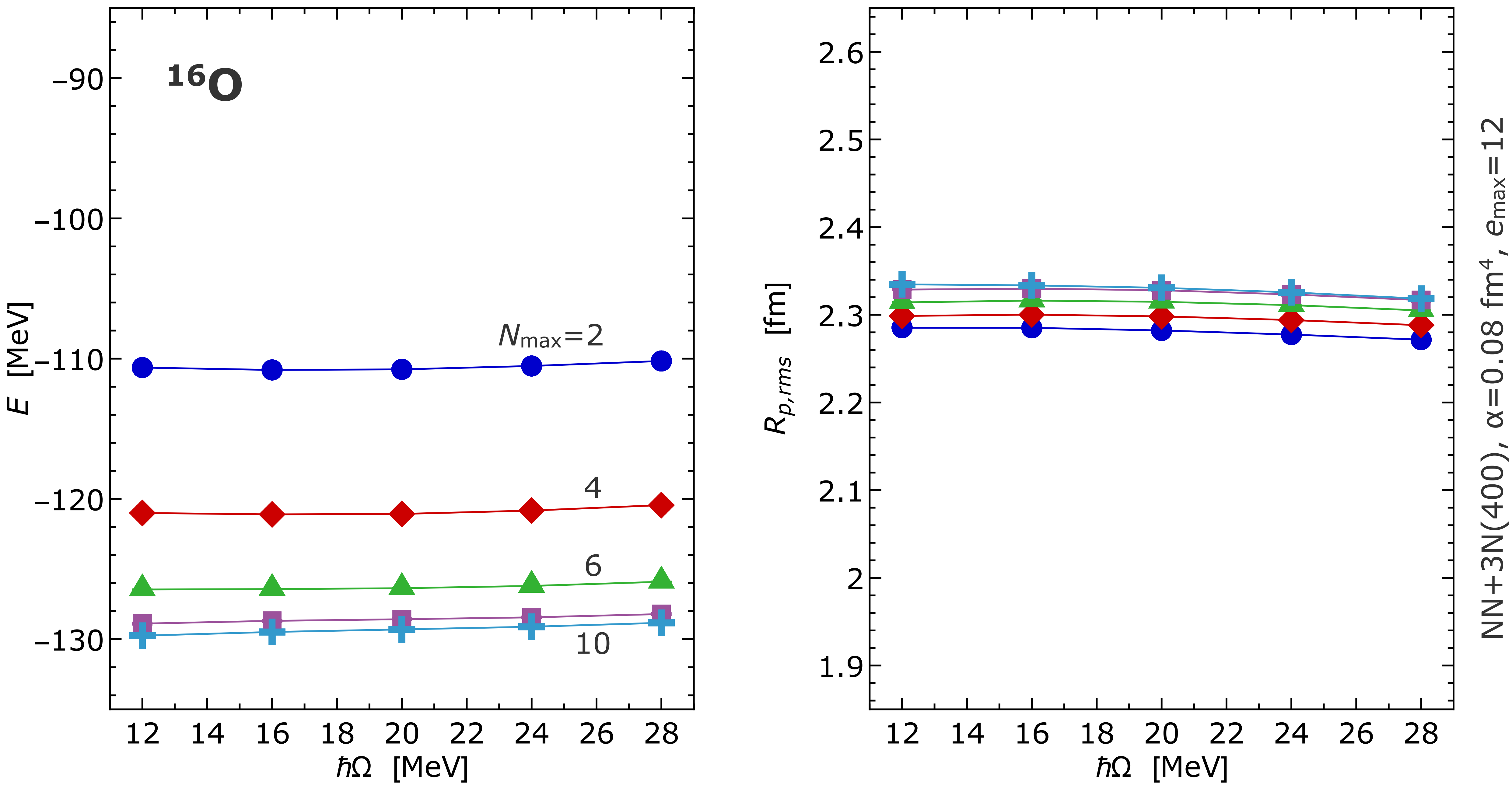
- construct HF basis in large single-particle space
- compute perturbative corrections to one-body density matrix up to second order
- determine natural orbitals from one-body density matrix and transform matrix elements

NCSM
many-body solution

- NCSM calculation with natural-orbital basis
- use importance truncation for large spaces and heavier nuclei (optional)
- use normal-ordered two-body approximation to include 3N interactions (optional)

Natural-Orbital NCSM: Convergence

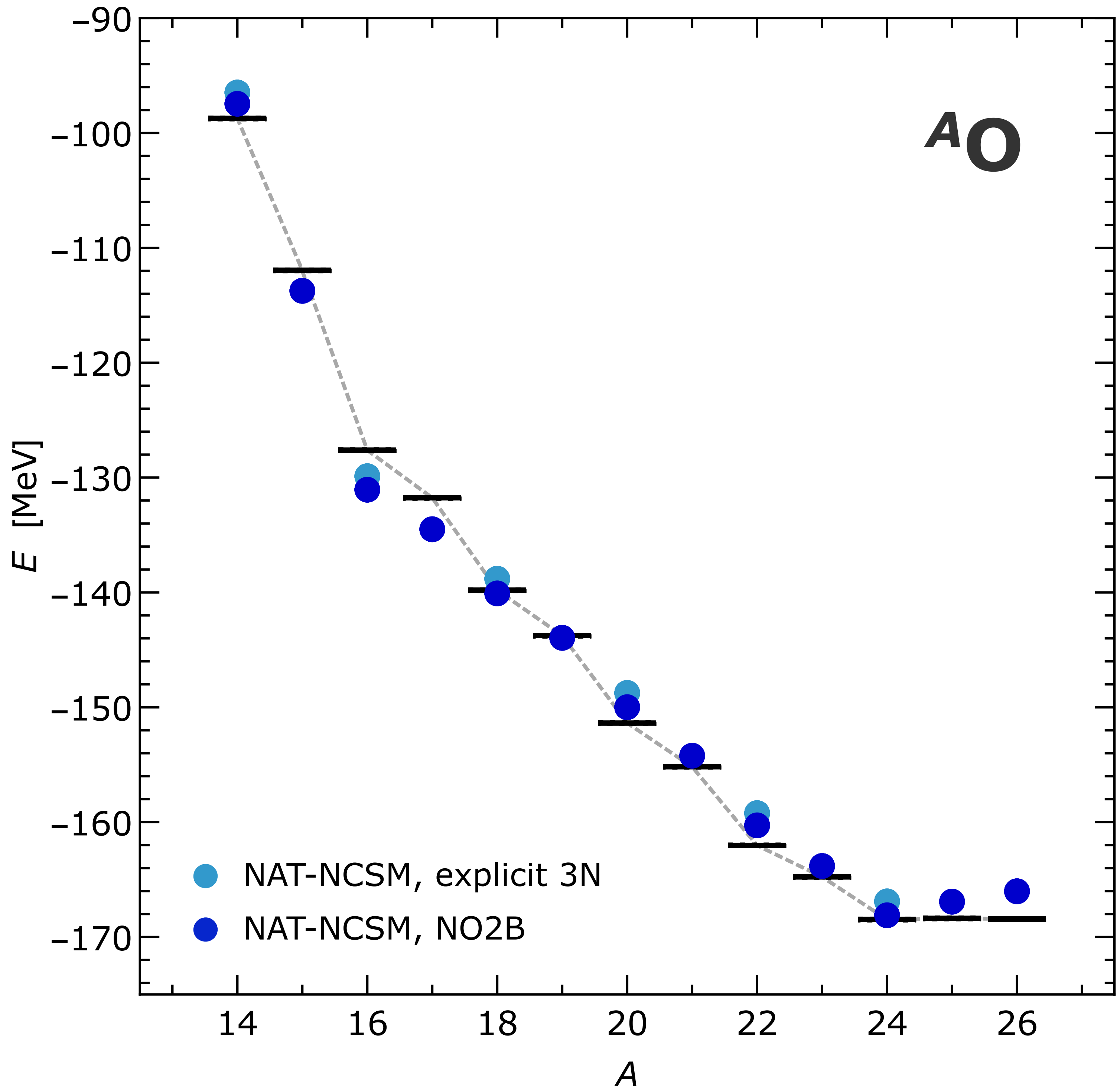
J. Müller, A. Tichai, K. Vobig, R. Roth, PRC (2019) in print



- natural-orbital basis eliminates frequency dependence and accelerates model-space convergence

Oxygen Isotopes

J. Müller, A. Tichai, K. Vobig, R. Roth, PRC (2019) in print



- excellent convergence with natural-orbital basis for all oxygen isotopes
- NO2B instead of explicit 3N causes ~1% overbinding

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

Perturbatively Improved NCSM

Tichai, Gebrerufael, Vobig, Roth; PLB 786, 448 (2018)

NCSM
many-body solution

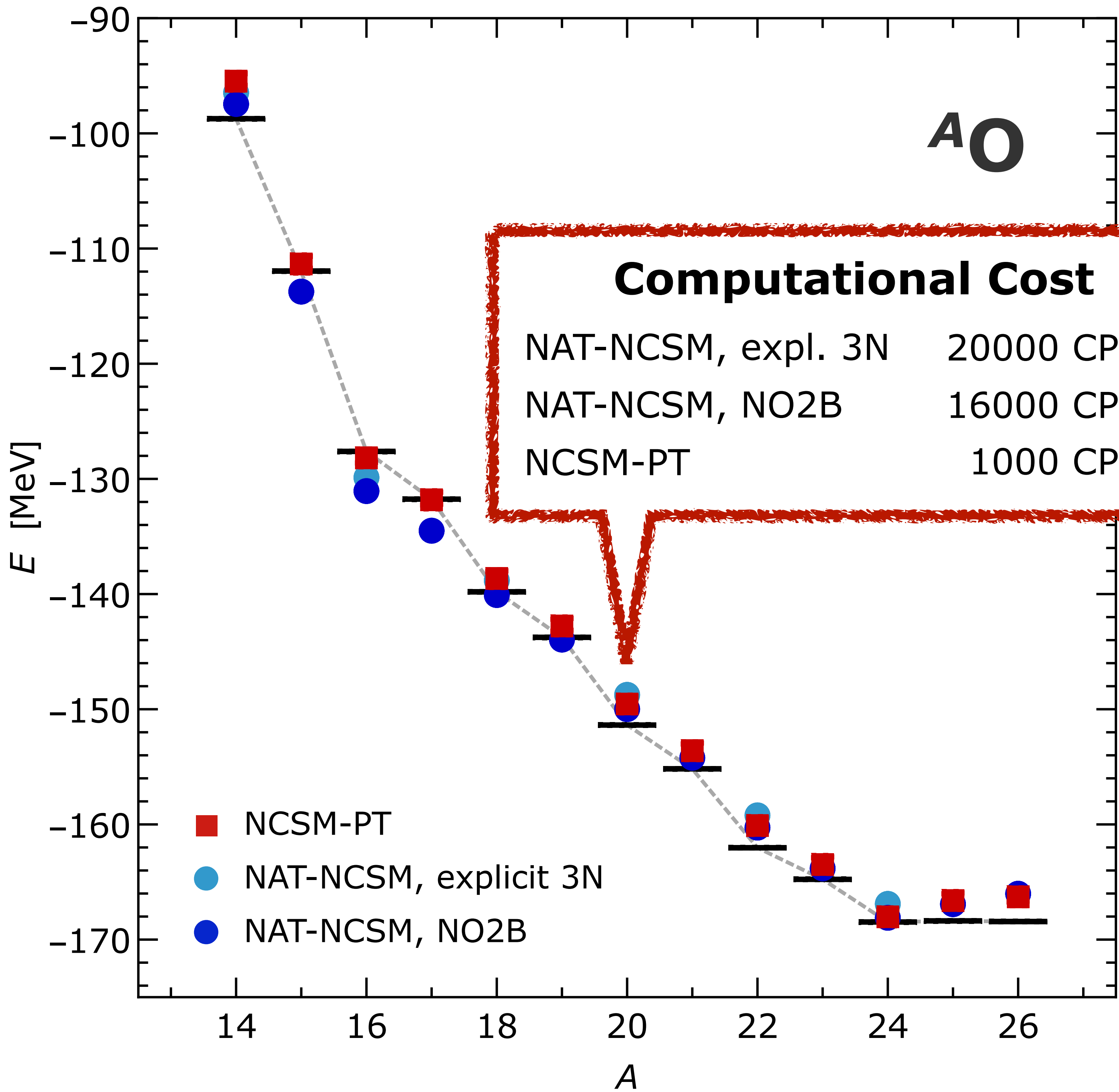
- eigenstates from NCSM at small N_{max} as unperturbed states
- access to all open-shell nuclei and systematically improvable

MBPT
convergence booster

- multi-configurational MBPT at second order for individual unperturbed states
- capture couplings in huge model-space through perturbative corrections

Oxygen Isotopes

Tichai, Gebrerufael, Vobig, Roth; PLB 786, 448 (2018)



Computational Cost

NAT-NCSM, expl. 3N	20000 CPU-h
NAT-NCSM, NO2B	16000 CPU-h
NCSM-PT	1000 CPU-h

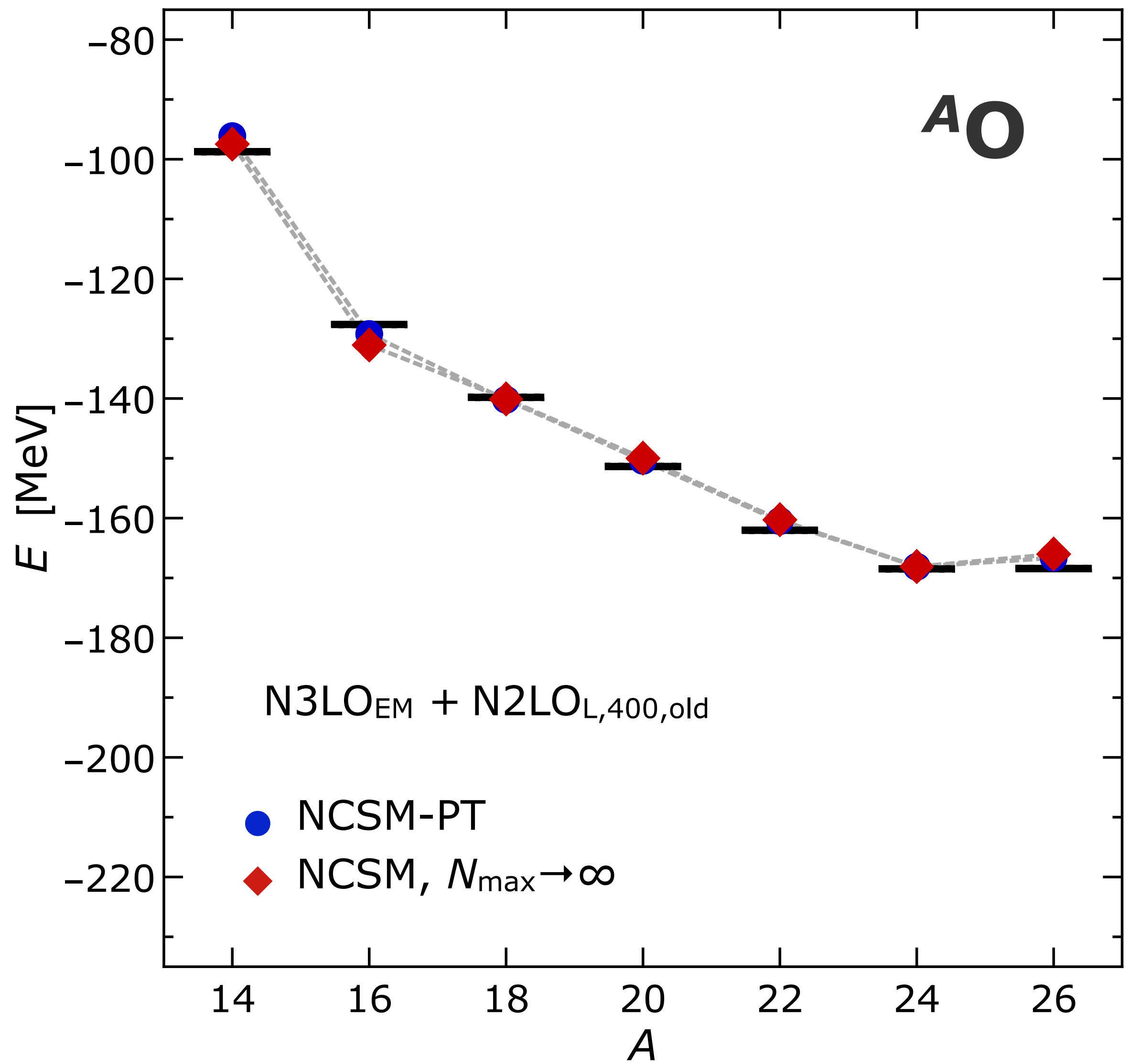
- excellent agreement with direct NCSM
- all isotopes are accessible due simple m-scheme implementation

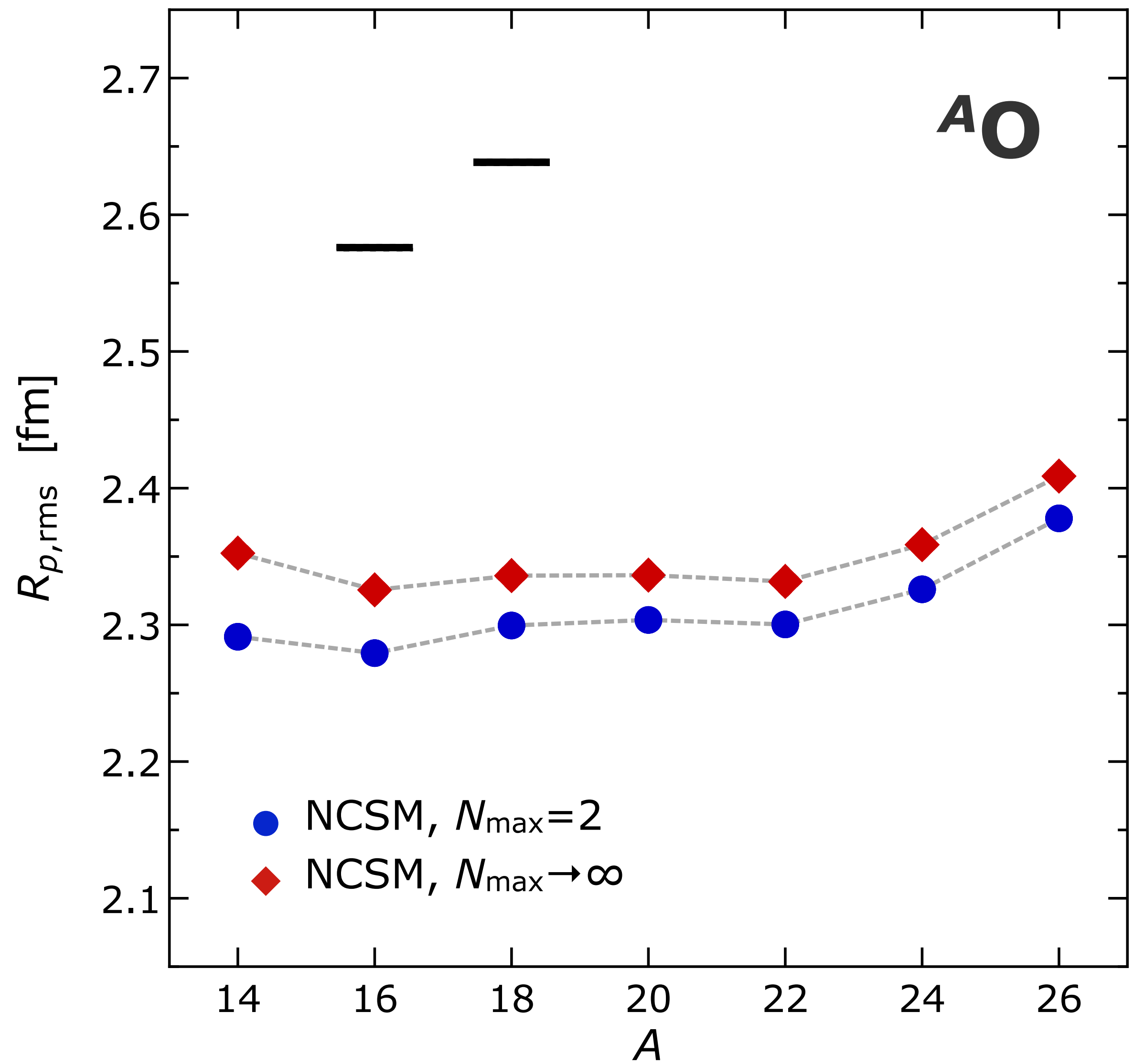
chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

HF basis
N_{max}=2 reference

Practitioner's View on Chiral Interactions

Baseline: N3LO$_{\mathrm{EM}}$ + N2LO$_{\mathrm{L,400,old}}$





NCSM-PT calculation for energy with N_{max}=2, e_{max}=12 and natural orbital basis

NCSM estimate for point-proton radius with N_{max}=2 and natural orbital basis

Chiral Interactions

Entem, Machleidt, PRC 68, 041001(R) (2003)

- **Entem-Machleidt (N3LO$_{EM}$)**
  - combine with different 3N interactions at N2LO
  - c_D from updated fit to triton half-life, c_E from t…

…96, 024004 (2017)

- **Entem-Machleidt-Nosyk (N*…**
  - use N2LO, N3LO, and …
  - combine with … N2LO, N3LO
  - c_D ran… radius

…RL 115, 122301 (2015); Reinhard, Epelbaum, Krebs, EPJA 54, 86 (2018)

- **Semi-Loc… …entum-Space (N*LO$_{SCS}$, N*LO$_{SMS}$)**
  - use N2LO … (N4LO$^+$) for R=1.0 fm or Λ=500 MeV
  - combine w… N2LO$_{SCS}$ and N2LO$_{SMS}$ 3N interaction
  - c_D determined from three-body scattering observables

- **for all interactions we use a free-space SRG evolution to α=0.08 fm^4 at the three-body level**
- induced many-body term are small on the energy scales relevant for the following discussion
- observables are evolved consistently

Chiral Interactions

Entem, Machleidt, PRC 68, 041001(R) (2003)

- **Entem-Machleidt ($N3LO_{EM}$)**
  - combine with different 3N interactions at N2LO
  - c_D from updated fit to triton half-life, c_E from triton energy

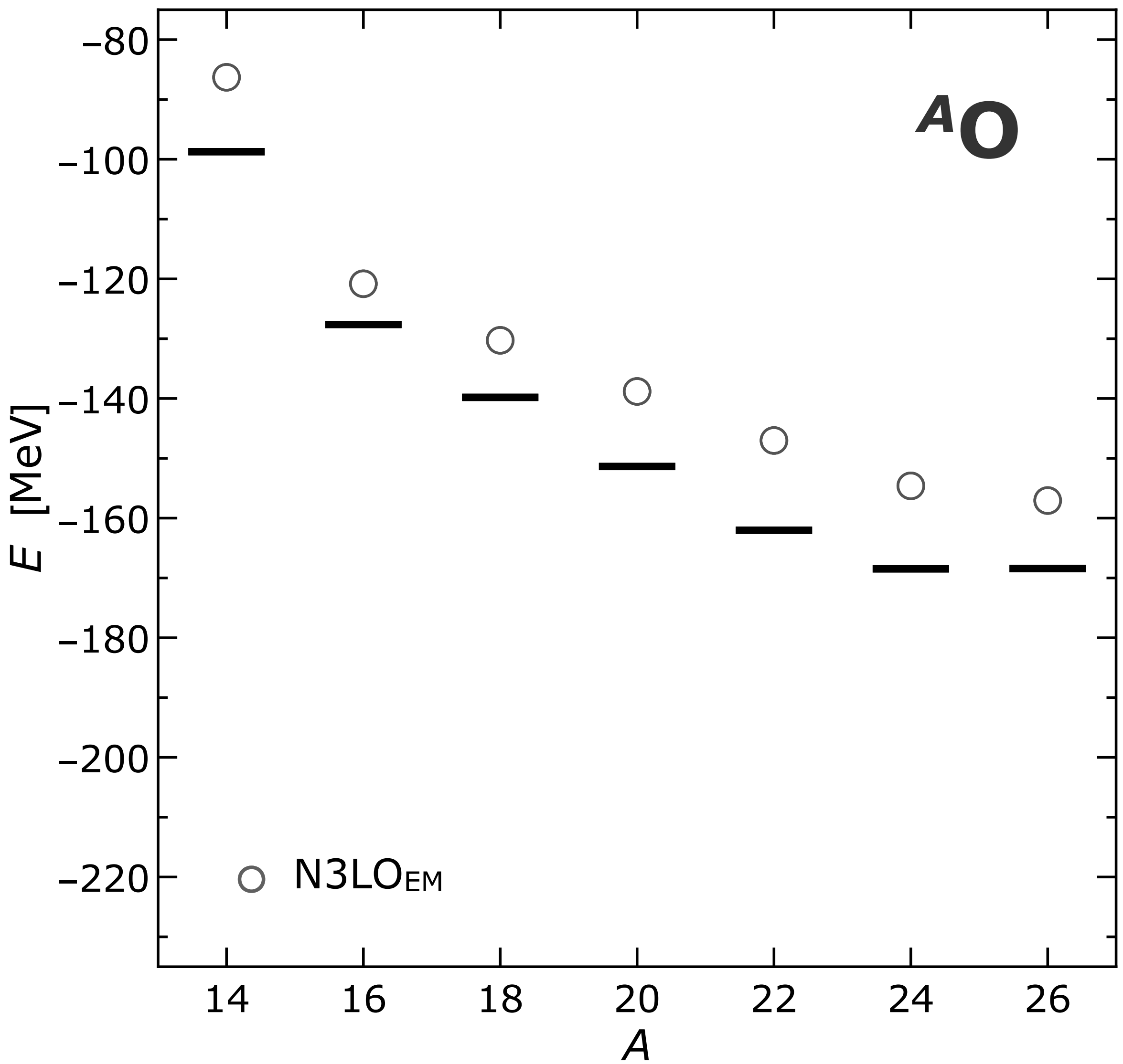
Entem, Machleidt, Nosyk, PRC 96, 024004 (2017)

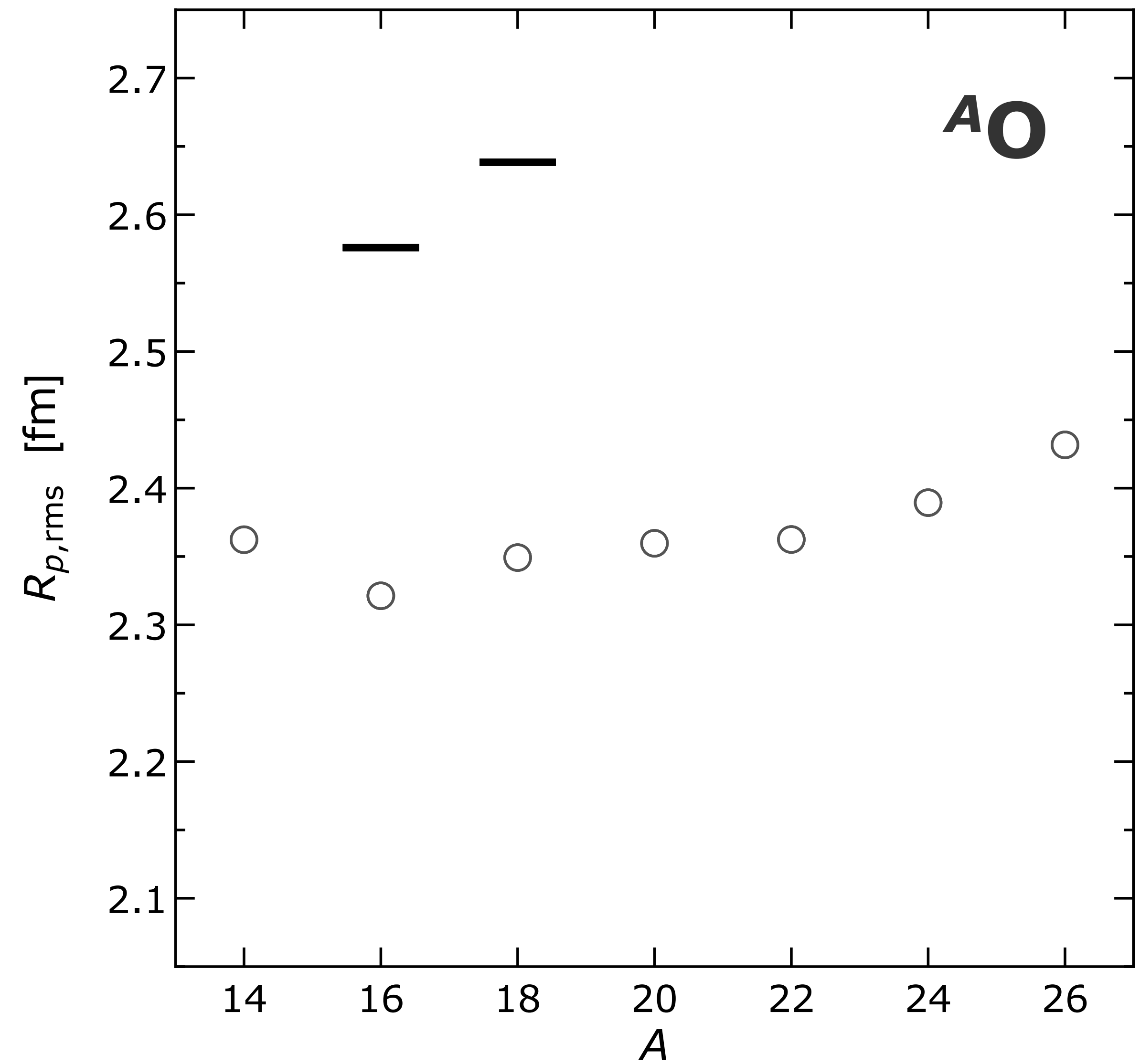
- **Entem-Machleidt-Nosyk ($N{*}LO_{EMN}$)**
  - use N2LO, N3LO, and N4LO for Λ=500 MeV
  - combine with 'consistent' non-local 3N interaction at N2LO, N3LO
  - c_D range extracted from ^{4}He binding energy and radius

Epelbaum, Krebs, Meißner, PRL 115, 122301 (2015); Reinhard, Epelbaum, Krebs, EPJA 54, 86 (2018)

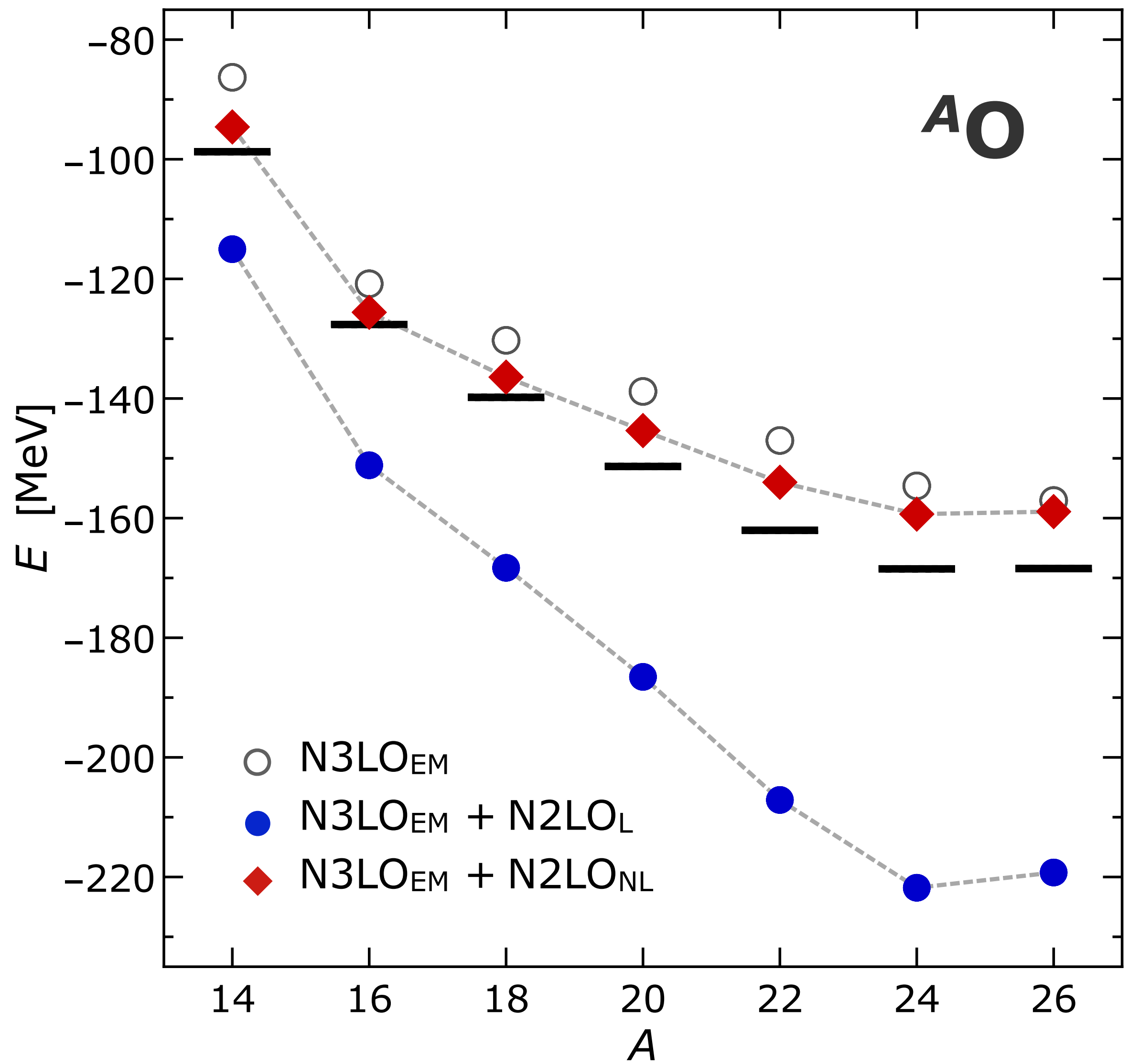
- **Semi-Local Coordinate/Momentum-Space ($N{*}LO_{SCS}$, $N{*}LO_{SMS}$)**
  - use N2LO, N3LO, N4LO ($N4LO^+$) for R=1.0 fm or Λ=500 MeV
  - combine with $N2LO_{SCS}$ and $N2LO_{SMS}$ 3N interaction
  - c_D determined from three-body scattering observables

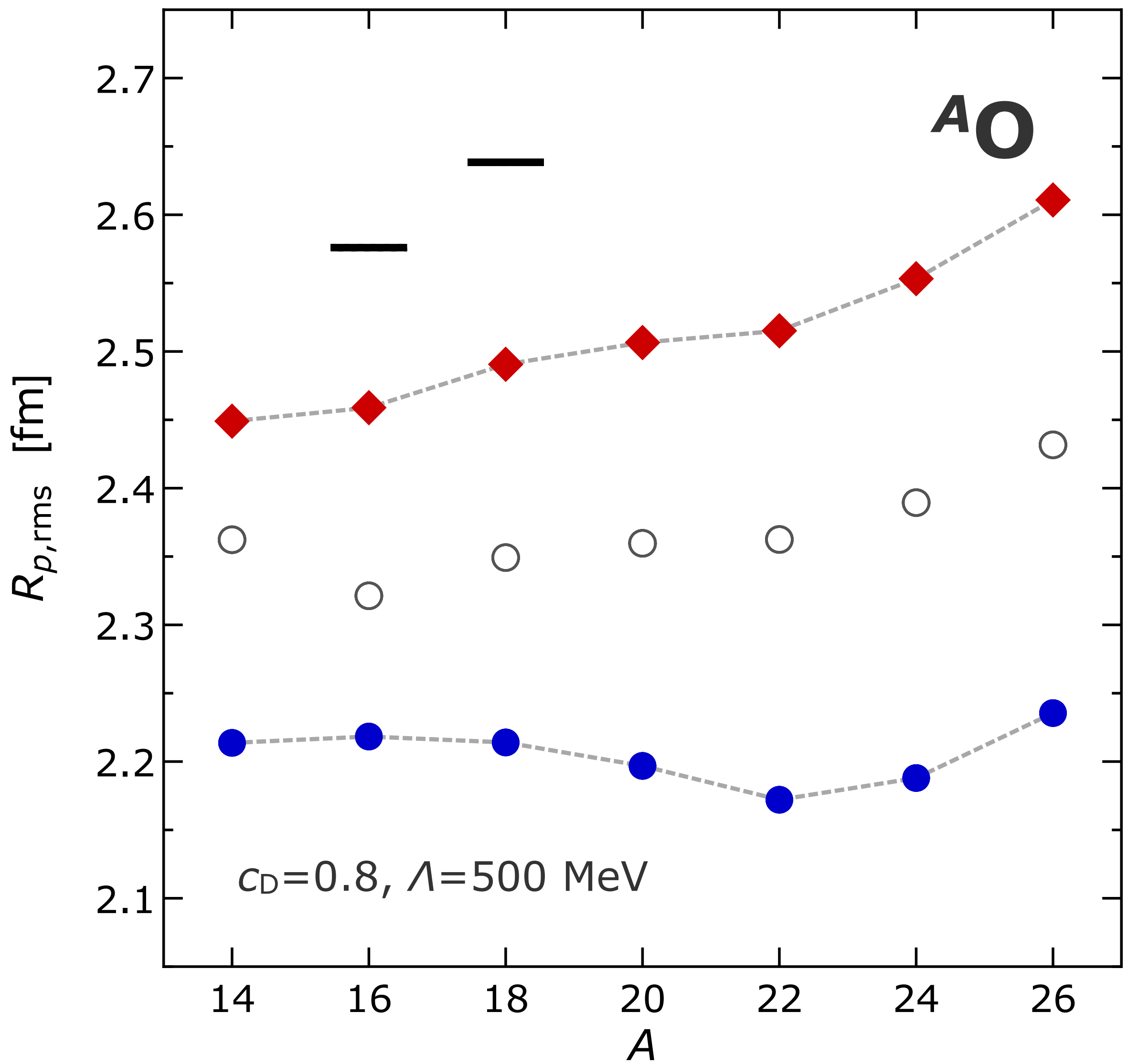
Local vs. Non-Local 3N Regulator





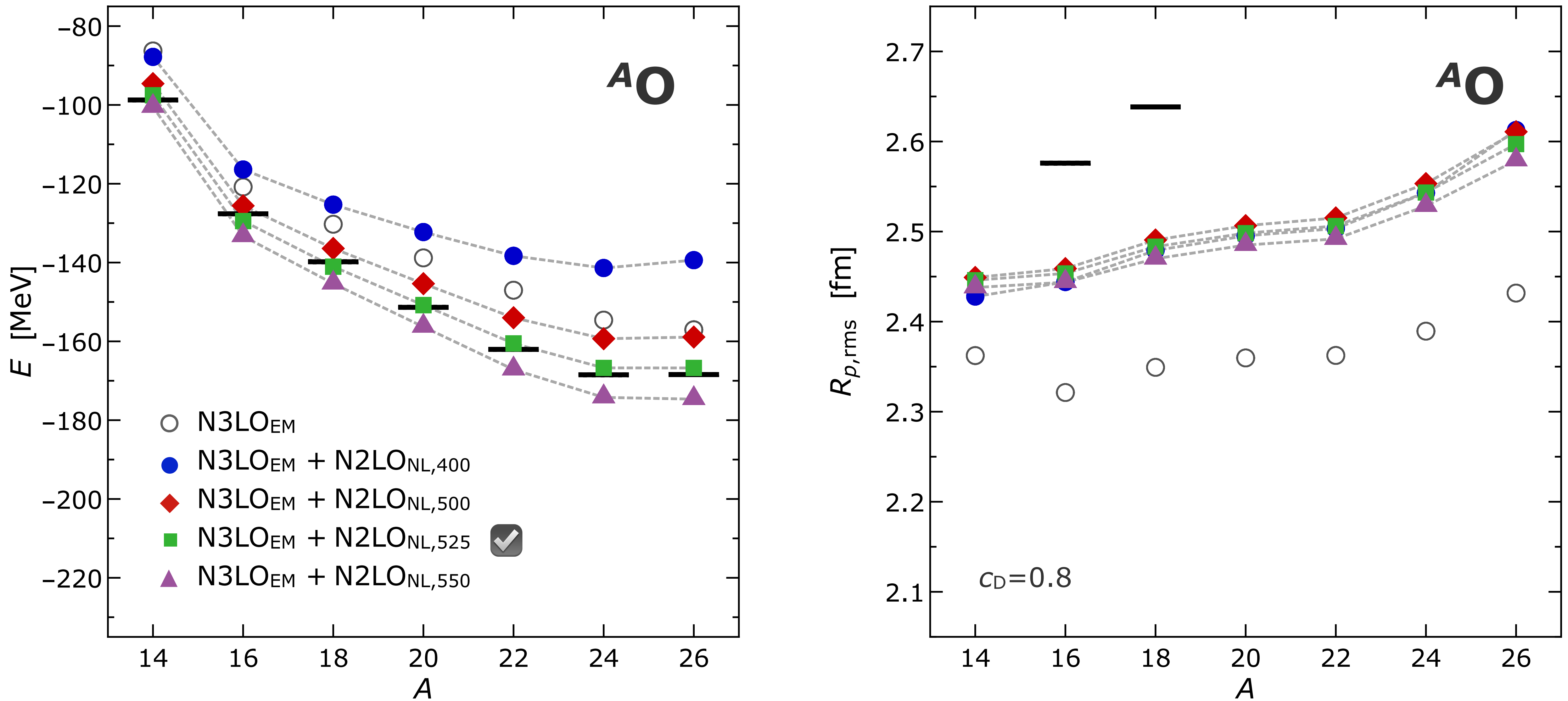
Local vs. Non-Local 3N Regulator





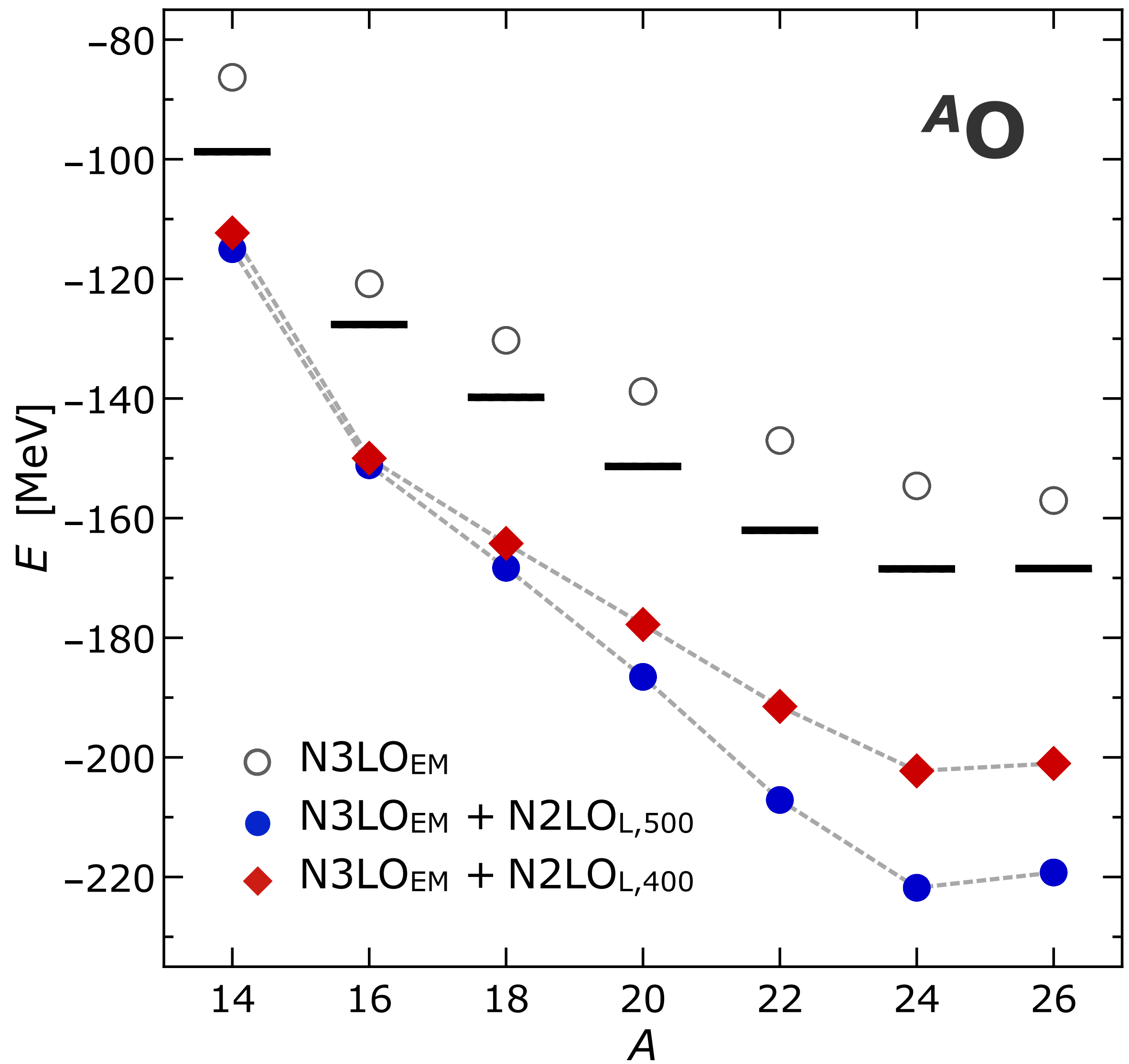
effect of 3N interactions with local and non-local regulators is completely different

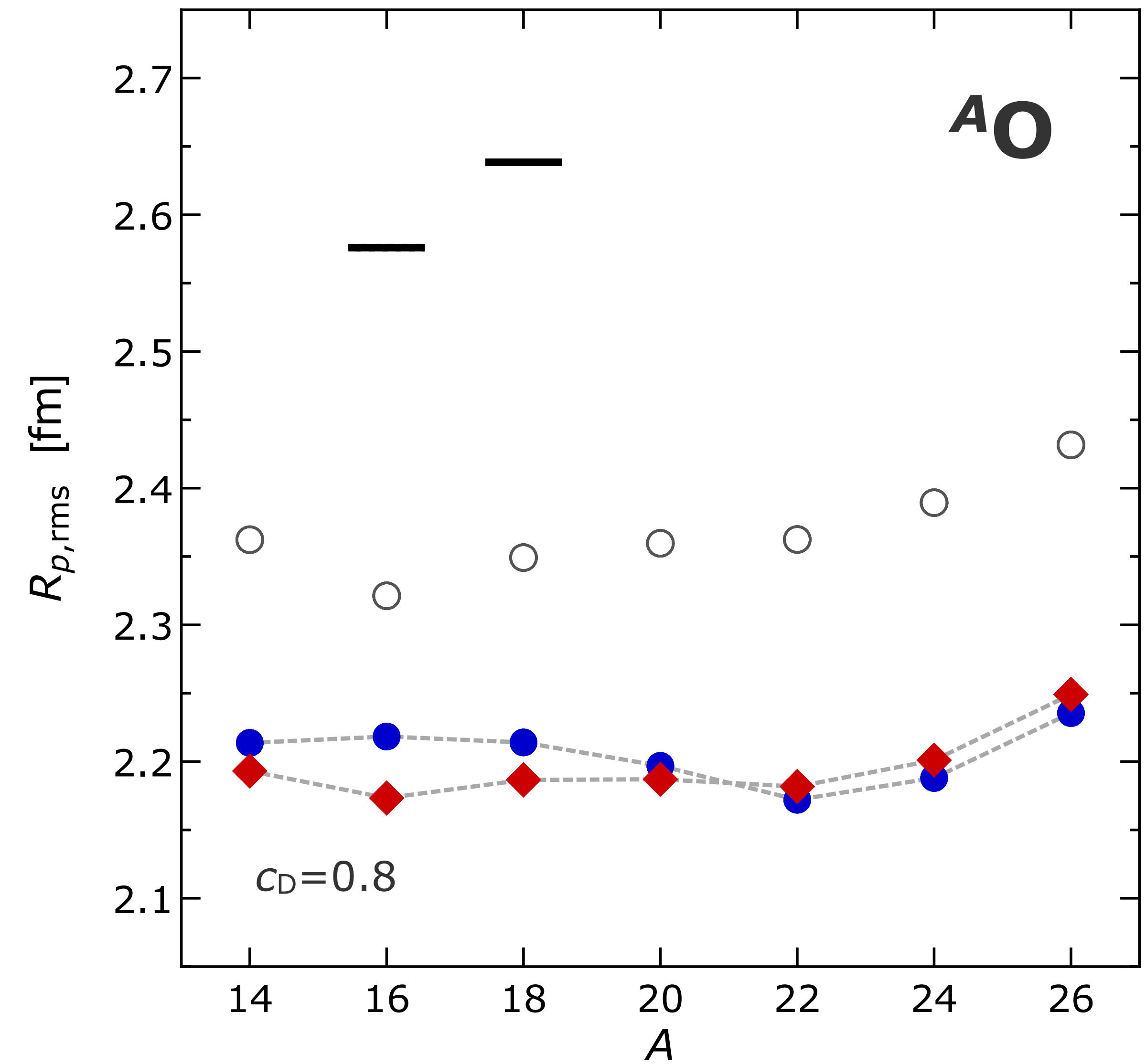
3N Cutoff Variation (Non-Local)



increase of the 3N cutoff provides systematically more binding without affecting radii

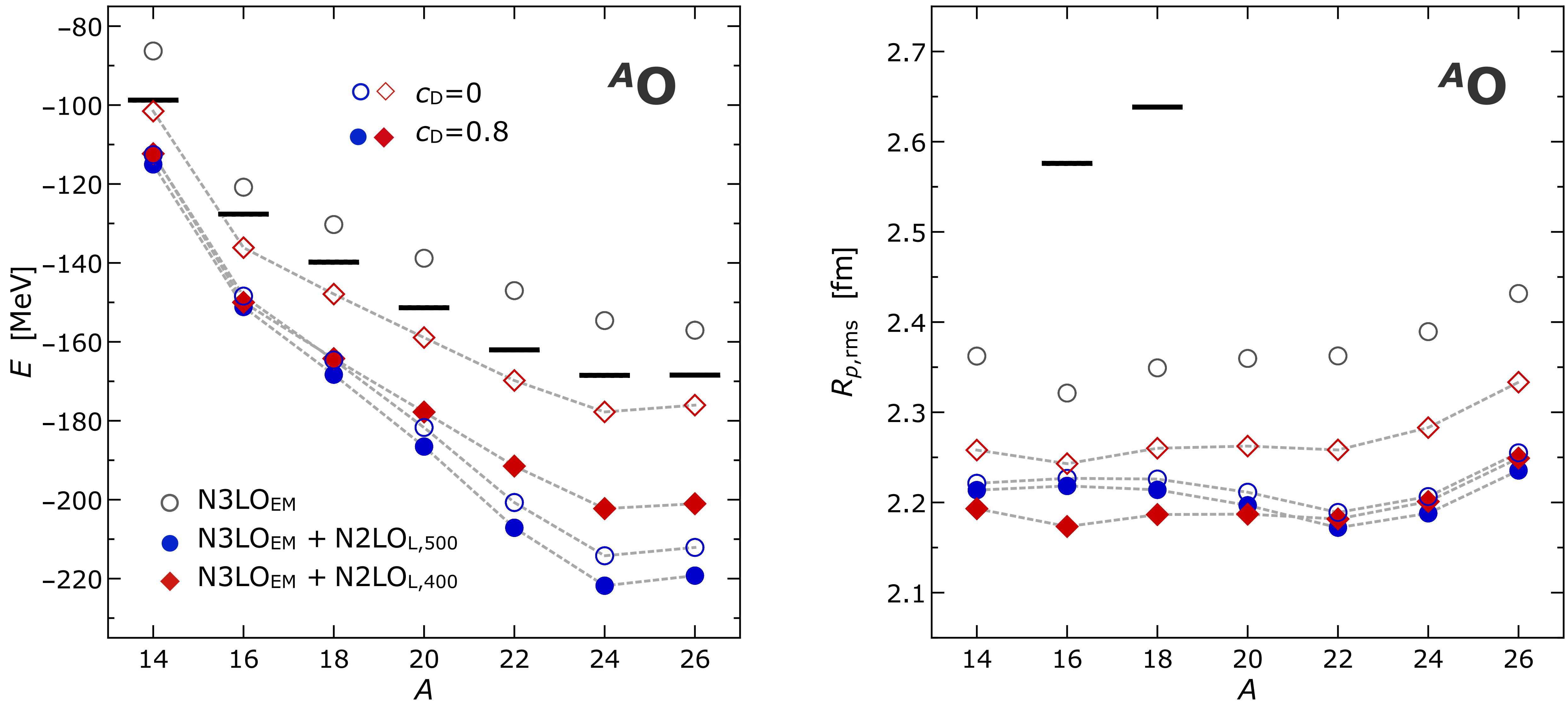
3N Cutoff Variation (Local)





decrease of the 3N cutoff reduces overbinding, but not enough to match experiment

c_D Variation (Local)



changing c_D from 0.8 to 0 reduces overbinding, particularly for Λ=400 MeV

A First Summary

- **Observations**
  - **local 3N regulators** produce overbinding and much too small radii
  - **non-local 3N regulators** produce underbinding and much better radii
  - underbinding can be fixed by slight increase of 3N cutoff
- **Chiral EFT Perspective**
  - non-local 3N regulators cut into long-range 2π physics
  - better use local regulators, at least for long-range terms (semi-local)
- **Practitioner’s Interpretation**
  - long-range 3N contributions at N2LO give too much attraction
  - larger radii require a delicate cancelation of 3N terms

Chiral Interactions

Entem, Machleidt, PRC 68, 041001(R) (2003)

- **Entem-Machleidt (N3LO$_{\text{EM}}$)**
  - combine with different 3N interactions at N2LO
  - c_D from updated fit to triton half-life, c_E from triton energy

Entem, Machleidt, Nosyk, PRC 96, 024004 (2017)

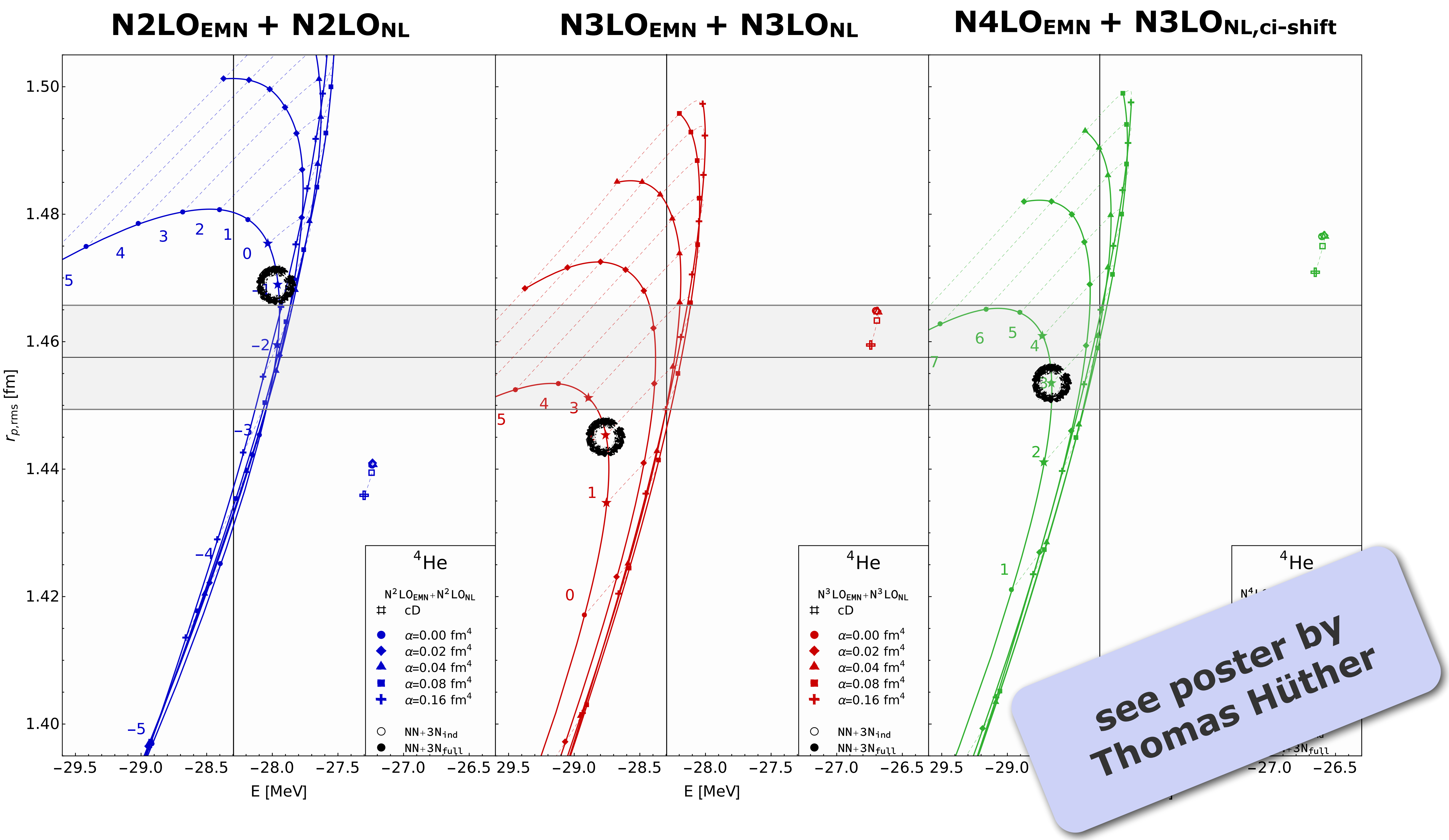
- **Entem-Machleidt-Nosyk (N*LO$_{\text{EMN}}$)**
  - use N2LO, N3LO, and N4LO for Λ=500 MeV
  - combine with 'consistent' non-local 3N interaction at N2LO, N3LO
  - c_D range extracted from ^{4}He binding energy and radius

Epelbaum, Krebs, Meißner, PRL 115, 122301 (2015); Reinhard, Epelbaum, Krebs, EPJA 54, 86 (2018)

- **Semi-Local Coordinate/Momentum-Space (N*LO$_{\text{SCS}}$, N*LO$_{\text{SMS}}$)**
  - use N2LO, N3LO, N4LO (N4LO$^+$) for R=1.0 fm or Λ=500 MeV
  - combine with N2LO$_{\text{SCS}}$ and N2LO$_{\text{SMS}}$ 3N interaction
  - c_D determined from three-body scattering observables

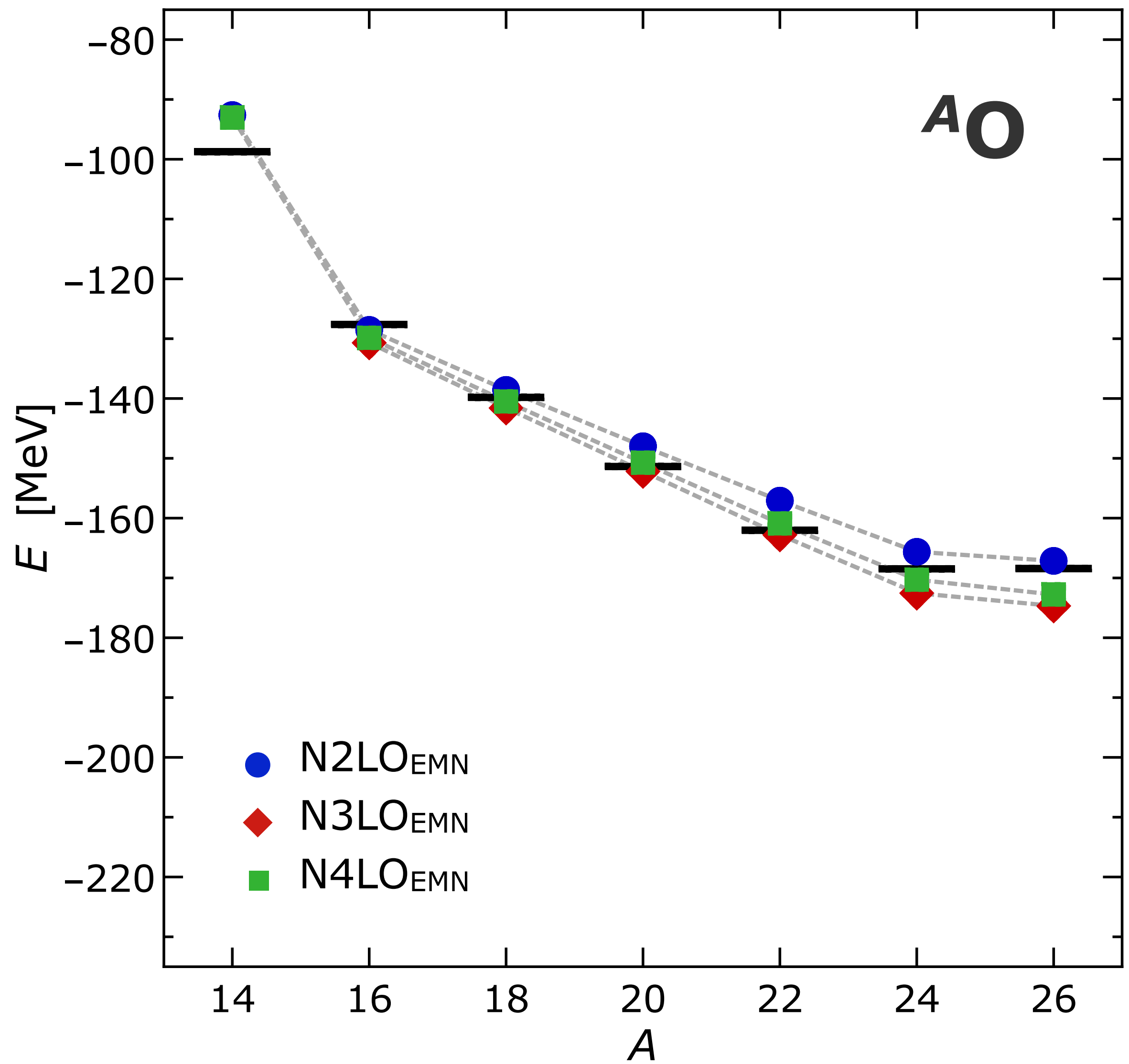
^{4}He Constraints on c_D

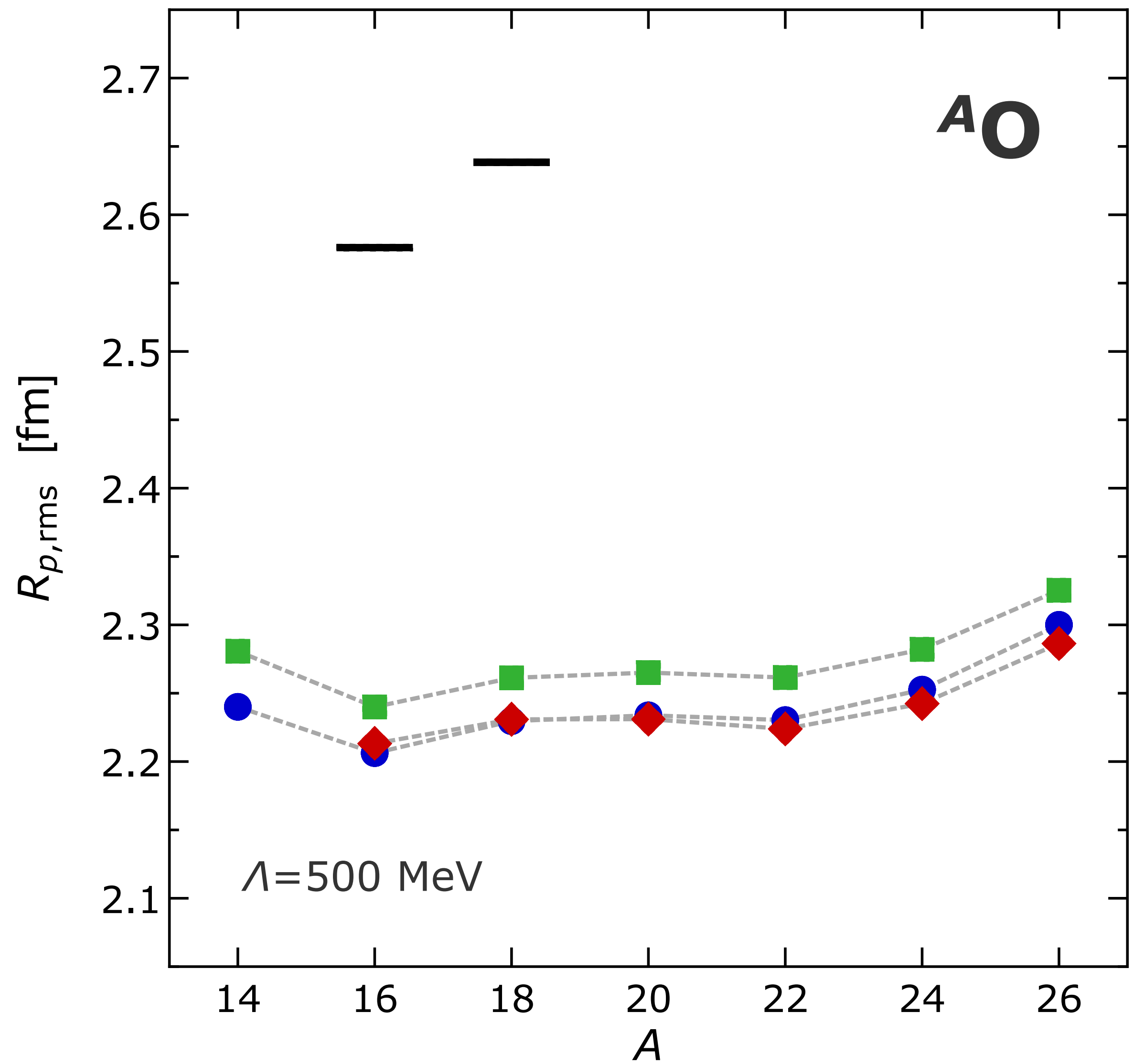
Hüther, Vobig, Roth, in prep.



c_E determined from triton energy fit for each c_D

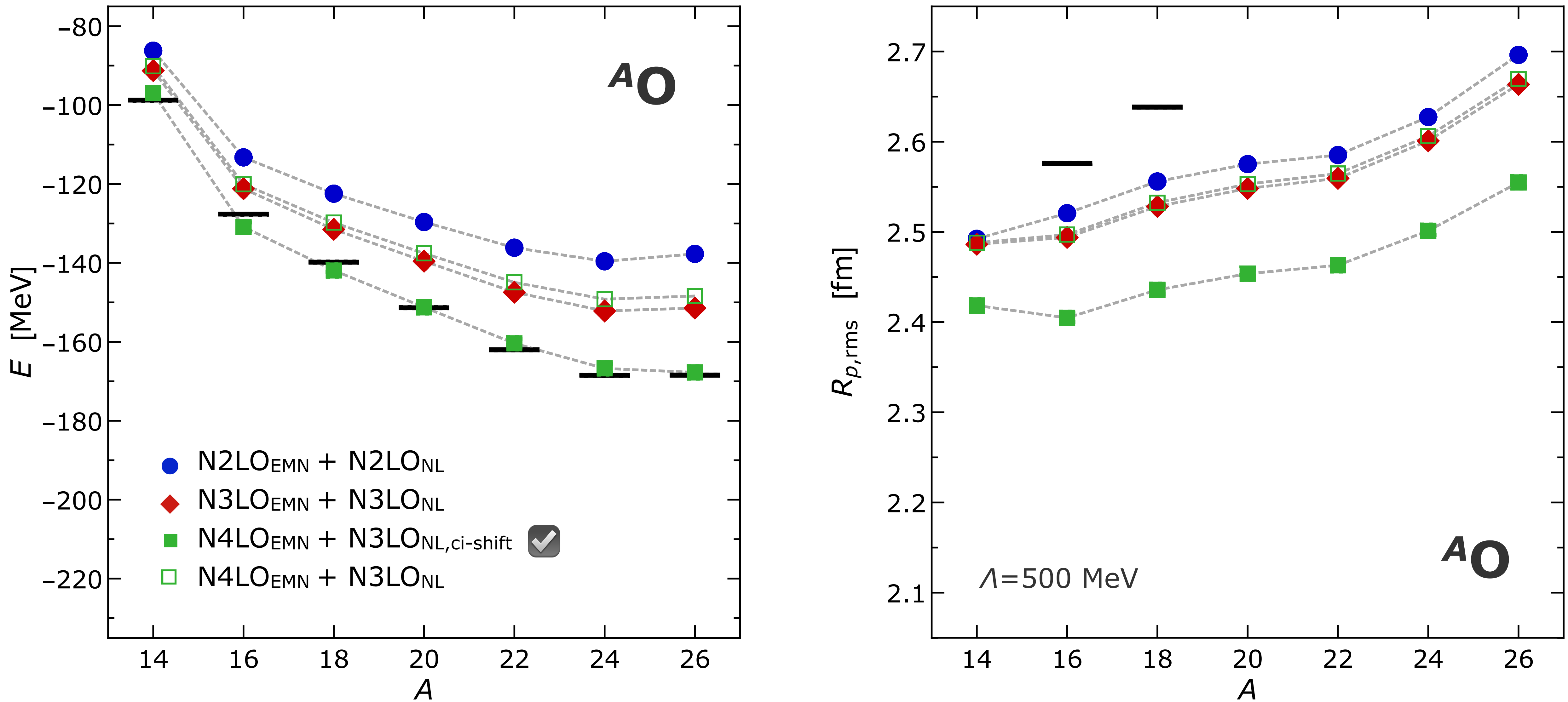
N*LO$_{EMN}$: Order-by-Order with NN





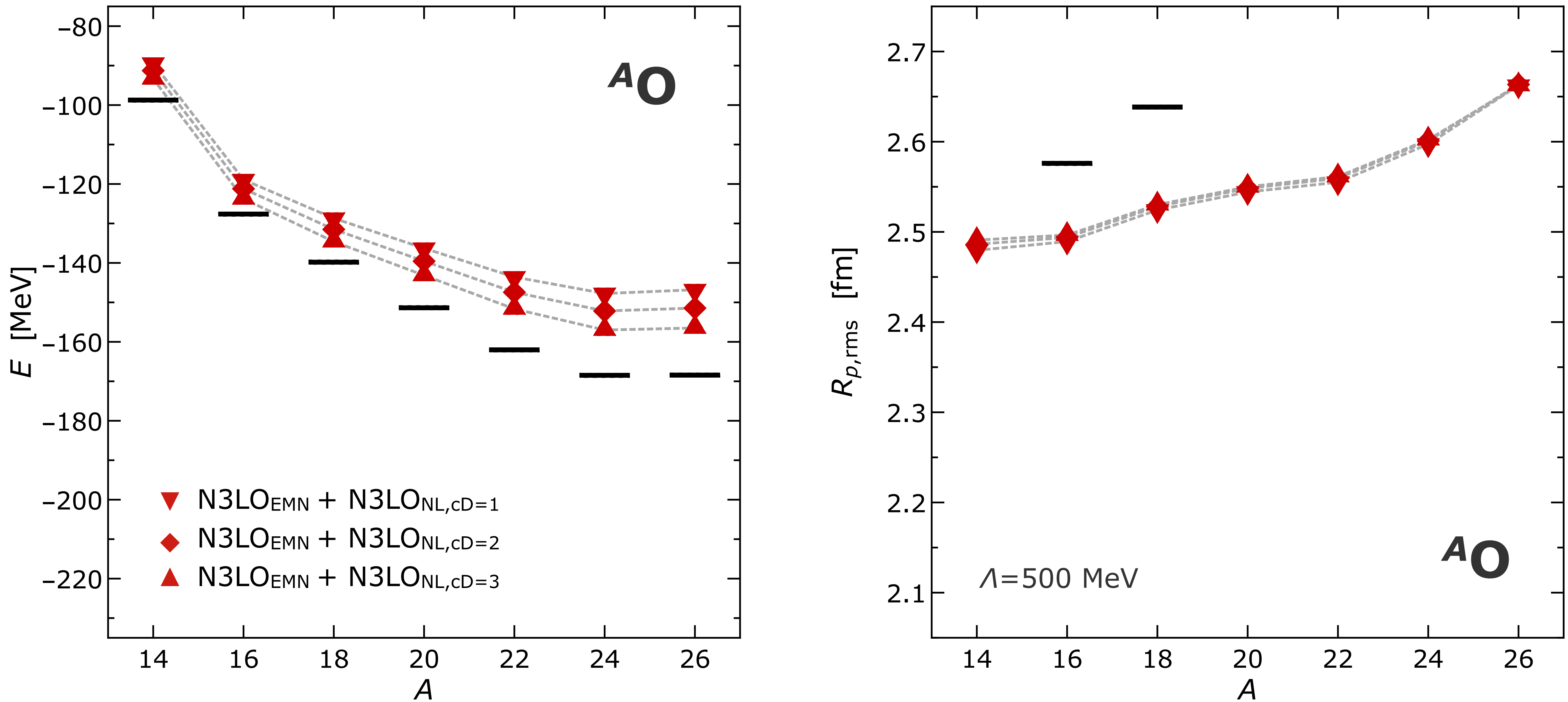
all NN interactions already reproduce ground-state energies, but severely underestimate radii

N*LO$_{EMN}$: Order-by-Order with NN+3N



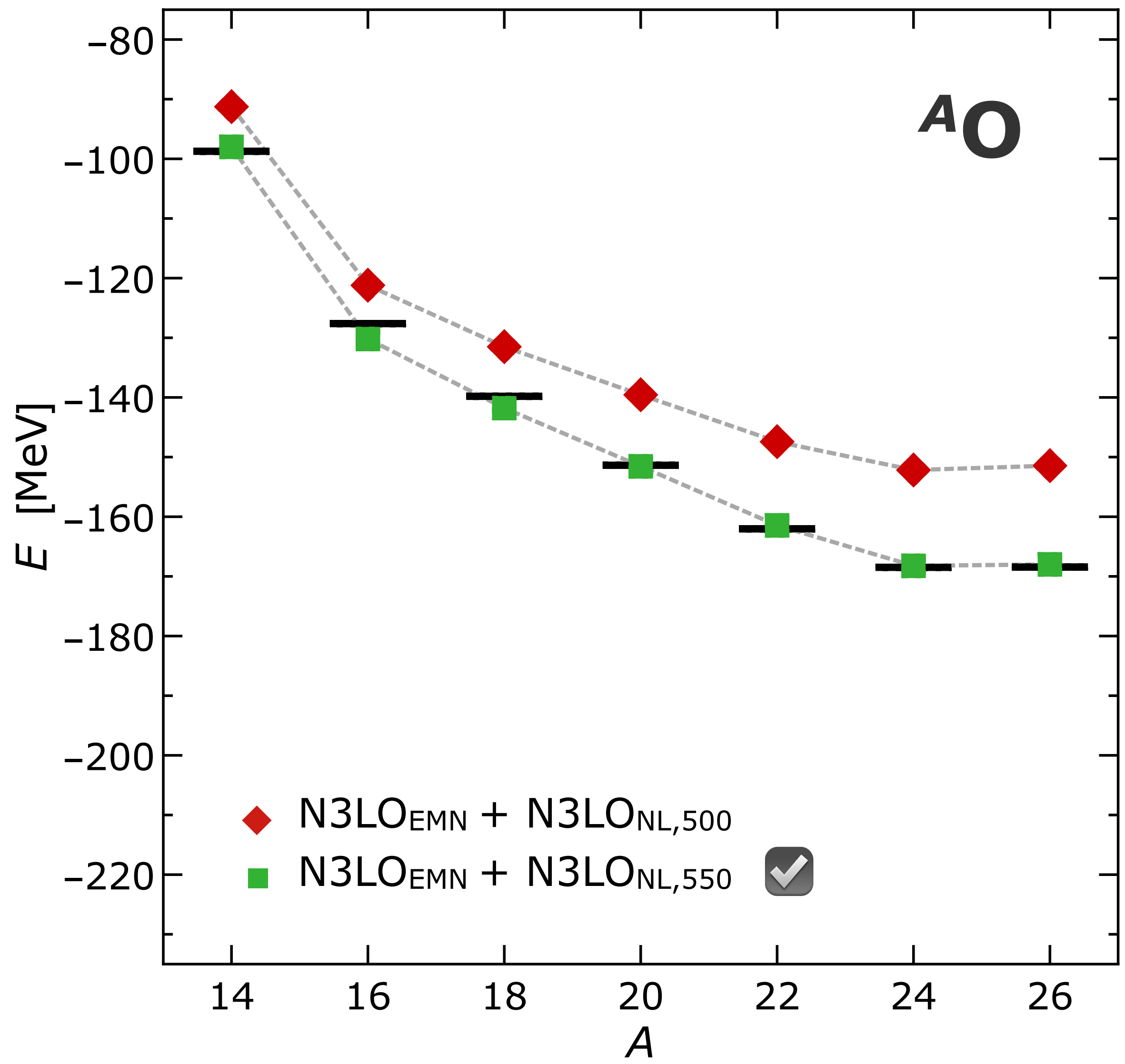
inclusion of the 3N interaction leads to underbinding and a significant increase of radii, except for highest order

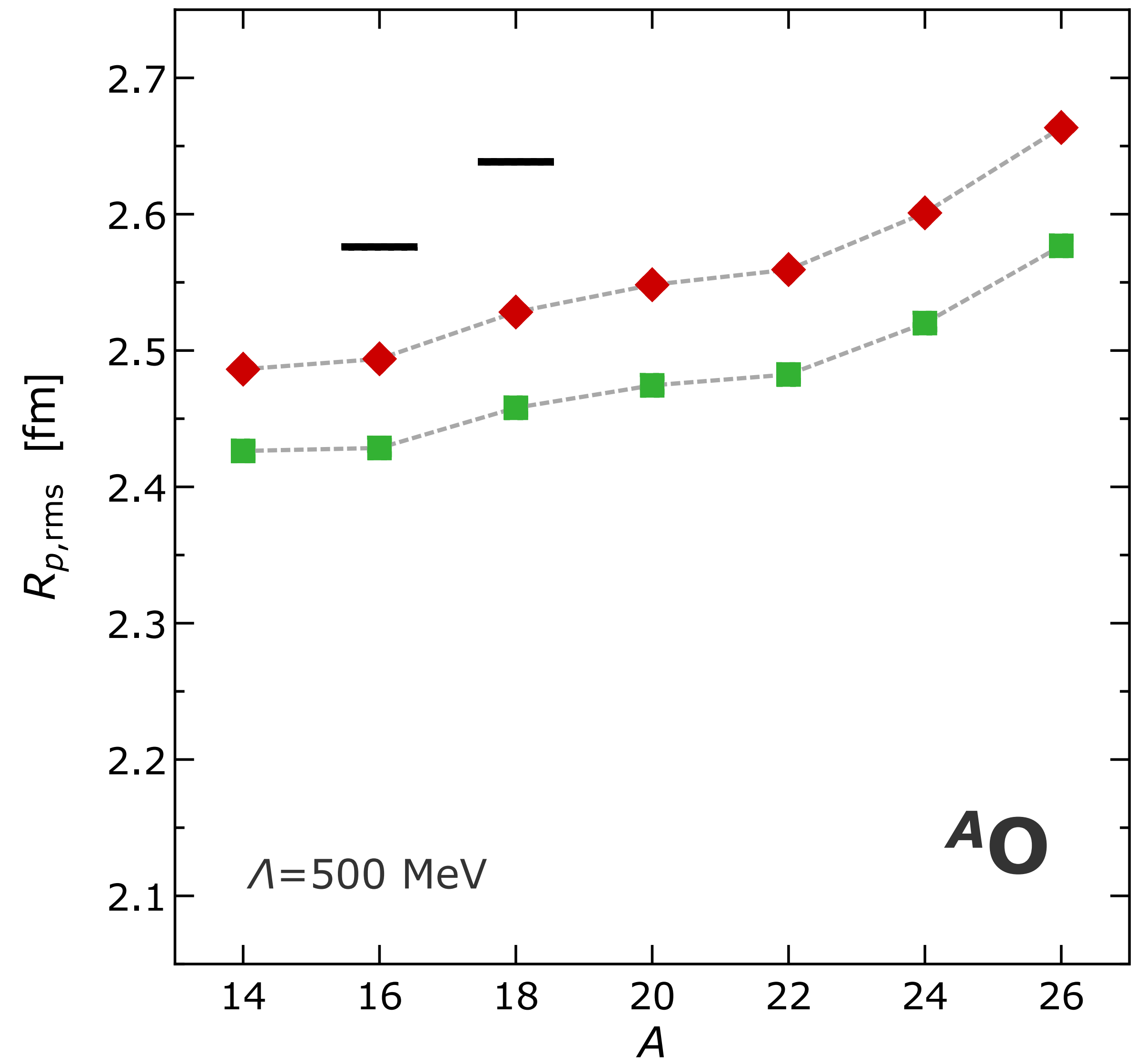
N3LO$_{\text{EMN}}$: Sensitivity to c_D



variation of c_D by ±1 has a moderate effect on binding energies and no effect on radii

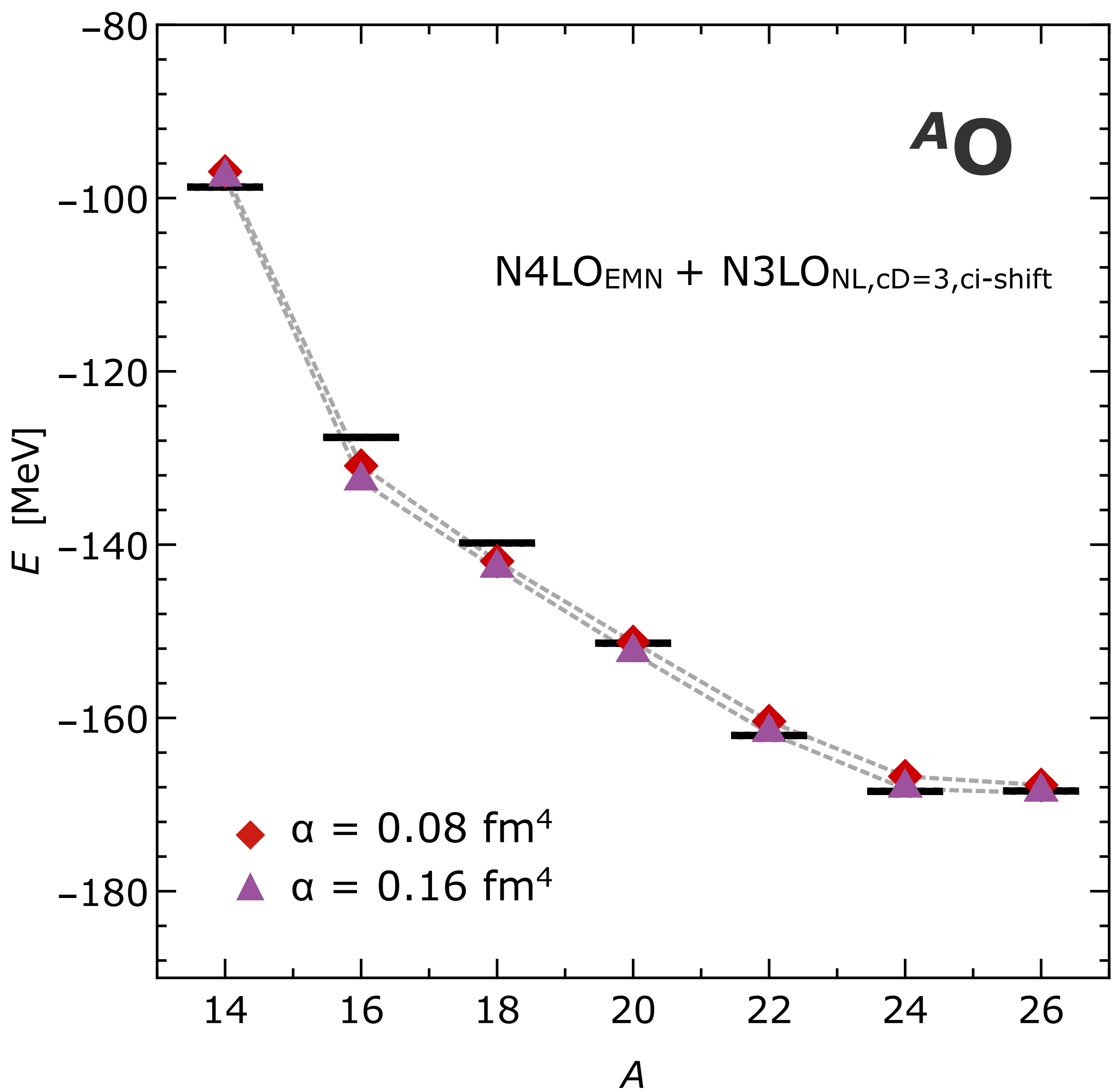
N3LO$_{\mathrm{EMN}}$: 3N Cutoff Variation

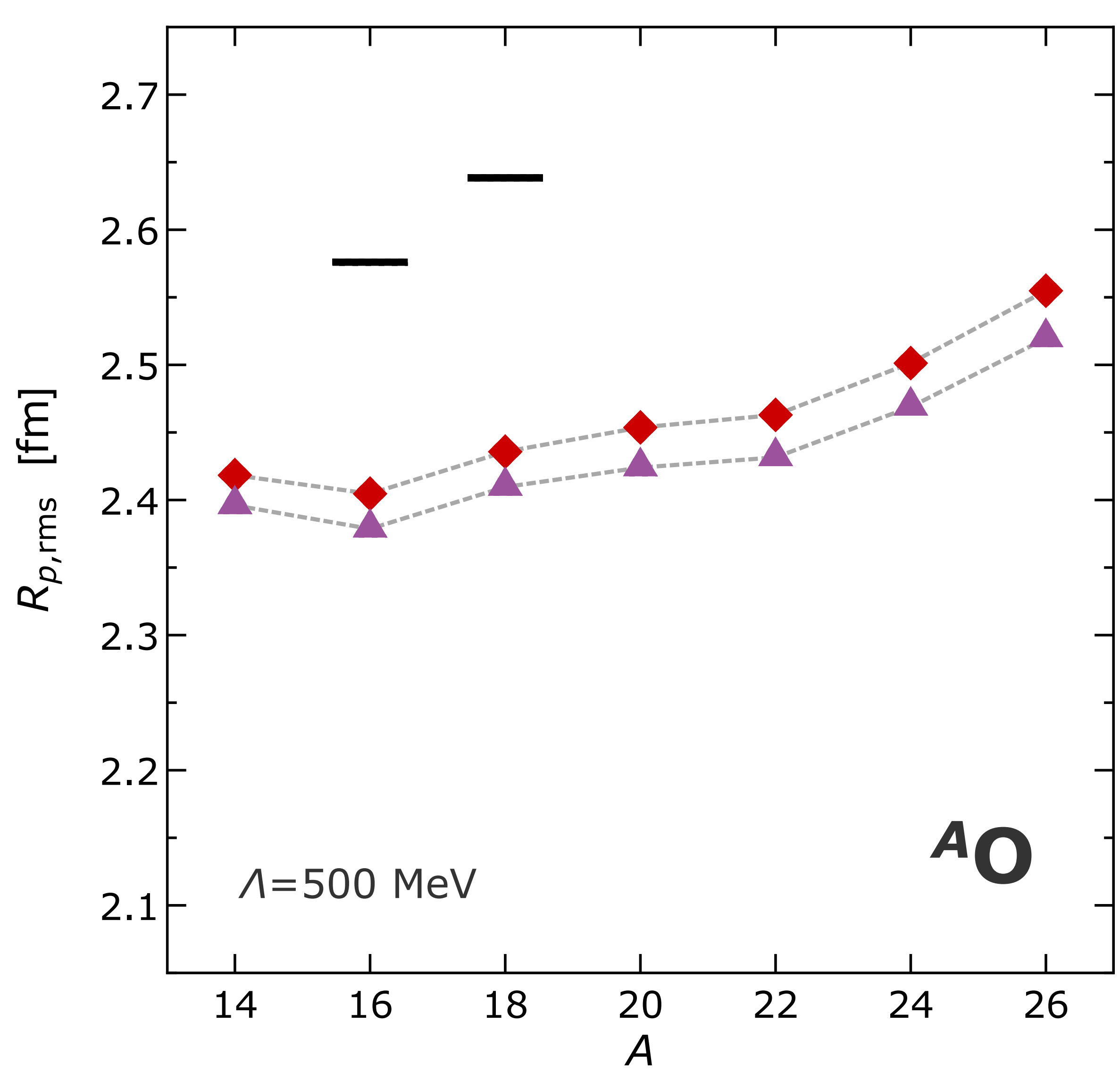




again, increase of 3N cutoff gives more binding
but also smaller radii

N4LO$_{EMN}$: SRG Flow Parameter





variation of flow parameter α has little effect on energies, effect on radius estimate larger

Chiral Interactions

Entem, Machleidt, PRC 68, 041001(R) (2003)

- **Entem-Machleidt (N3LO$_{EM}$)**
  - combine with different 3N interactions at N2LO
  - c_D from updated fit to triton half-life, c_E from triton energy

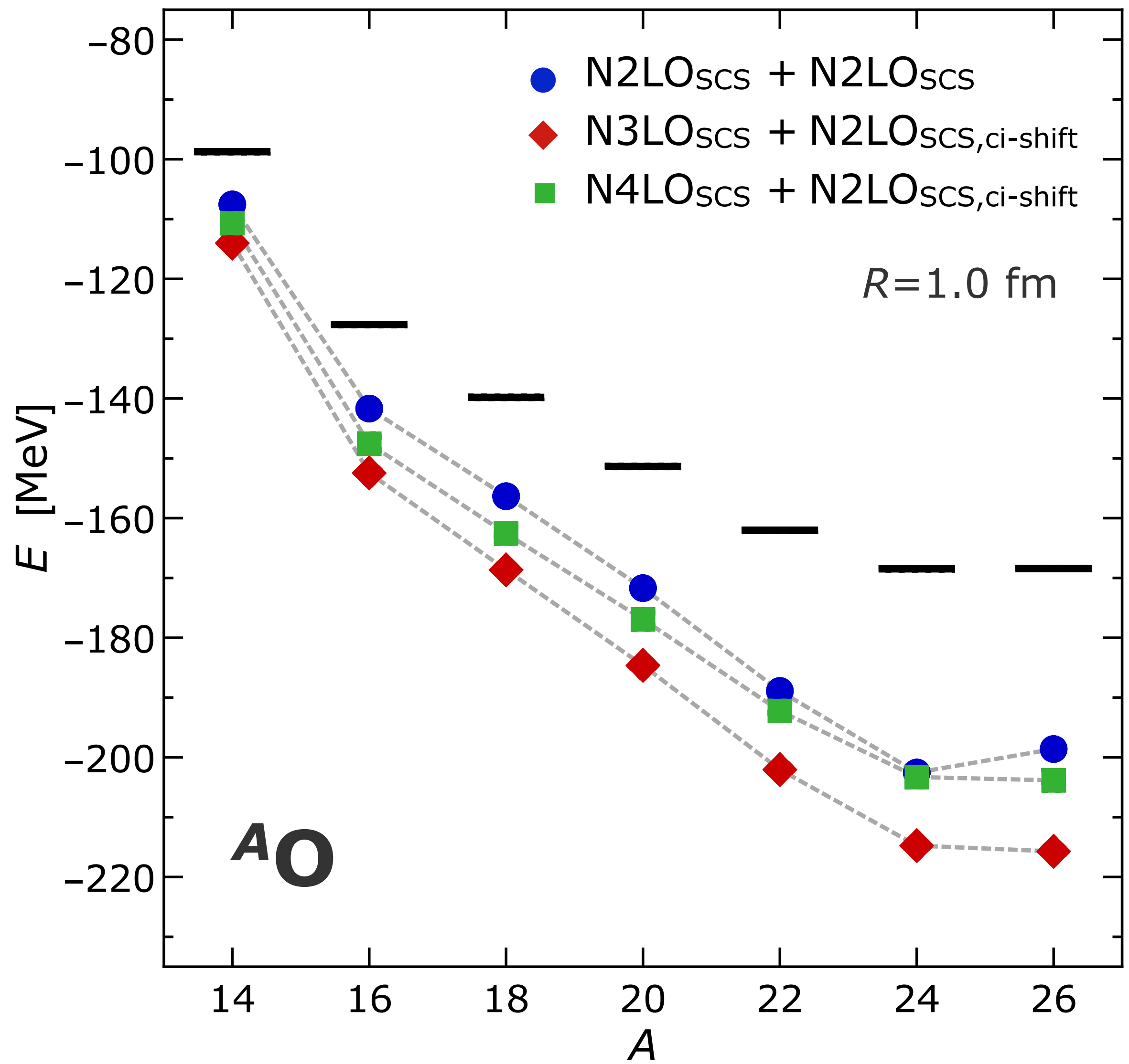
Entem, Machleidt, Nosyk, PRC 96, 024004 (2017)

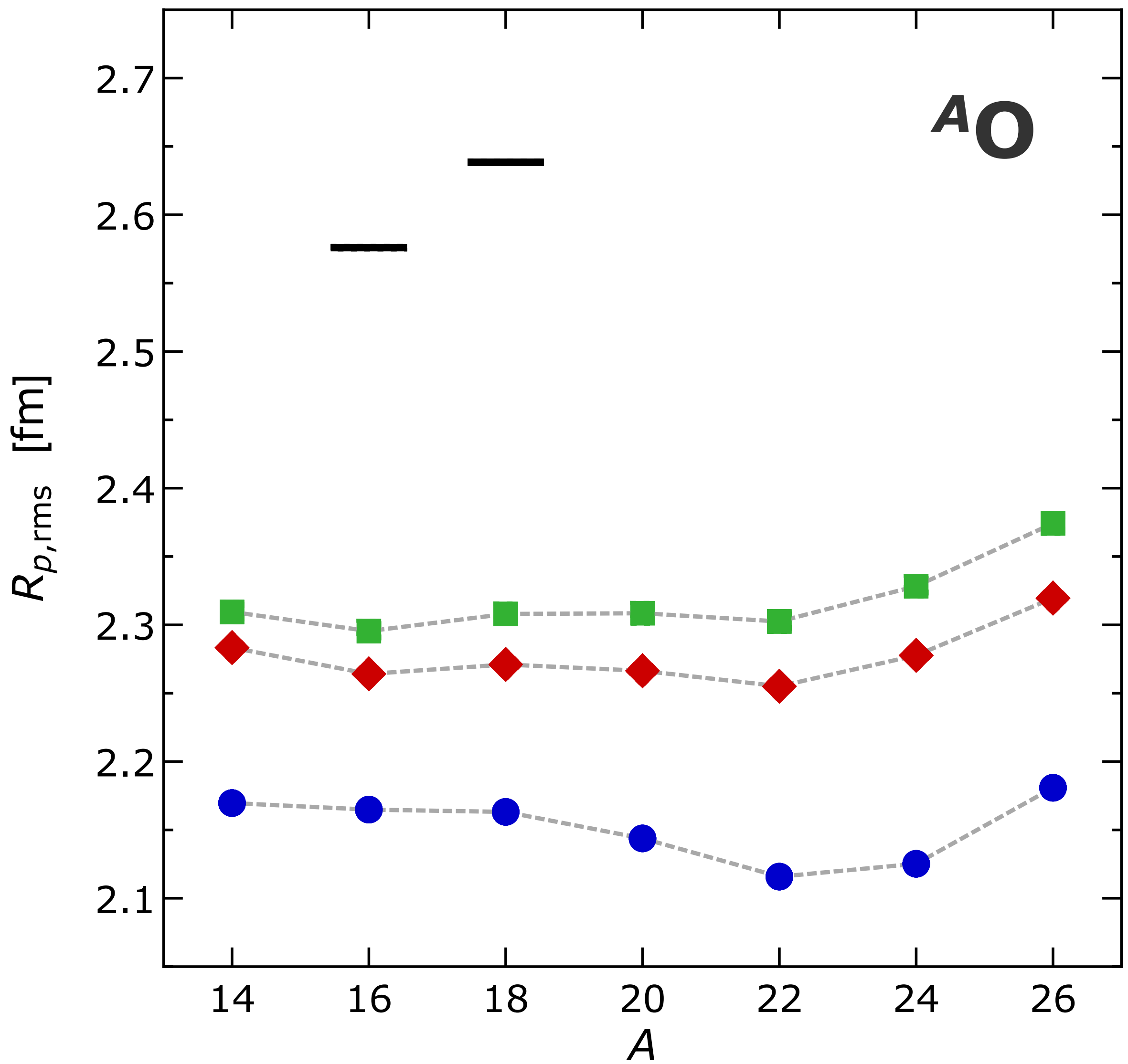
- **Entem-Machleidt-Nosyk (N*LO$_{EMN}$)**
  - use N2LO, N3LO, and N4LO for Λ=500 MeV
  - combine with ‘consistent’ non-local 3N interaction at N2LO, N3LO
  - c_D range extracted from ^{4}He binding energy and radius

Epelbaum, Krebs, Meißner, PRL 115, 122301 (2015); Reinhard, Epelbaum, Krebs, EPJA 54, 86 (2018)

- **Semi-Local Coordinate/Momentum-Space (N*LO$_{SCS}$, N*LO$_{SMS}$)**
  - use N2LO, N3LO, N4LO (N4LO$^+$) for R=1.0 fm or Λ=500 MeV
  - combine with N2LO$_{SCS}$ and N2LO$_{SMS}$ 3N interaction
  - c_D determined from three-body scattering observables

N*LOscs: Order-by-Order

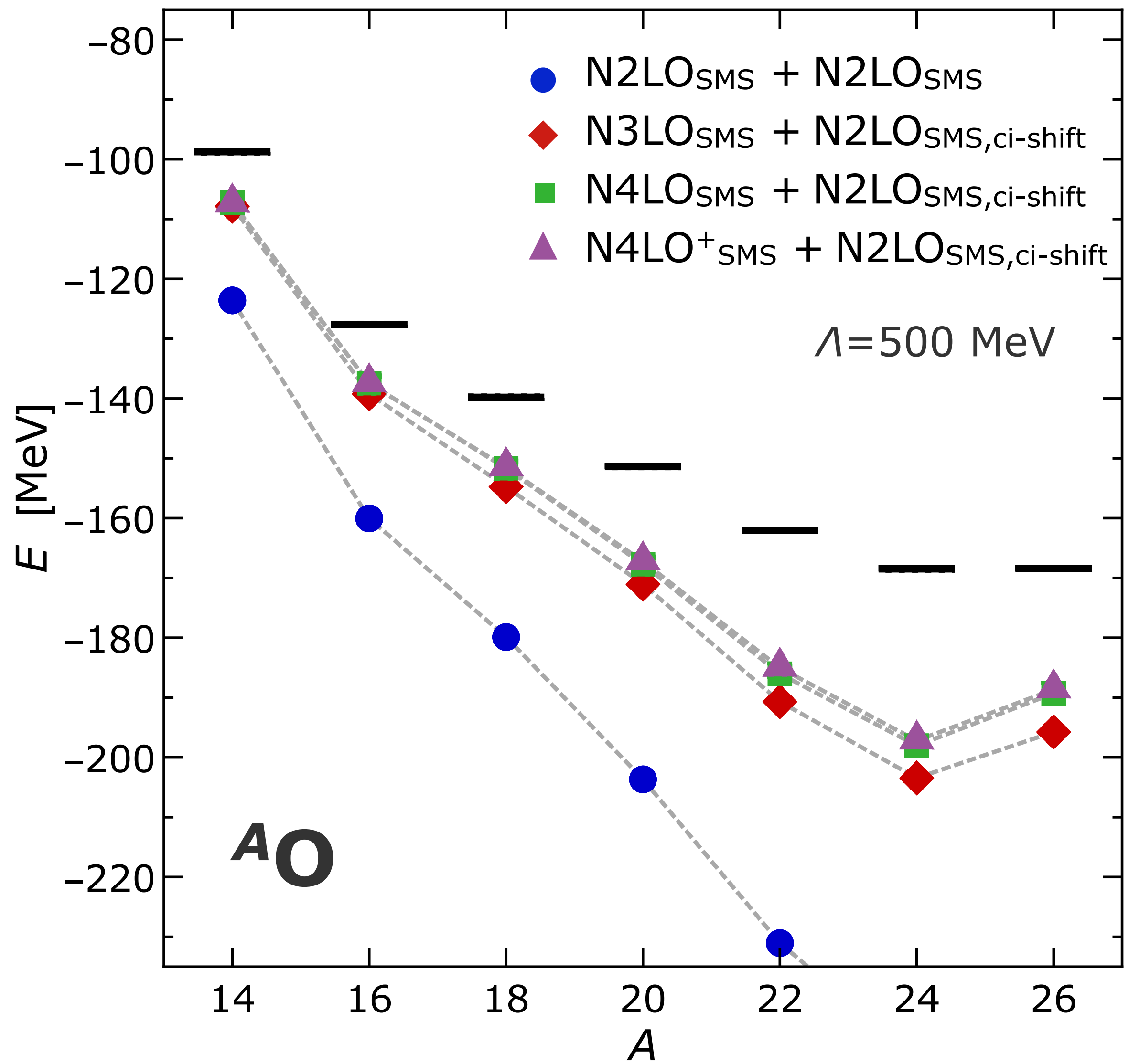


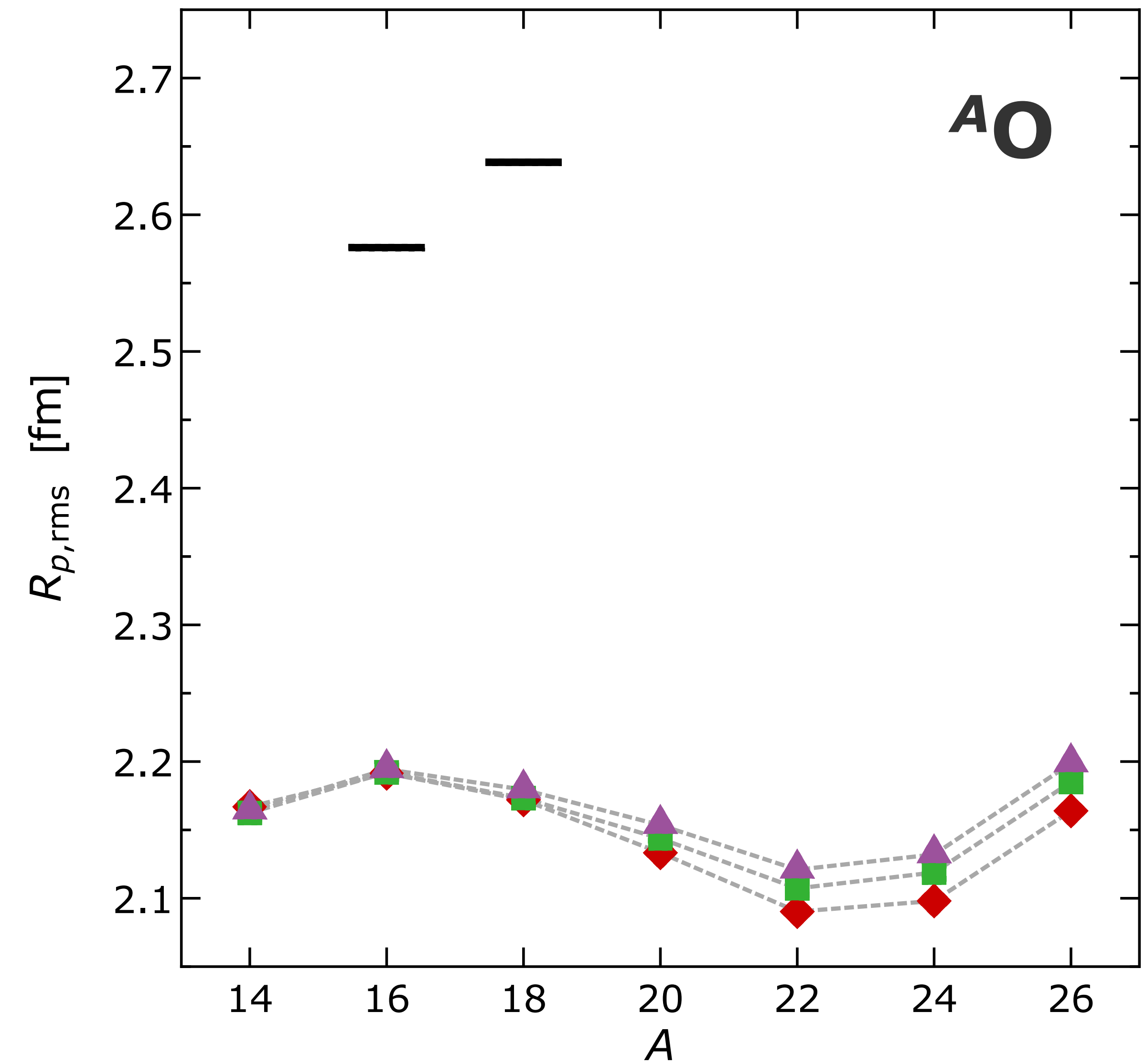


overbinding and too small radii at all orders, similar to the simple local interactions

cf. recent LENPIC paper: PRC 99, 024313 (2019)

N*LO$_{SMS}$: Order-by-Order





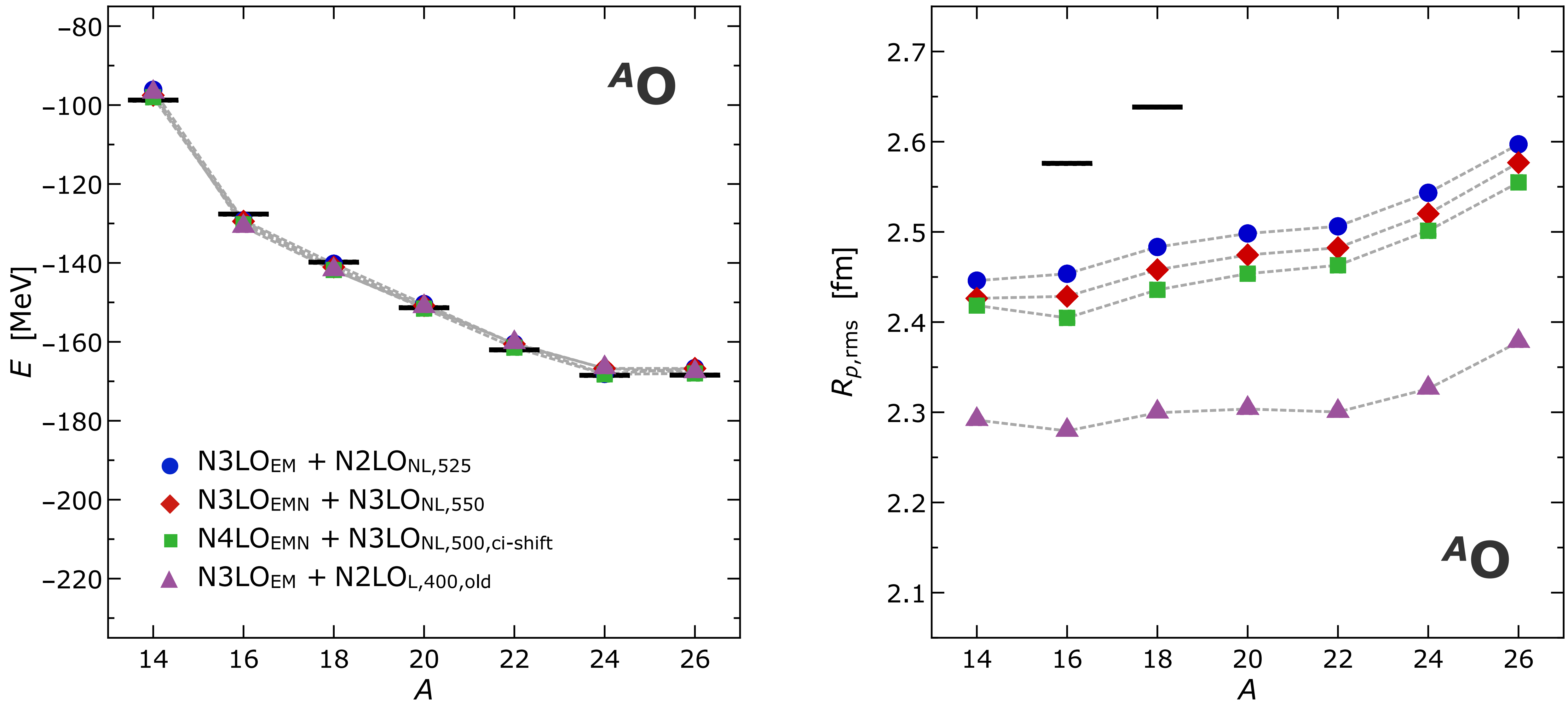
overbinding and even smaller radii at all orders,
similar to the simple local interactions

Summary

- from practical point of view, non-local regulators perform consistently better than local or semi-local ones
- several candidate interactions with good ground-state energies in oxygen chain and improved radii (still not perfect)
  - $\mathrm{N3LO}_{\mathrm{EM}} + \mathrm{N2LO}_{\mathrm{NL,525}}$
  - $\mathrm{N3LO}_{\mathrm{EMN}} + \mathrm{N3LO}_{\mathrm{NL,550}}$
  - $\mathrm{N4LO}_{\mathrm{EMN}} + \mathrm{N3LO}_{\mathrm{NL,500,ci\text{-}shift}}$
- from a conceptual point of view, several open questions:
  - do local or semi-local interactions improve with higher-order 3N terms?
  - which mechanism will increase radii further?
  - is the delicate cancelation with non-local 3N a problem?

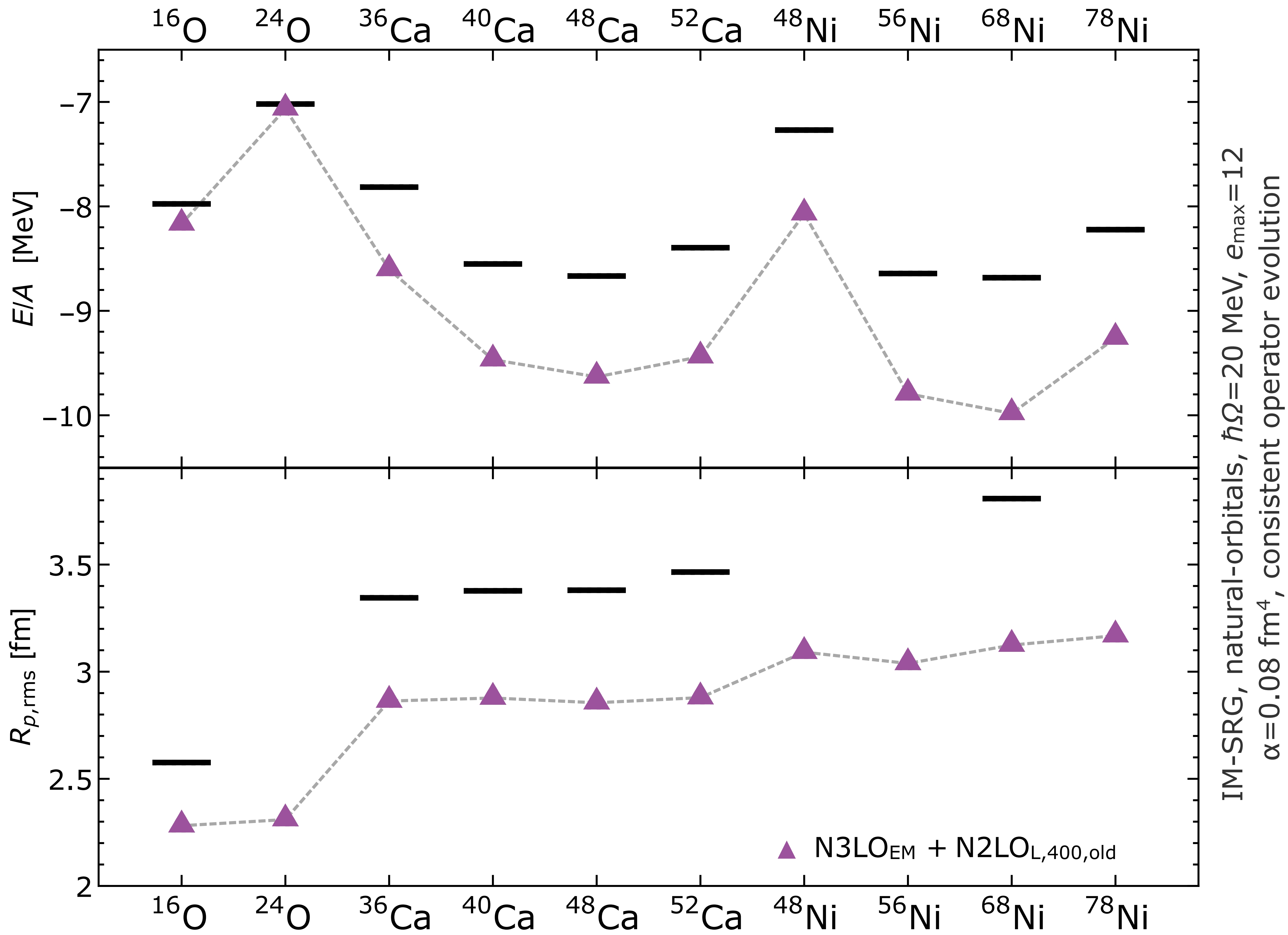
Outlook

Best-Of Interactions

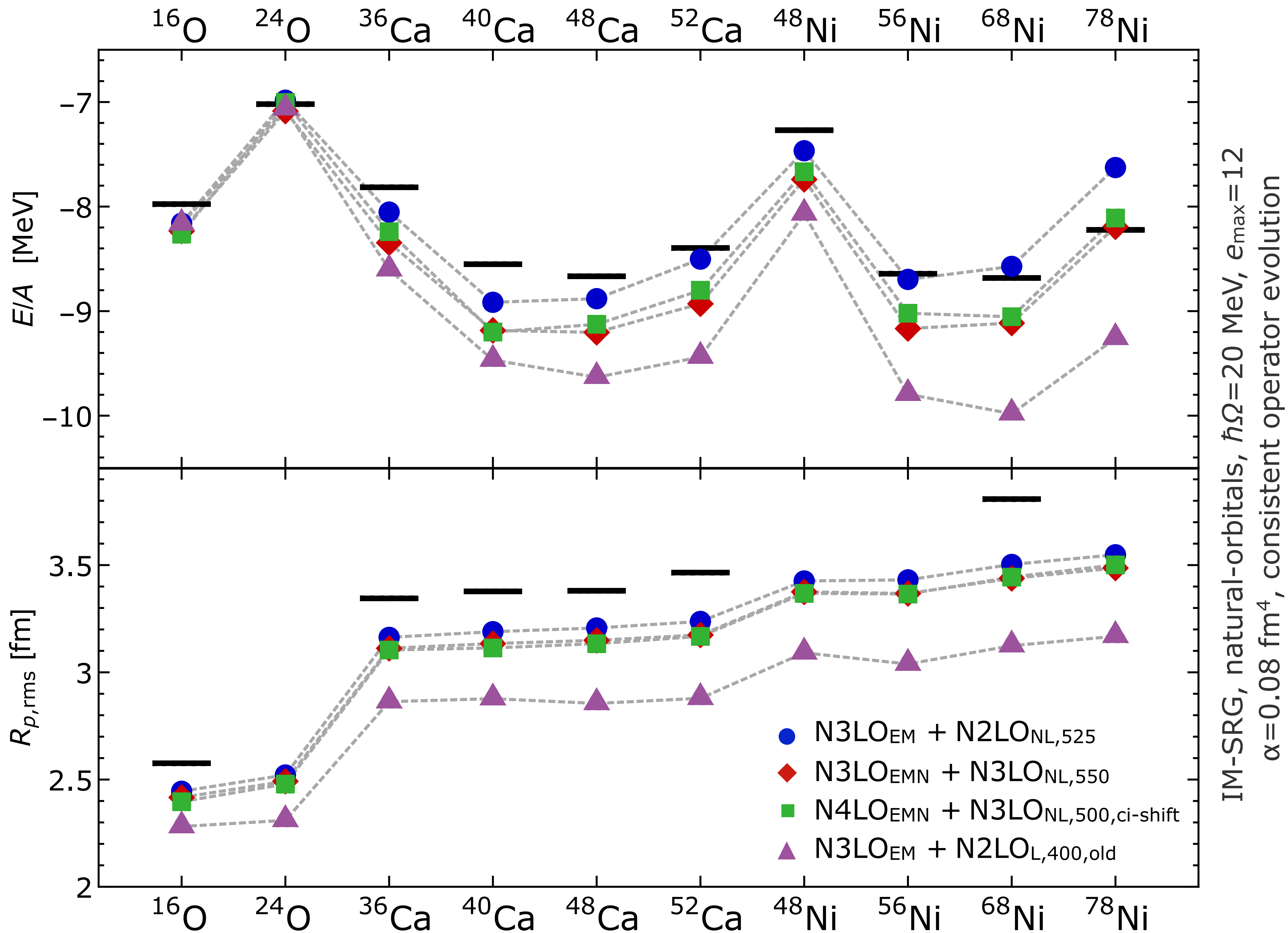


set of different NN+3N interactions that reproduce binding energies equally well, but differ significantly for radii

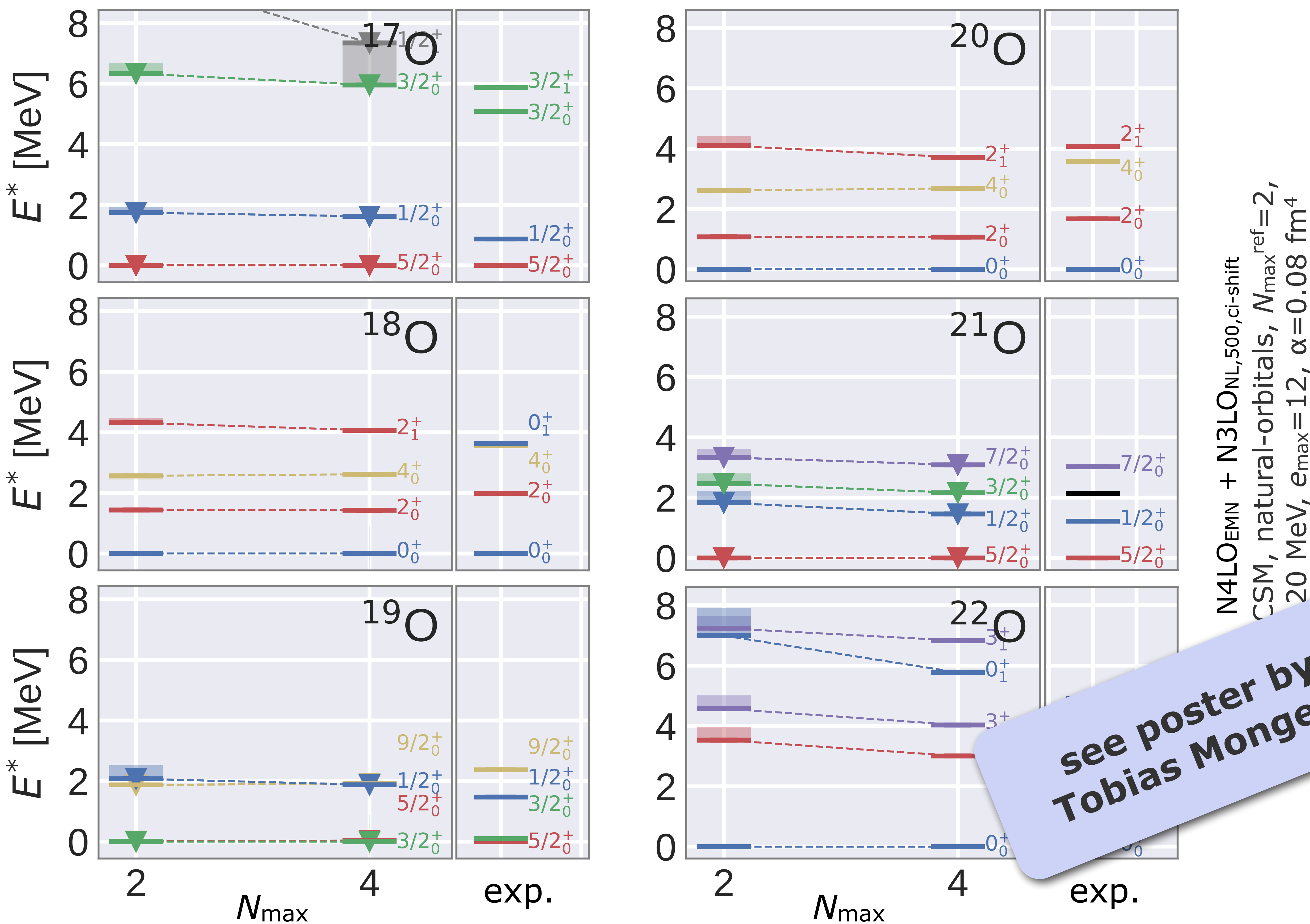
IM-SRG: Medium-Mass Nuclei



IM-SRG: Medium-Mass Nuclei



IM-NCSM: Oxygen Spectra



see poster by Tobias Mongelli

Epilogue

- **thanks to my group and my collaborators**
  - S. Alexa, M. Deuker, **T. Hüther**, P. Käse, M. Knöll, L. Mertes, T. Mongelli, J. Müller, K. Vobig, C. Walde, T. Wolfgruber & **K. Hebeler**
    Technische Universität Darmstadt
  - A. Tichai
    CEA Saclay
  - P. Navrátil
    TRIUMF, Vancouver
  - H. Hergert, R. Wirth
    NSCL / Michigan State University
  - J. Vary, P. Maris
    Iowa State University
  - E. Epelbaum, H. Krebs, P. Reinhard & the LENPIC Collaboration
    Universität Bochum, …

LENPIC

SFB 1245
Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung