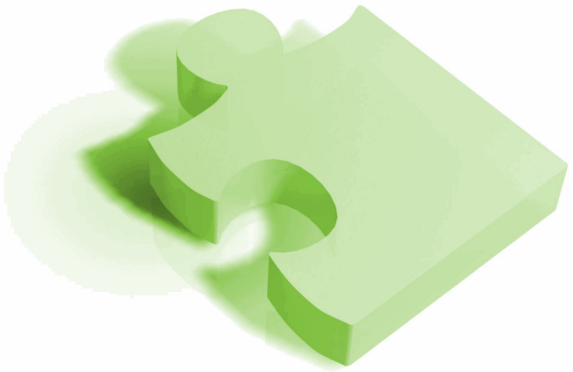
Ab Initio Nuclear Structure Theory from Chiral Interactions

Robert Roth

TECHNISCHE
UNIVERSITÄT
DARMSTADT

New Era of Nuclear Structure Theory



- **QCD at low energies**

  improved understanding through effective field theories & lattice simulations

New Era of Nuclear Structure Theory

- **QCD at low energies**

  improved understanding through effective field theories & lattice simulations

- **quantum many-body methods**

  advances in ab initio treatment of the nuclear many-body problem

New Era of Nuclear Structure Theory

- **QCD at low energies**

  improved understanding through effective field theories & lattice simulations

- **quantum many-body methods**

  advances in ab initio treatment of the nuclear many-body problem

- **computing & algorithms**

  increase of computational resources & improved algorithms

New Era of Nuclear Structure Theory

- **QCD at low energies**

  improved understanding through effective field theories & lattice simulations

- **quantum many-body methods**

  advances in ab initio treatment of the nuclear many-body problem

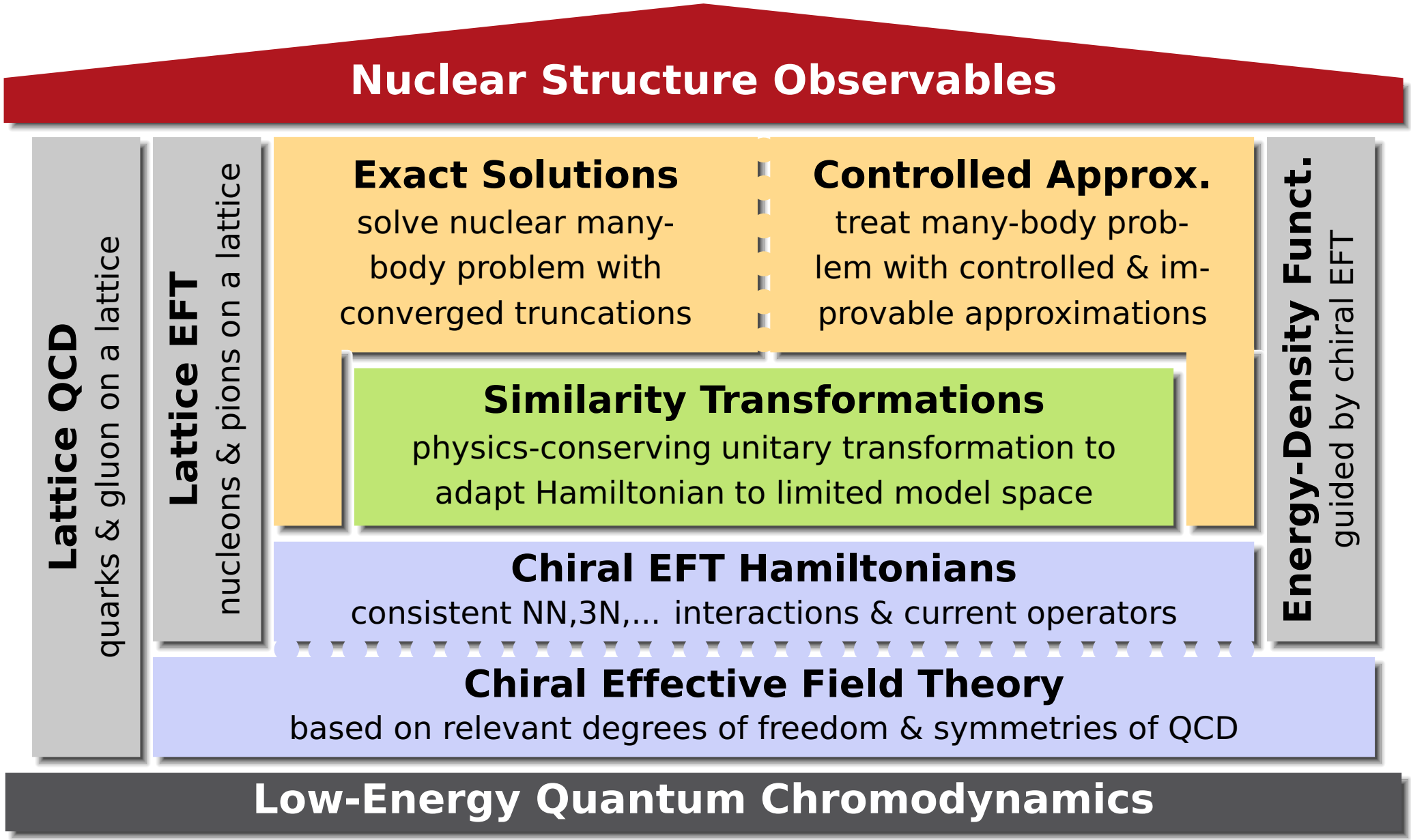
- **computing & algorithms**

  increase of computational resources & improved algorithms

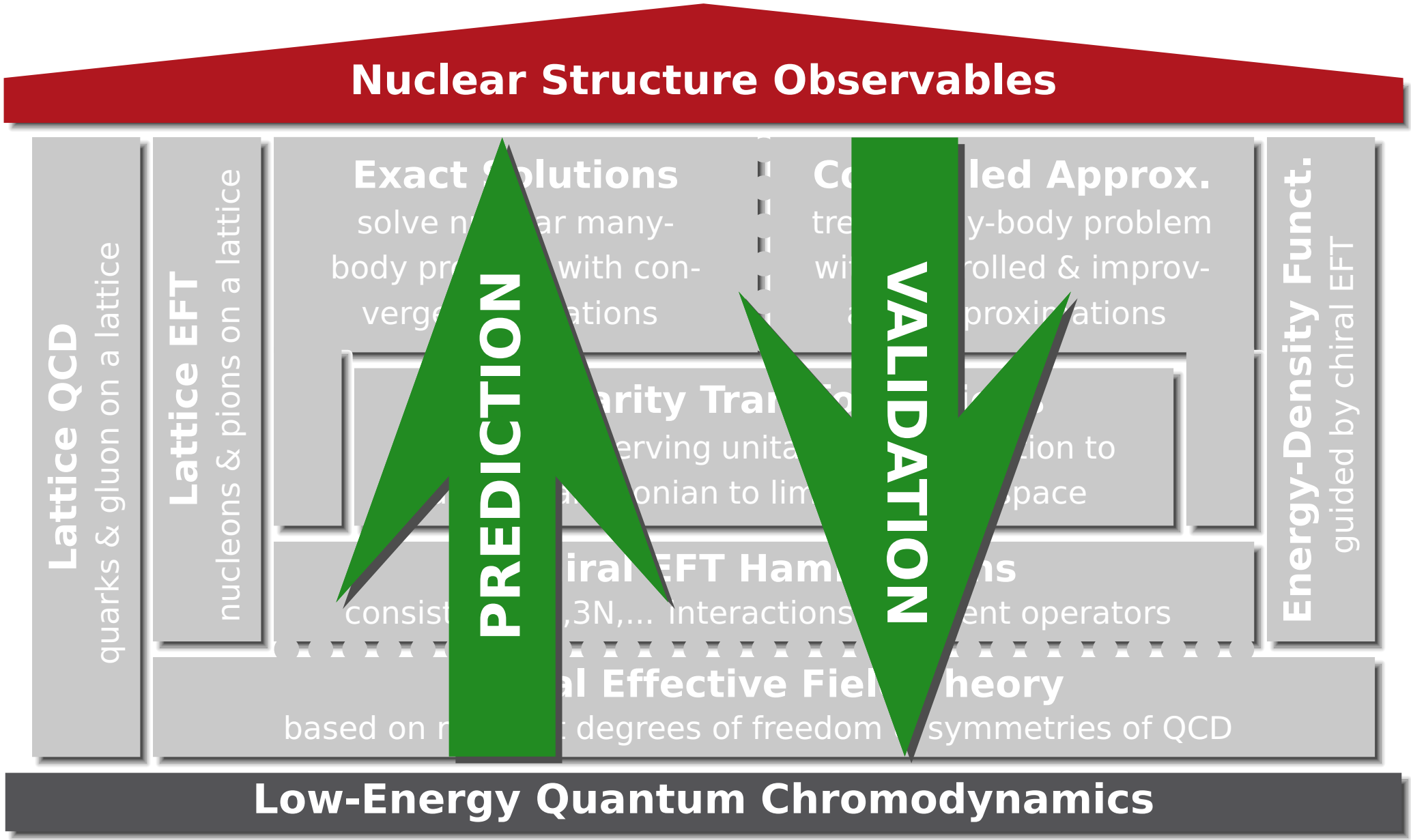
- **experimental facilities**

  amazing perspectives for the study of nuclei far-off stability

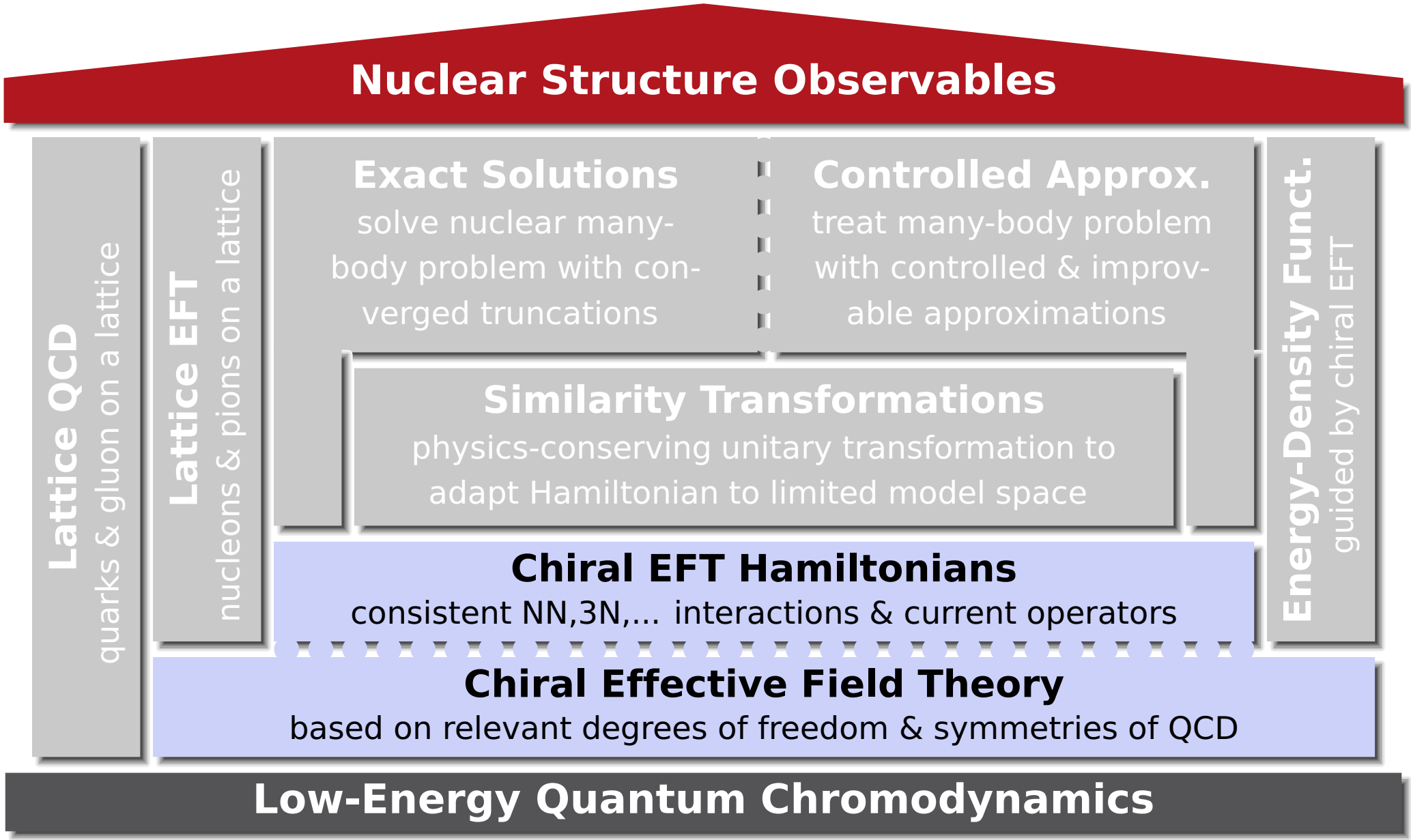
Ab Initio Nuclear Structure



Ab Initio Nuclear Structure



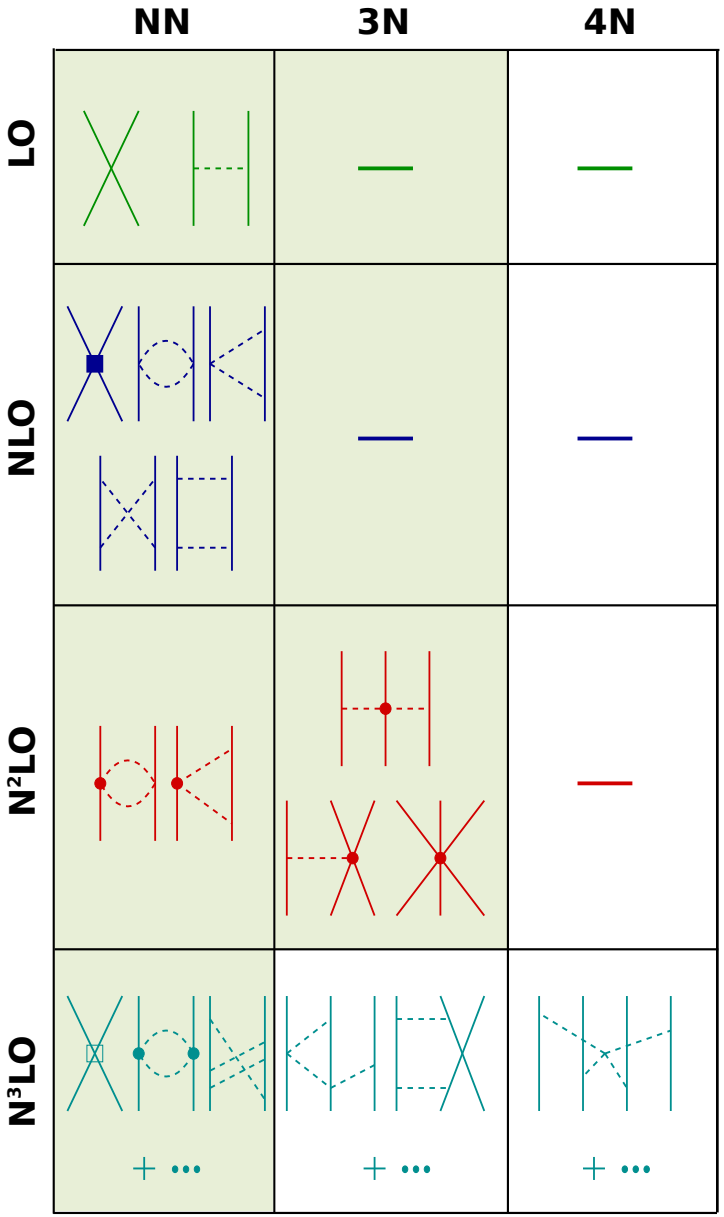
Ab Initio Nuclear Structure



Nuclear Interactions from Chiral EFT

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...

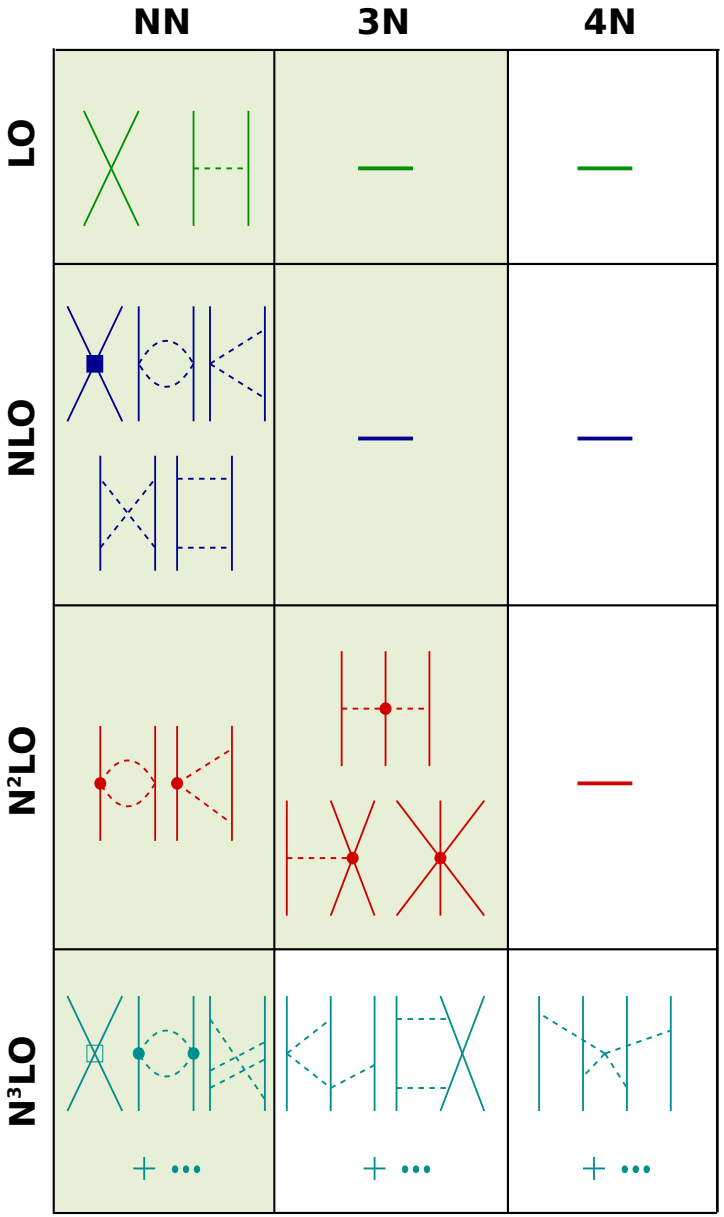
- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- long-range **pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment (NN, πN,...)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at N3LO, N4LO,...
  - explicit inclusion of Δ-resonance
  - YN- & YY-interactions
  - remaining issues: power counting, renormalization, cutoff choice,...



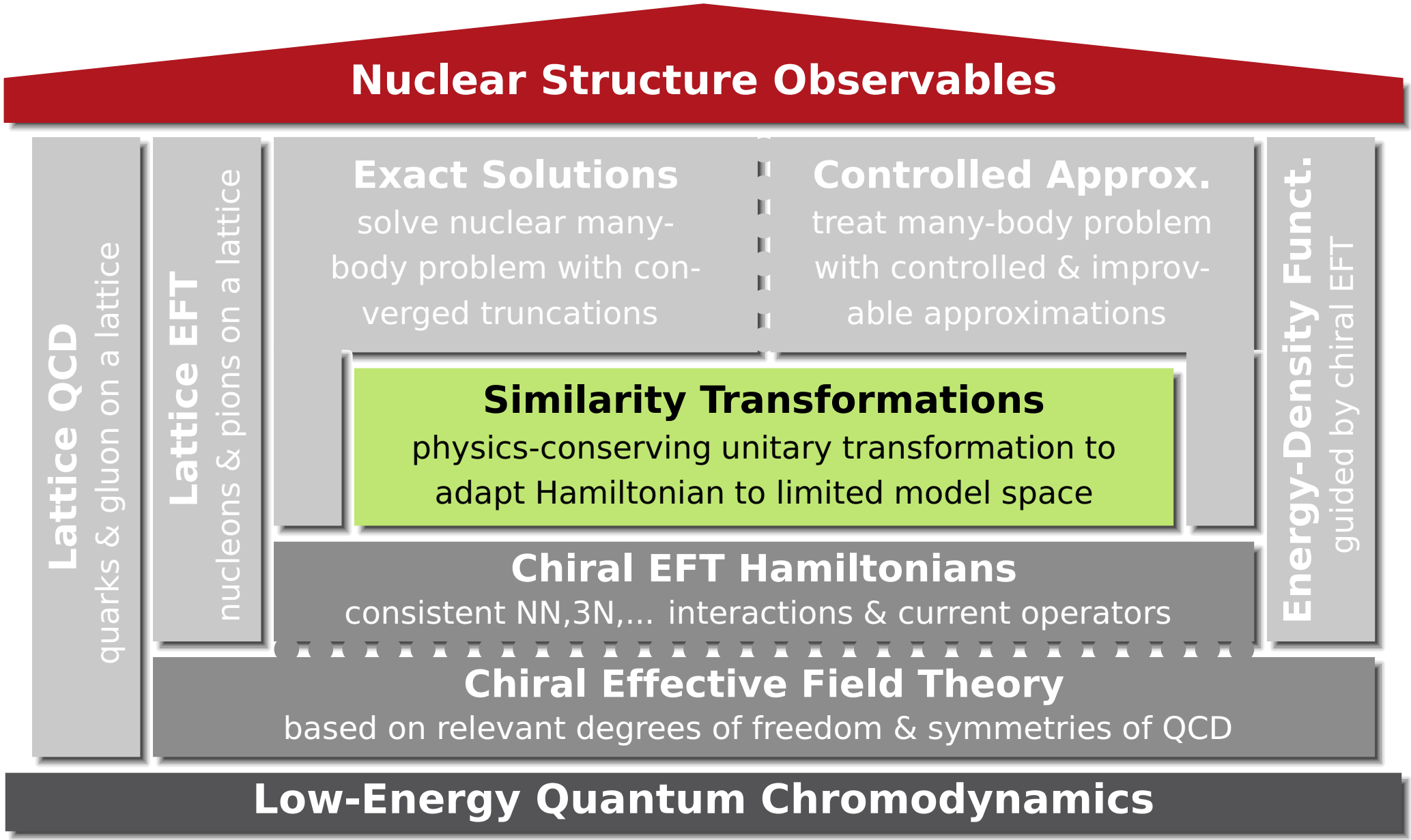
Nuclear Interactions from Chiral EFT

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...

- **standard Hamiltonian**:
  - NN at N3LO:
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N2LO:
    Navrátil, A=3 fit, 500 MeV cutoff
- **present alternatives**:
  - modified 3N interaction at N2LO
    (cutoff & LECs variations)
  - consistent Hamiltonians at N2LO
    (NN: Epelbaum, POUNDERs-opt.)
- **next generation**:
  - consistent Hamiltonians at N3LO
    (LENPIC Collaboration)
  - Δ-full chiral EFT, N4LO contribu-
    tions,...



Ab Initio Nuclear Structure



Similarity Renormalization Group

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

continuous transformation driving
Hamiltonian to band-diagonal form
with respect to a uncorrelated basis

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hami

$$H_\alpha = U_\alpha^\dagger H U_\alpha \qquad U_\alpha$$

- **evolution equations** for H_α and U

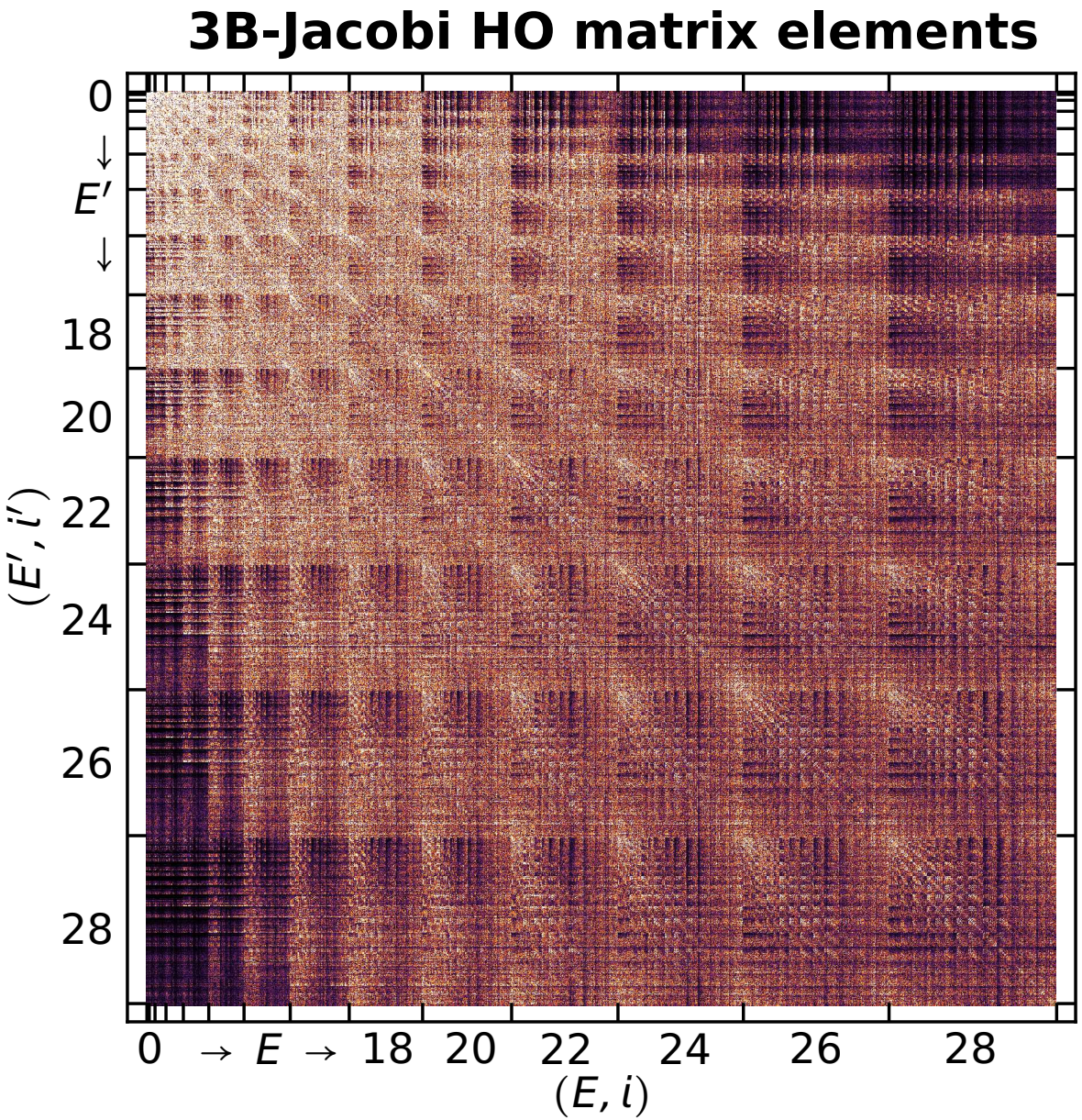
$$\frac{d}{d\alpha} H_\alpha = \left[\eta_\alpha, H_\alpha\right]$$

solve SRG evolution equations using two-, three- & four-body matrix representation

- **dynamic generator**: commutator with the operator in whose eigenbasis H_α shall be diagonalized

$$\eta_\alpha = (2\mu)^2 \left[T_{\text{int}}, H_\alpha\right]$$

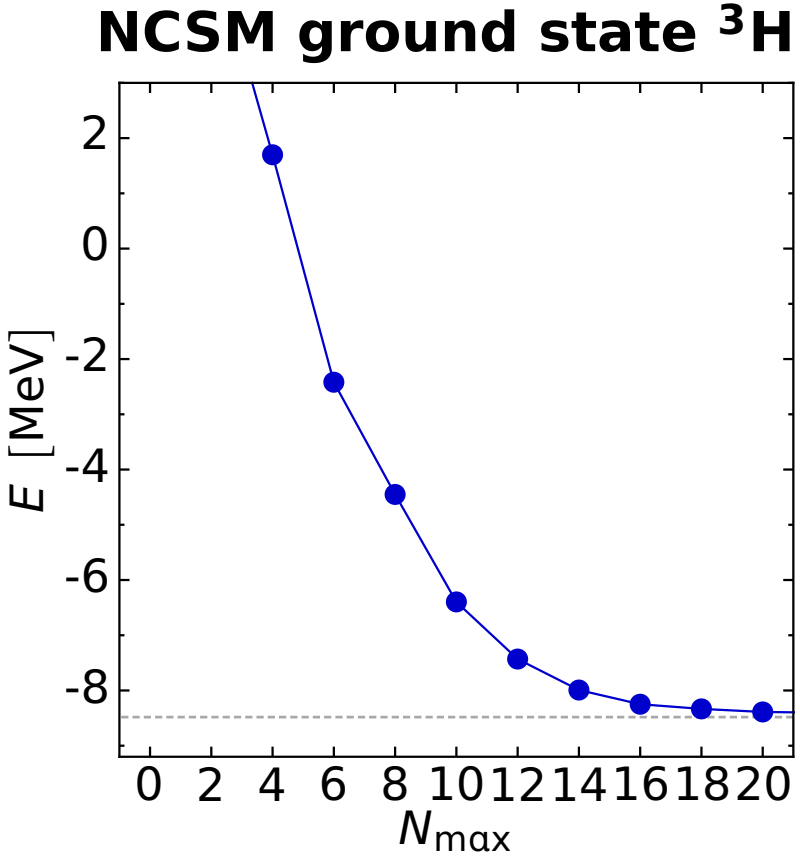
SRG Evolution in Three-Body Space



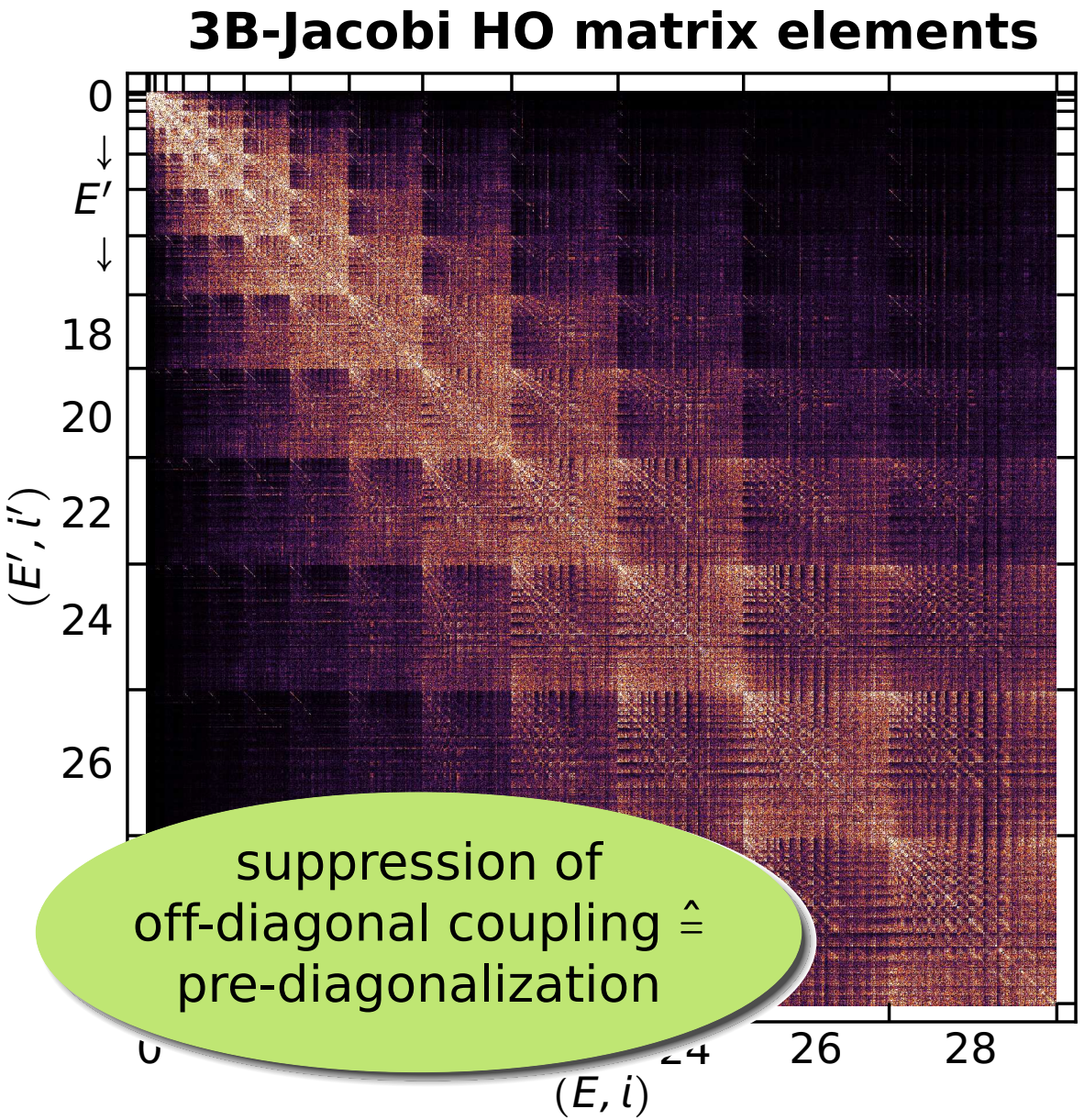
$\alpha = 0.000\,\mathrm{fm}^4$

$\Lambda = \infty\,\mathrm{fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



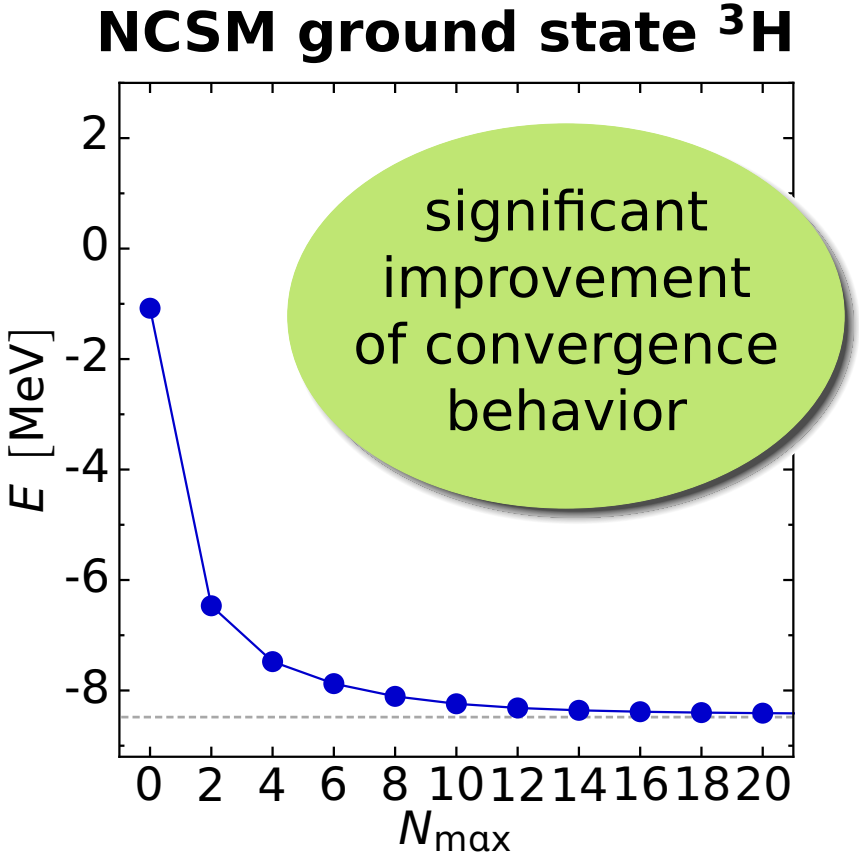
SRG Evolution in Three-Body Space



$\alpha = 0.320\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



Hamiltonian in A-Body Space

- evolution **induces n-body contributions** $\mathrm{H}_\alpha^{[n]}$ to Hamiltonian

$$\mathrm{H}_\alpha = \mathrm{H}_\alpha^{[1]} + \mathrm{H}_\alpha^{[2]} + \mathrm{H}_\alpha^{[3]} + \mathrm{H}_\alpha^{[4]} + \mathrm{H}_\alpha^{[5]} + \ldots$$

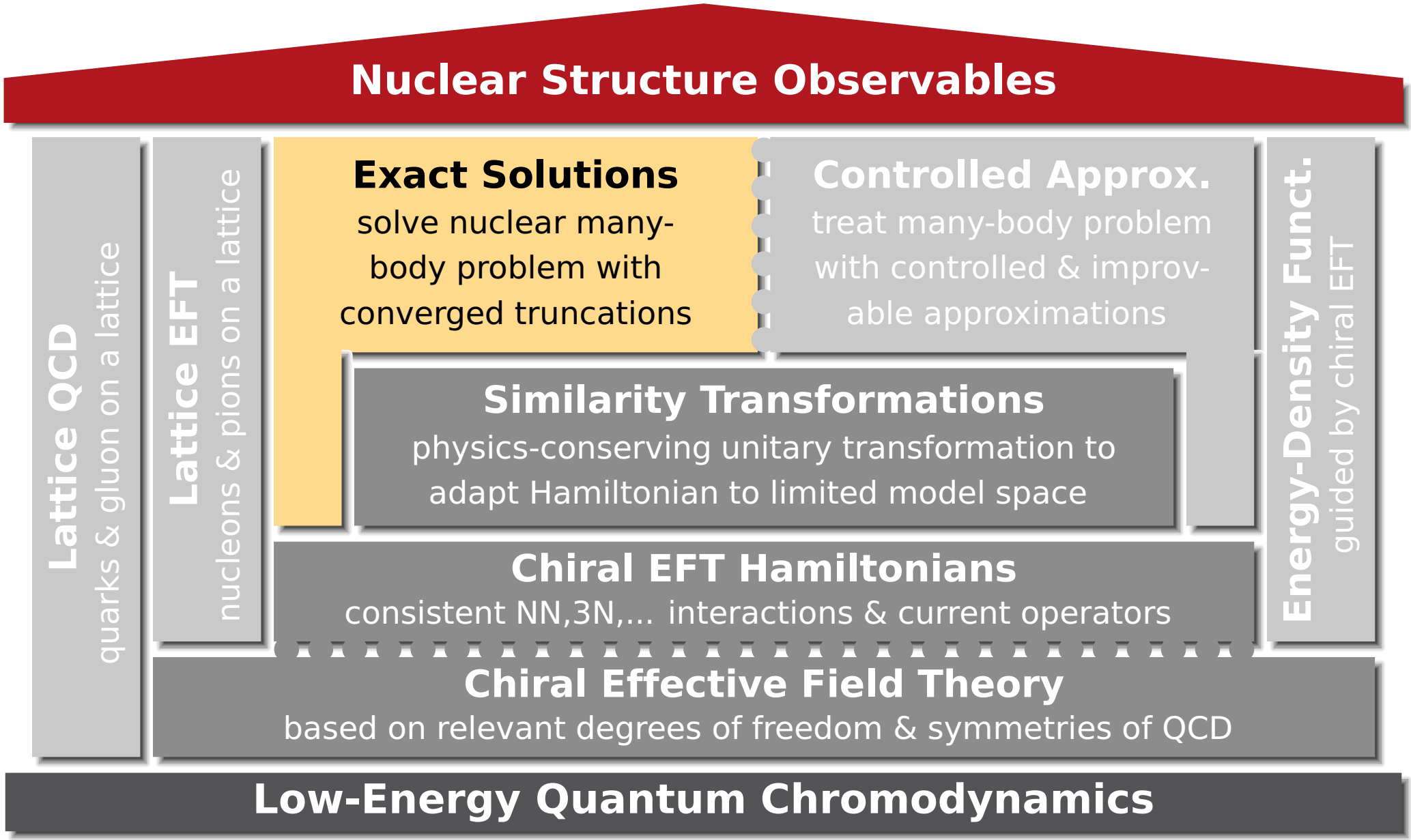
- **truncation of cluster series** formally destroys unitarity and invariance of energy eigenvalues (independence of α)

- flow-parameter α provides **diagnostic tool** to assess neglected higher-order contributions

SRG-Evolved Hamiltonians

$\mathbf{NN_{only}}$	use initial NN, keep evolved NN
$\mathbf{NN + 3N_{ind}}$	use initial NN, keep evolved NN+3N
$\mathbf{NN + 3N_{full}}$	use initial NN+3N, keep evolved NN+3N
$\mathbf{NN + 3N_{full} + 4N_{ind}}$	use initial NN+3N, keep evolved NN+3N+4N

Ab Initio Nuclear Structure



No-Core Shell Model

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

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

- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **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

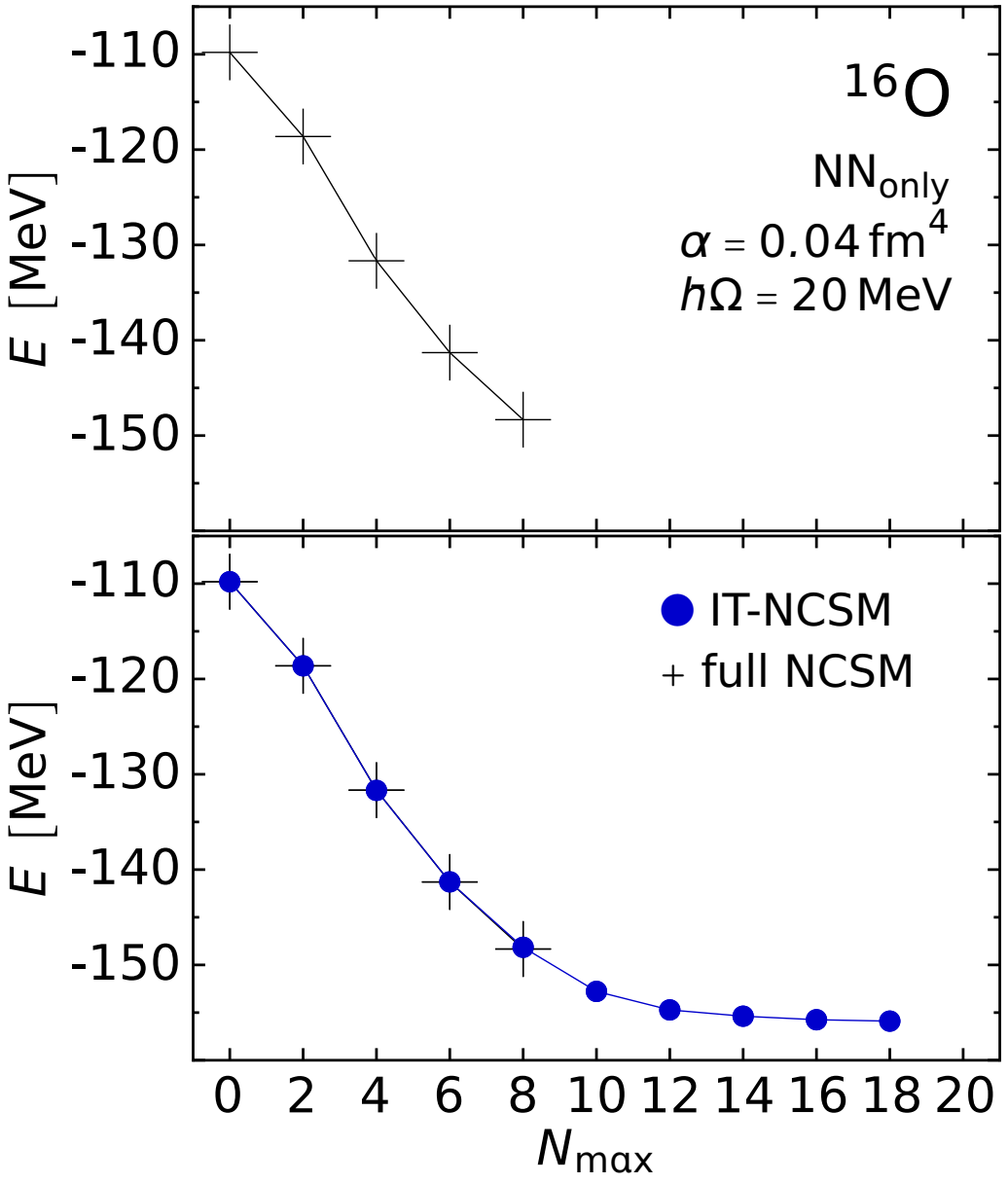
Importance Truncated NCSM

Roth, PRC 79, 064324 (2009); PRL 99, 092501 (2007)

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $N_{max} = 10$ calculation for ^{16}O very difficult (basis dimension $> 10^{10}$)

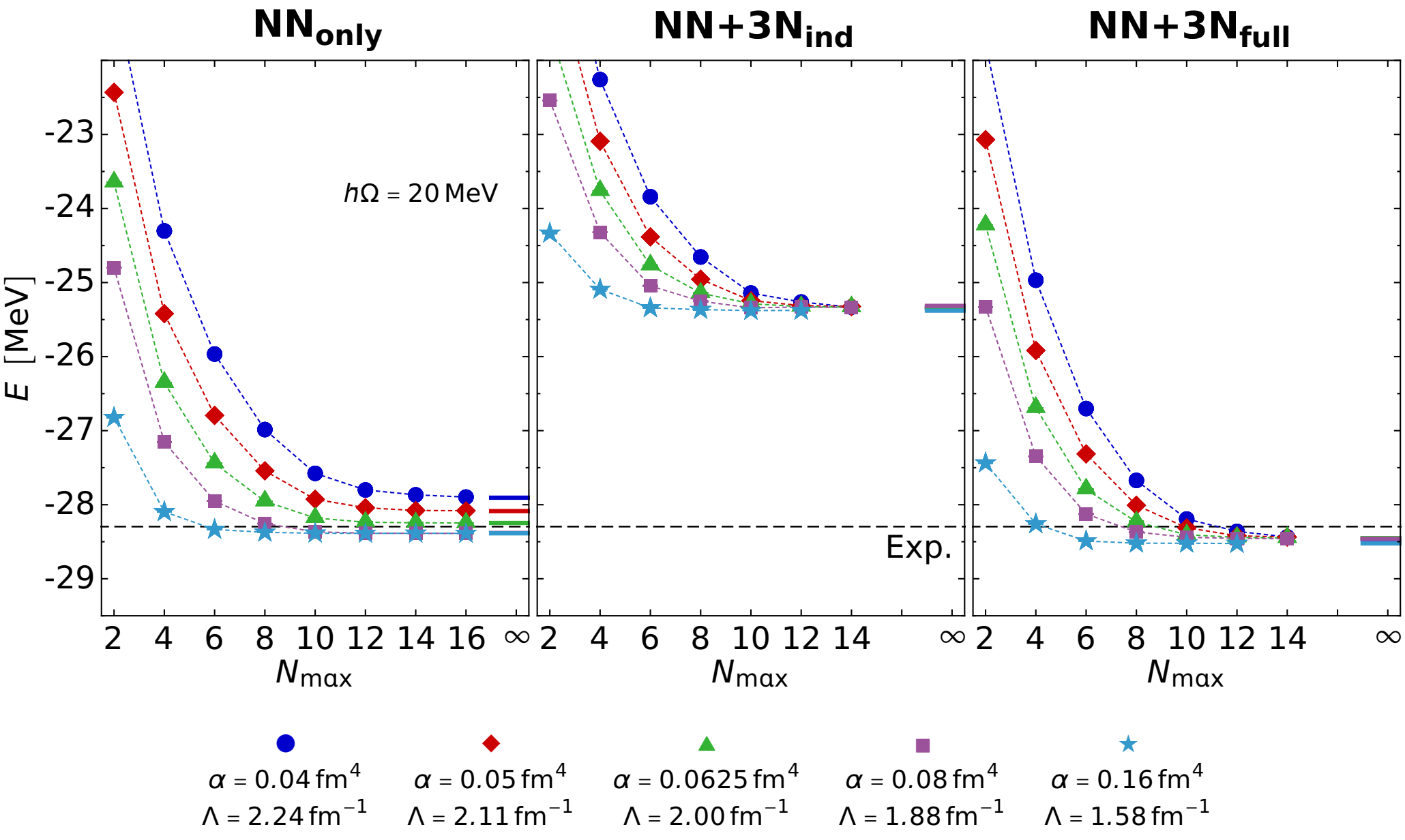
Importance Truncation

reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



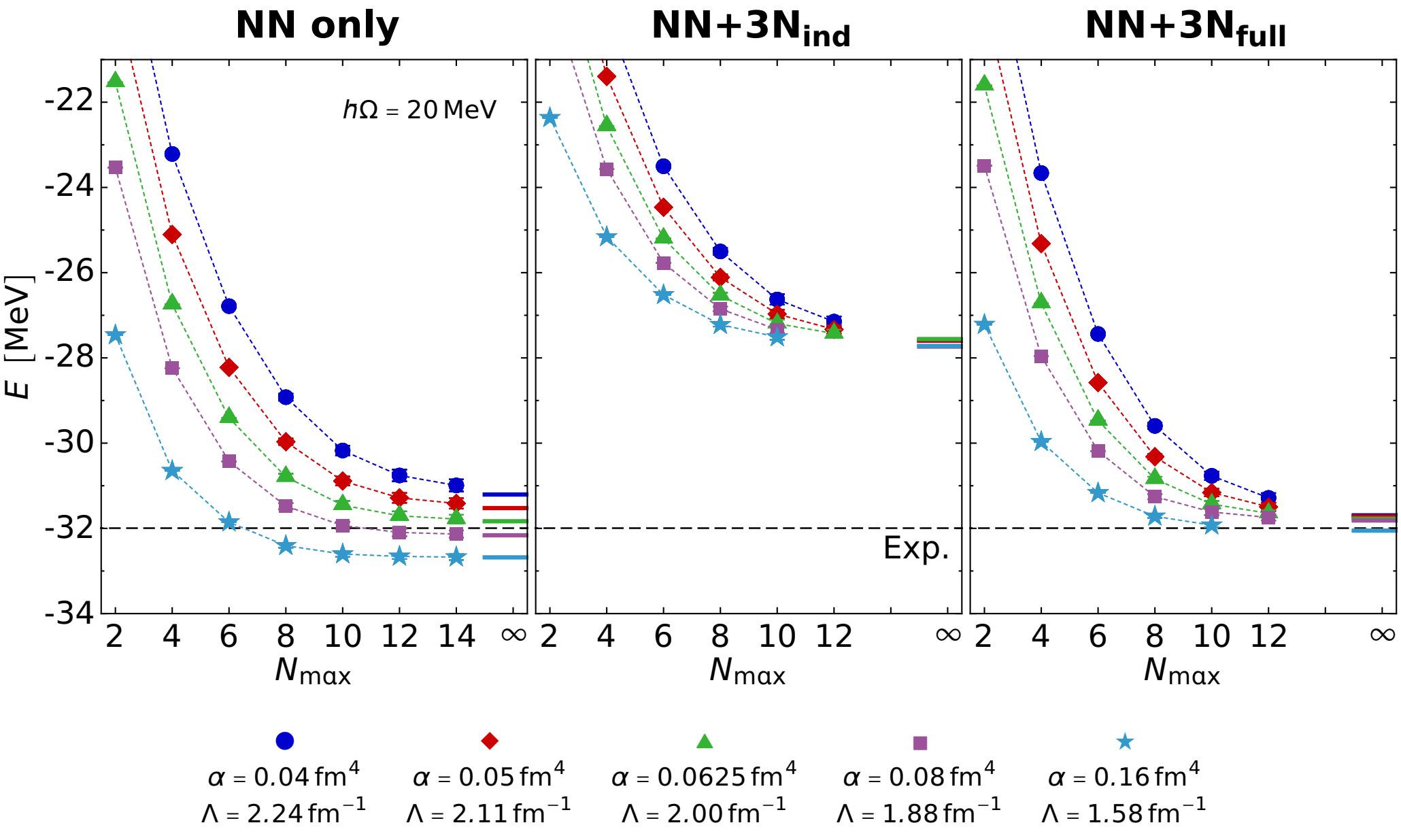
^{4}He: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



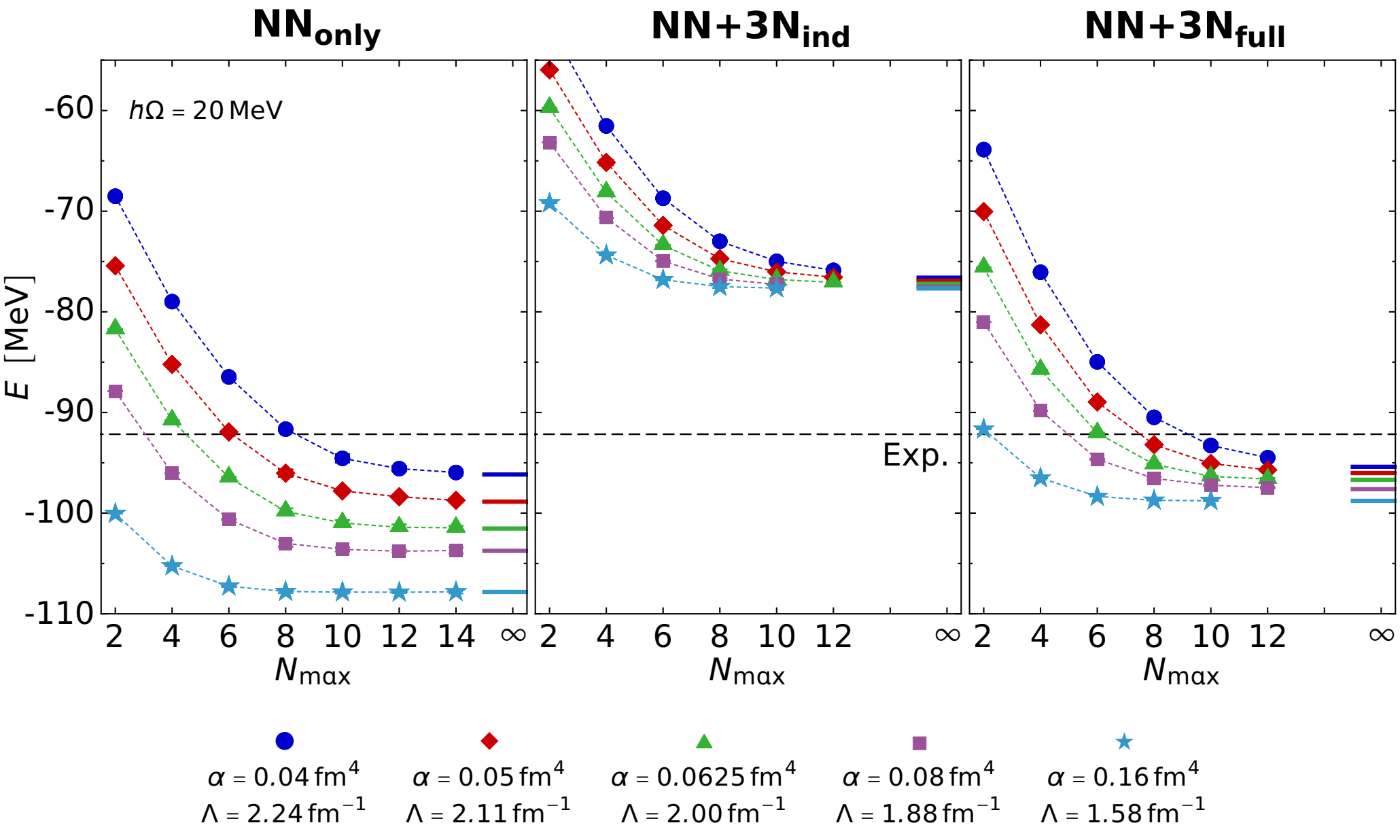
^{6}Li: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



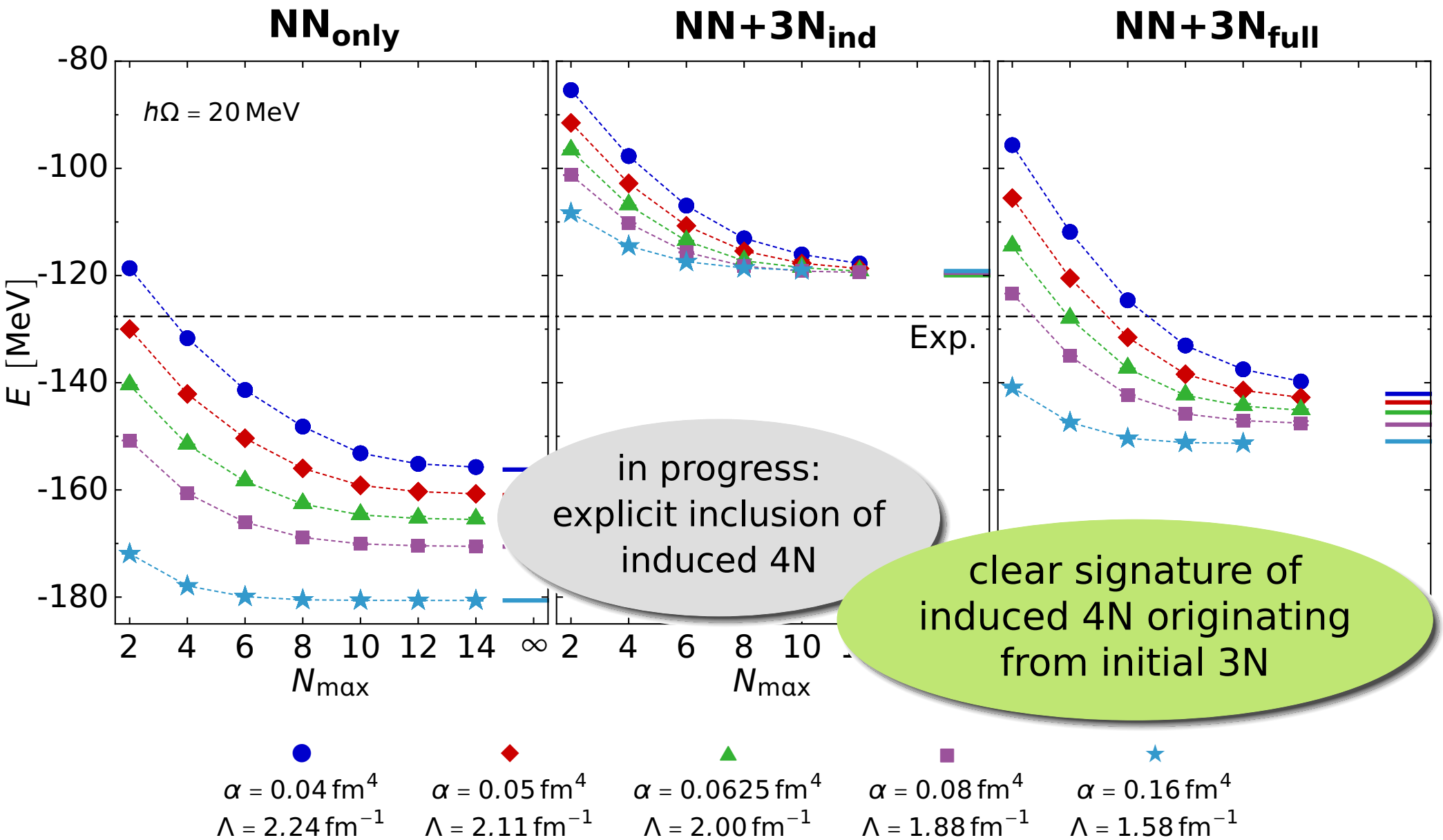
^{12}C: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



^{16}O: Ground-State Energies

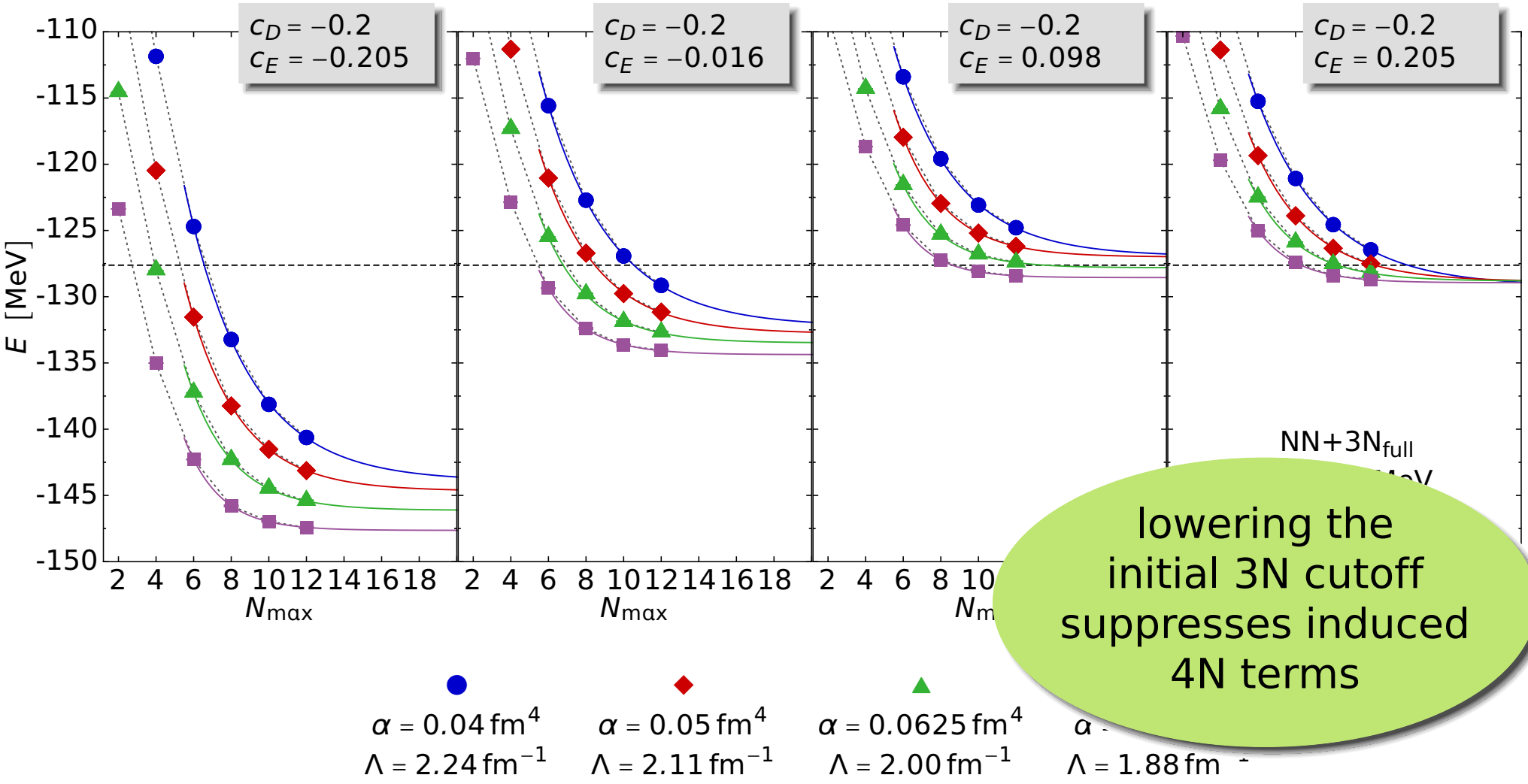
Roth, et al; PRL 107, 072501 (2011)



^{16}O: Lowering the Initial 3N Cutoff

standard

reduced 3N cutoff
(c_E refit to ^{4}He binding energy)



lowering the initial 3N cutoff suppresses induced 4N terms

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)

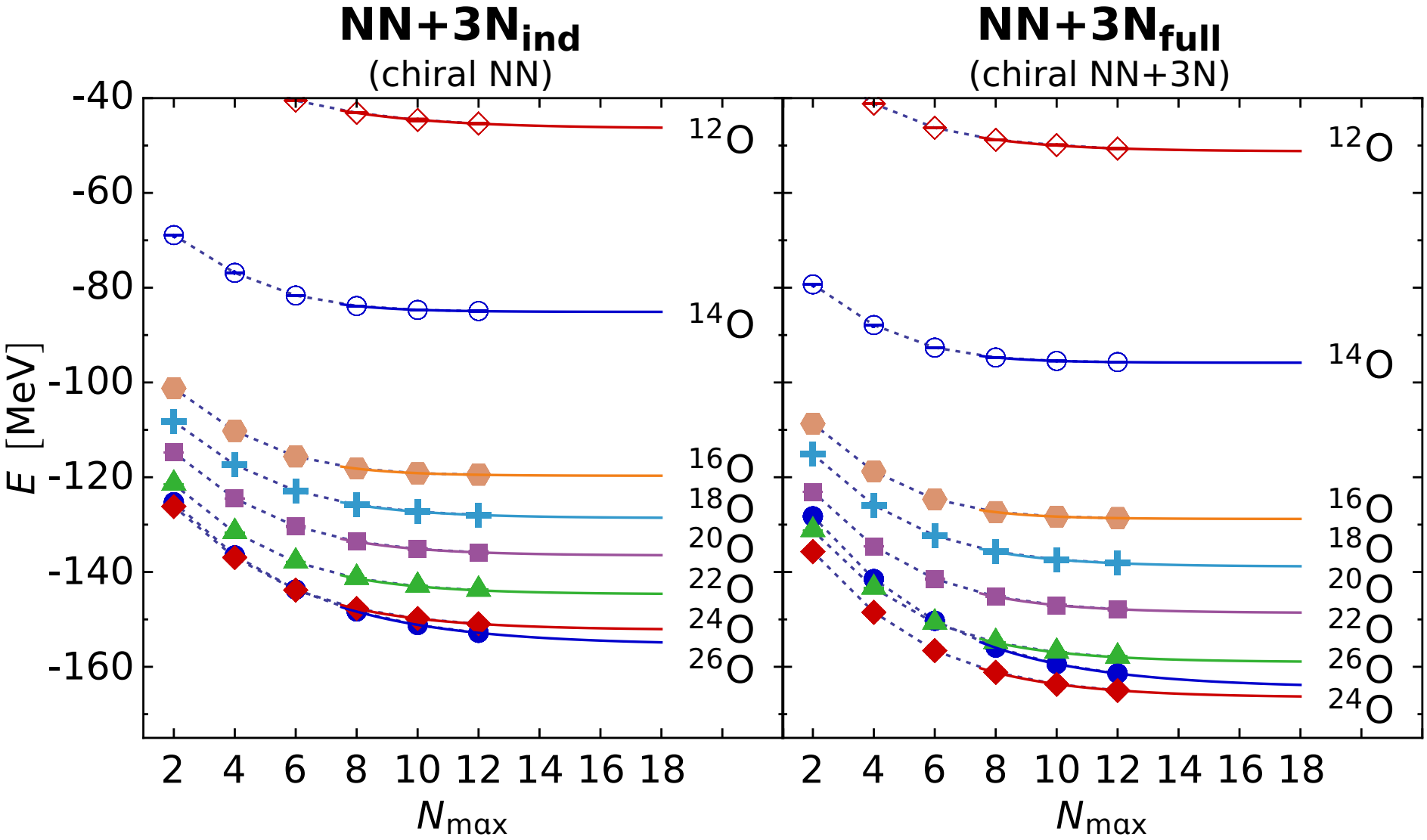
- 2012: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

Hergert, Binder, Calci, Langhammer, Roth, PRL 110, 242501 (2013)

- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions...

Ground States of Oxygen Isotopes

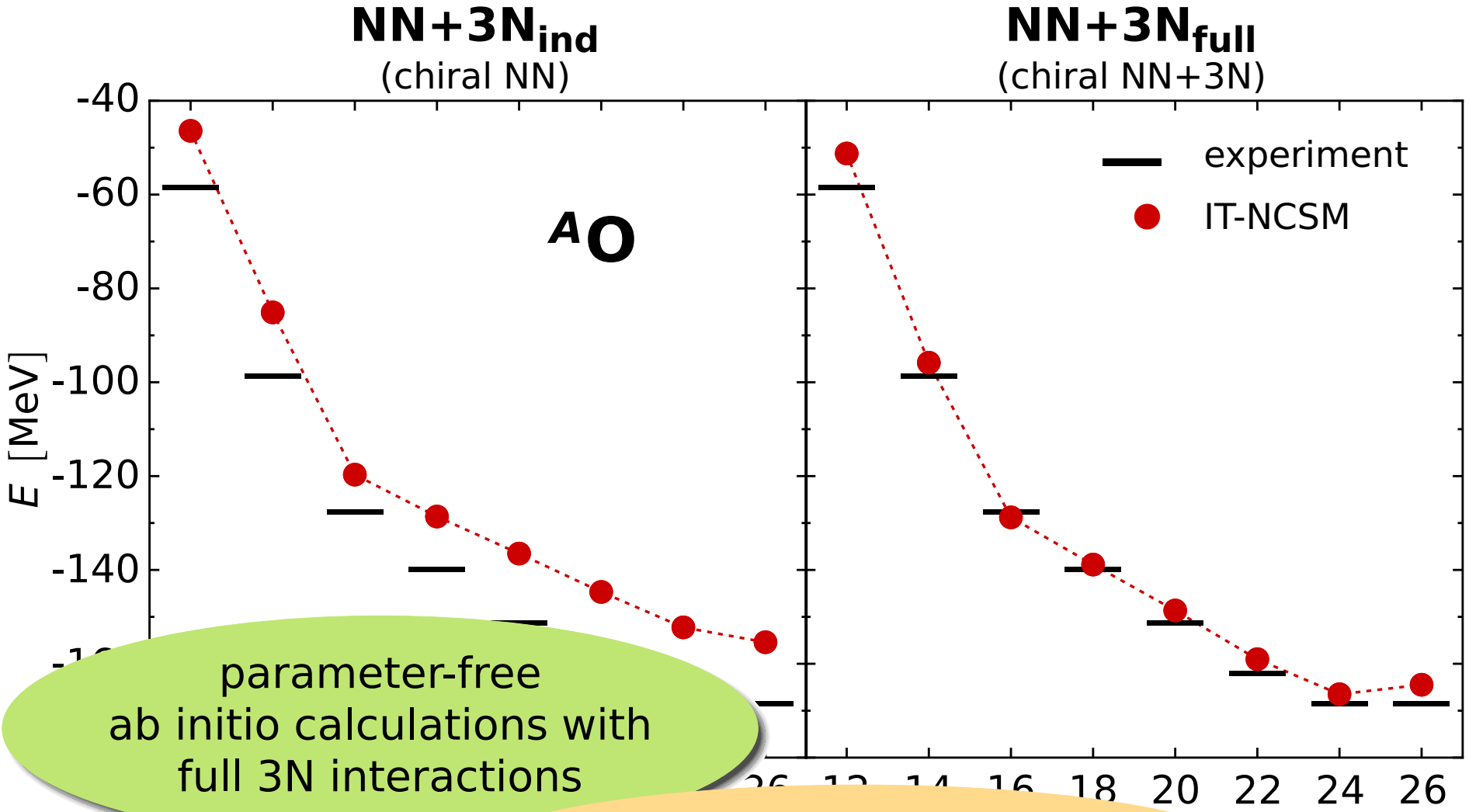
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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)



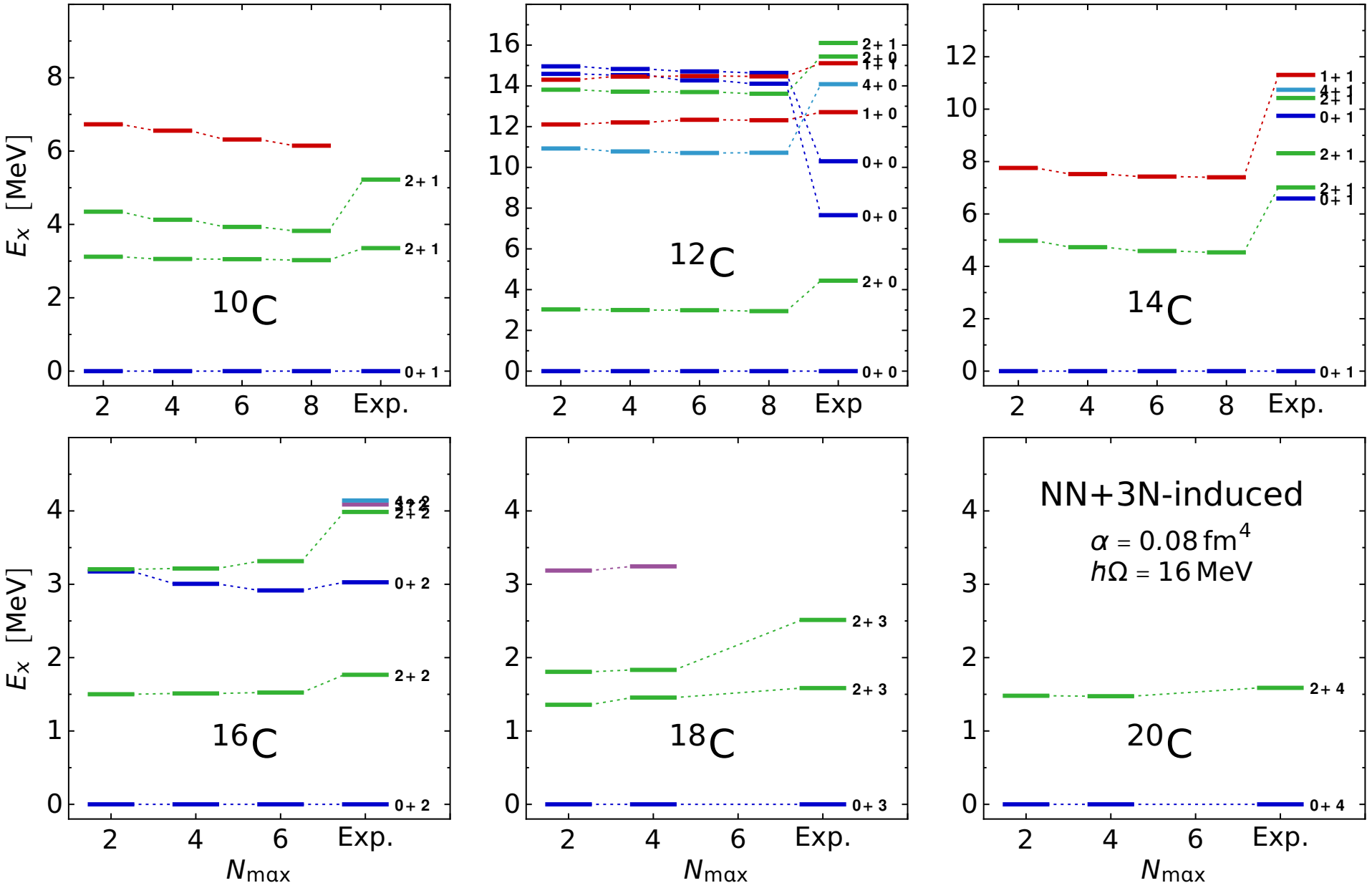
parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

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

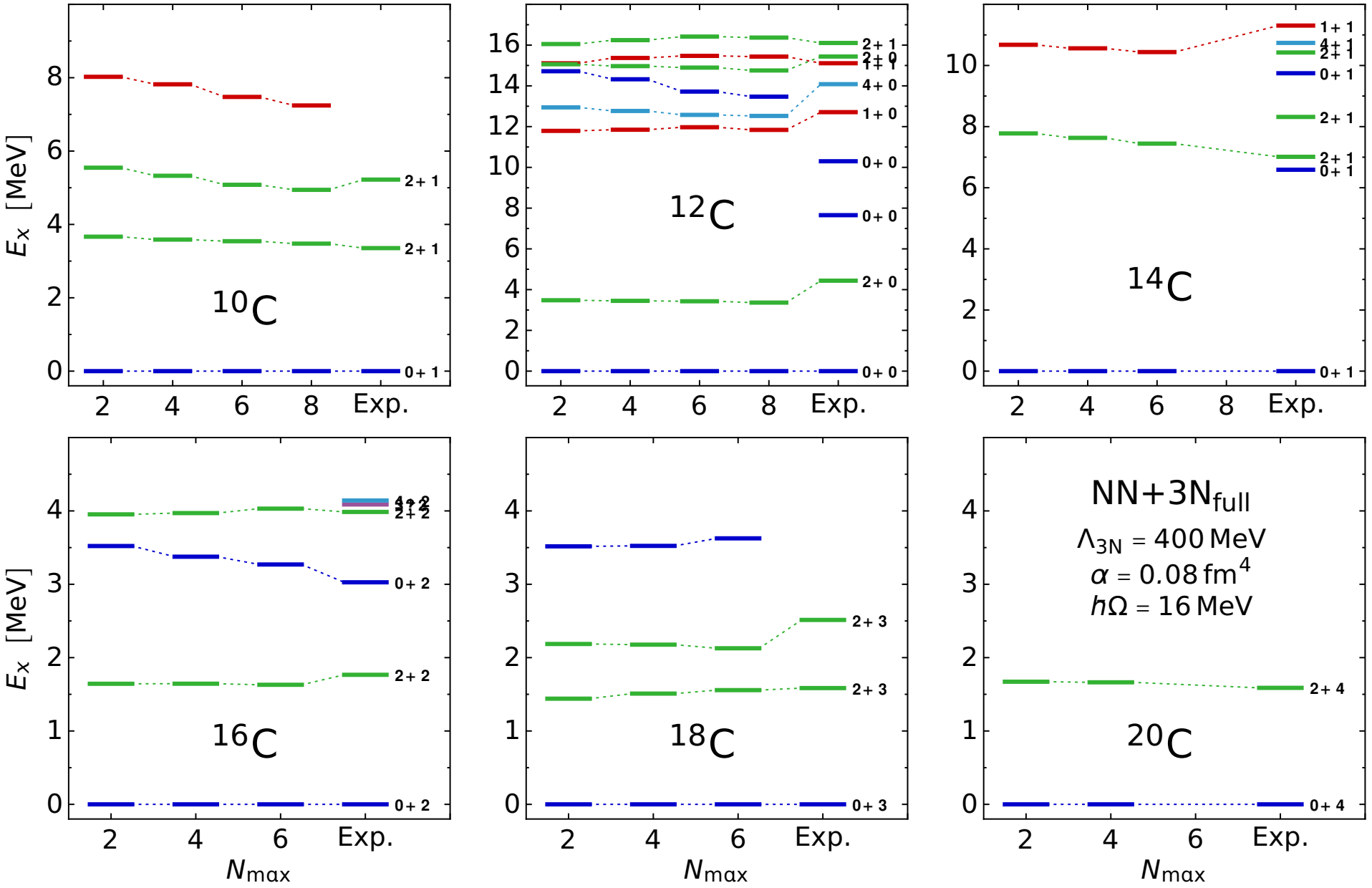
Spectroscopy of Carbon Isotopes

Forssen et al., JPG 40, 055105 (2013); Roth et al., in prep.

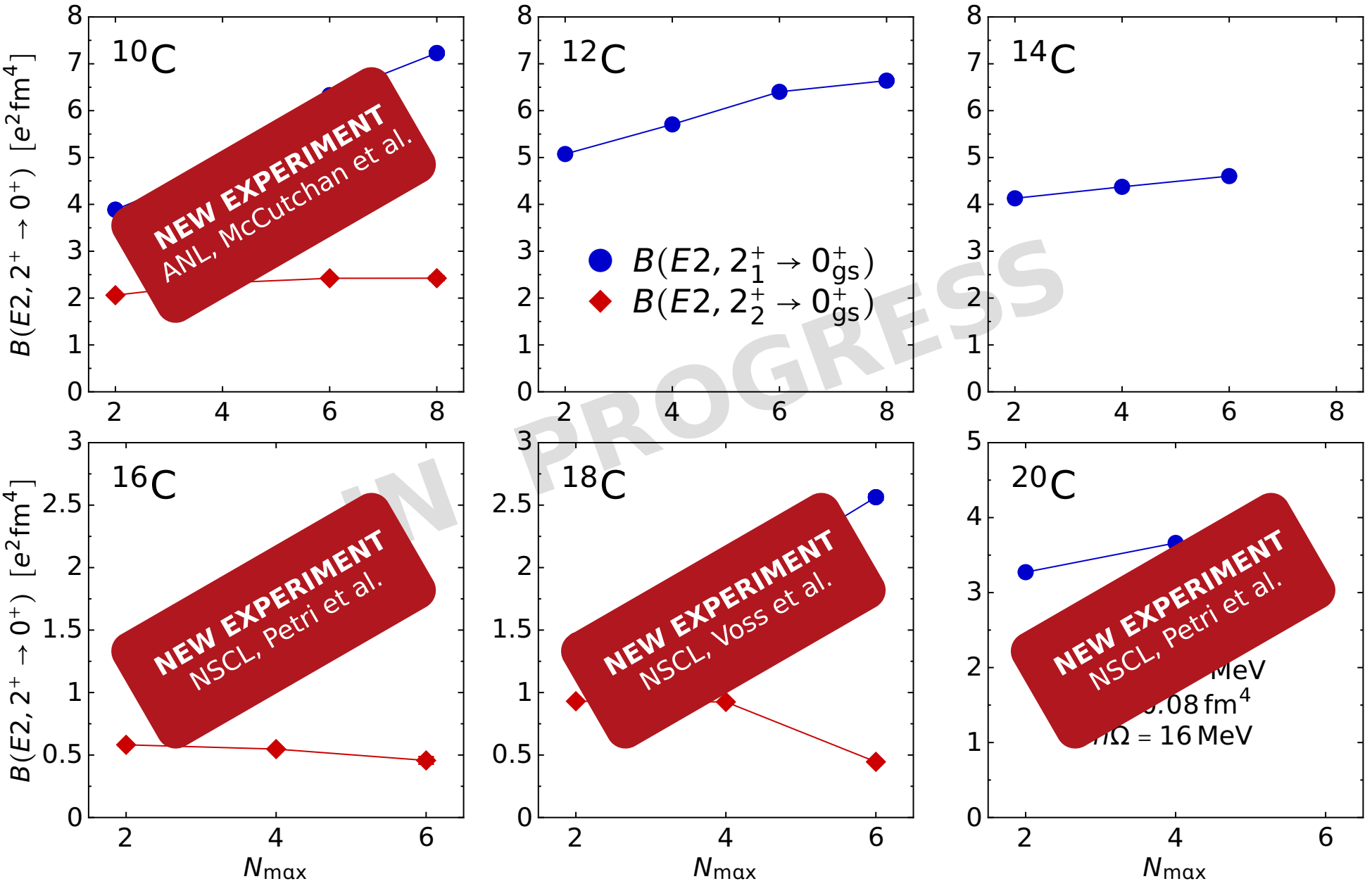


Spectroscopy of Carbon Isotopes

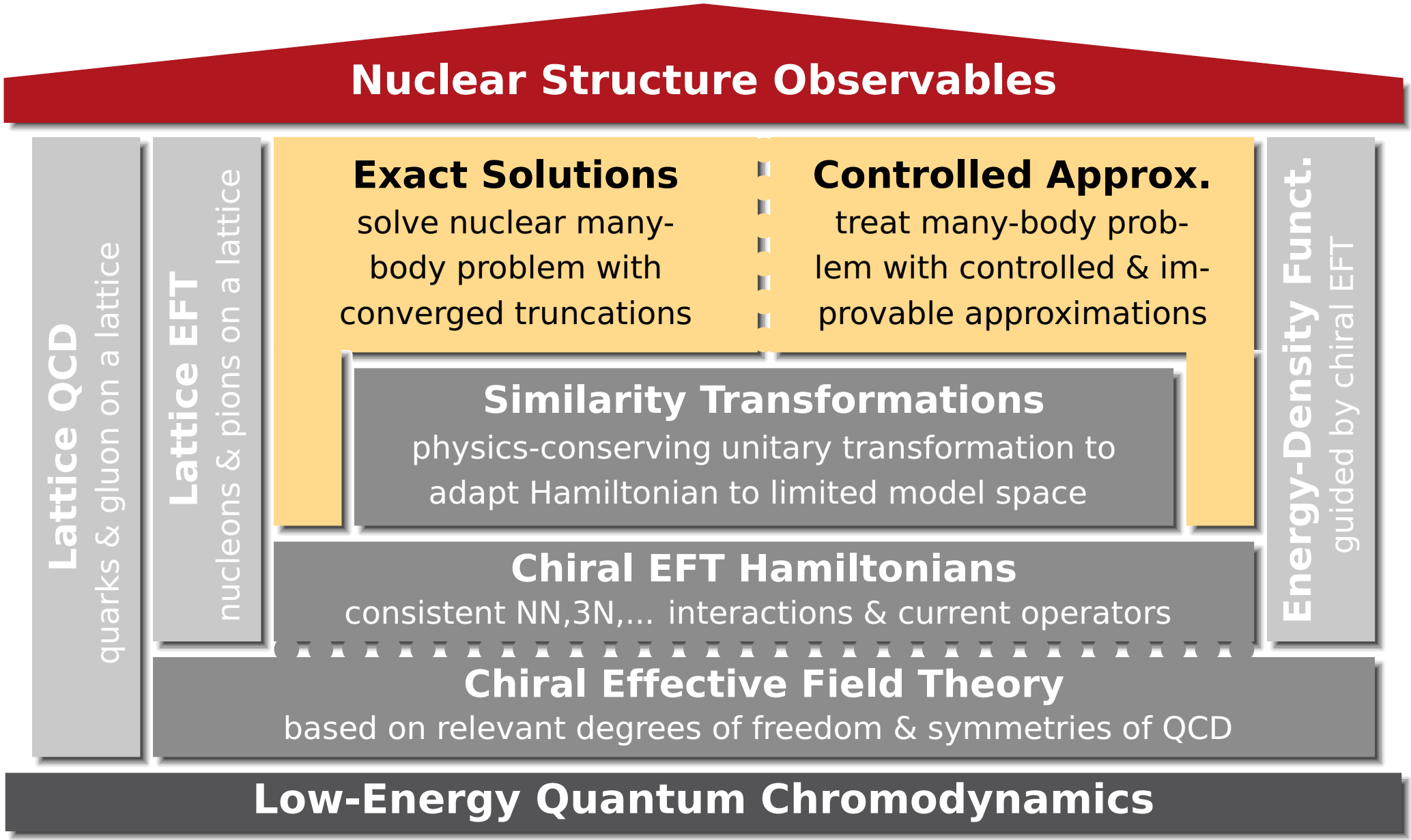
Forssen et al., JPG 40, 055105 (2013); Roth et al., in prep.



Spectroscopy of Carbon Isotopes



Ab Initio Nuclear Structure



Frontier: Medium-Mass Nuclei

advent of novel ab initio many-body approaches applicable in the medium-mass regime

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

- **coupled-cluster theory**: ground-state parametrized by exponential wave operator applied to single-determinant refer
  - truncation at doubles level (CCSD) plus tri D(T))
  - equations of motion for excited s

...iyama, Schwenk, Hergert,...

- **in-medium SR** ible excitations from many-bod ation
  - normal-o Hamiltonian truncated at two-body level
  - both close ground states; excitations via EOM or SM

Barbieri, Soma, Duguet,...

- self-consistent Green's function approaches

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

Inclusion of 3N Interactions

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013), Binder et al. arXiv:1309.1123

- **premium option: explicit 3N**
  - extend coupled-cluster equations for explicit 3N interactions
  - CCSD-3B, Λ-CCSD(T)-3B are feasible, but much more expensive

- **low-cost option: normal-ordered two-body approximation**
  - write 3N interaction in normal-ordered form with respect to the actual *A*-body reference determinant (HF state)

$$V_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ}\, a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ a_\circ$$

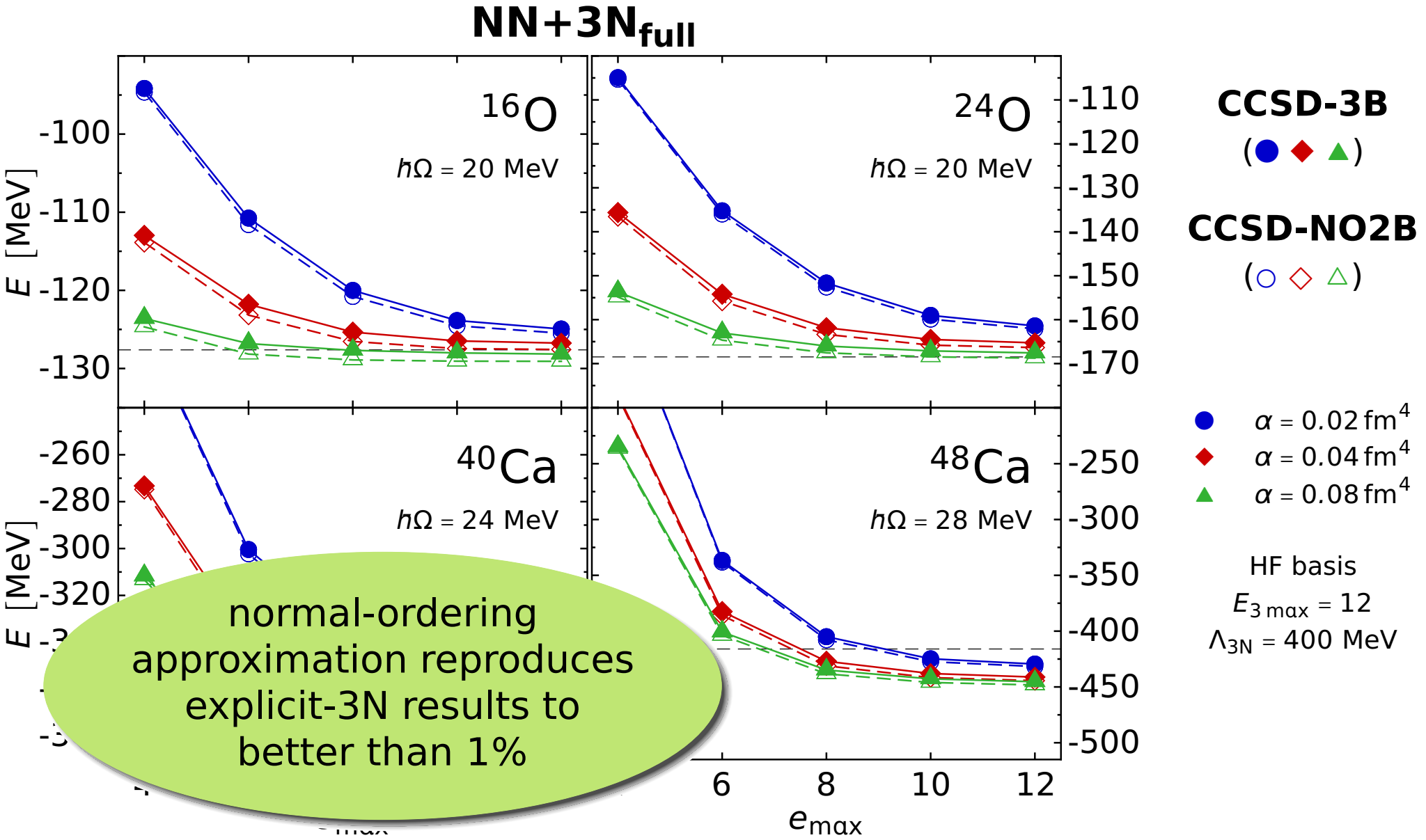
$$= W^{0B} + \sum W^{1B}_{\circ\circ}\, \{a^\dagger_\circ\, a_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ\}$$

$$+ \sum W^{3B}_{\circ\circ\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ a_\circ\}$$

  - discard normal-ordered three-body term and use two-body formalism

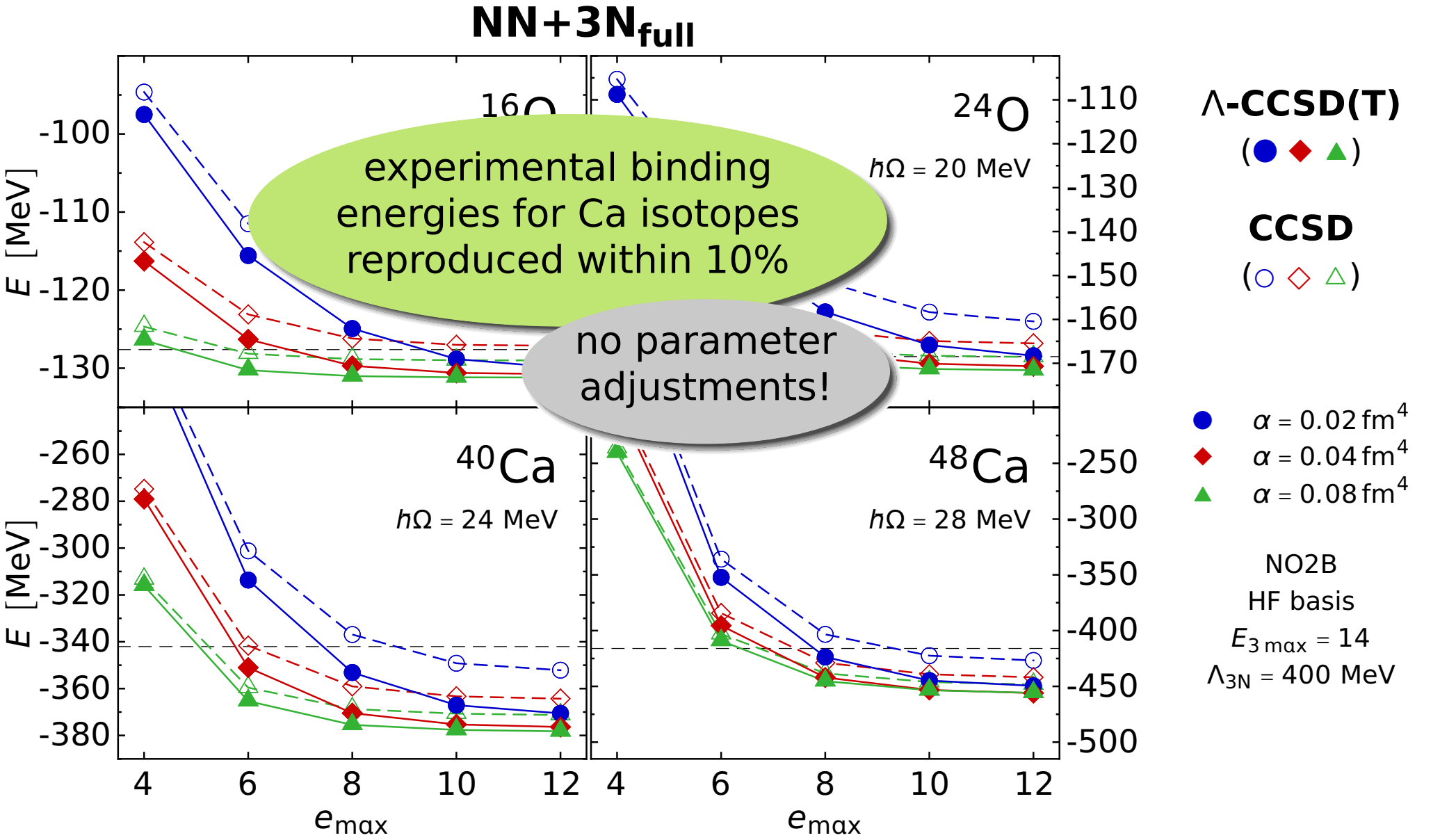
CCSD with Explicit 3N Interactions

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)



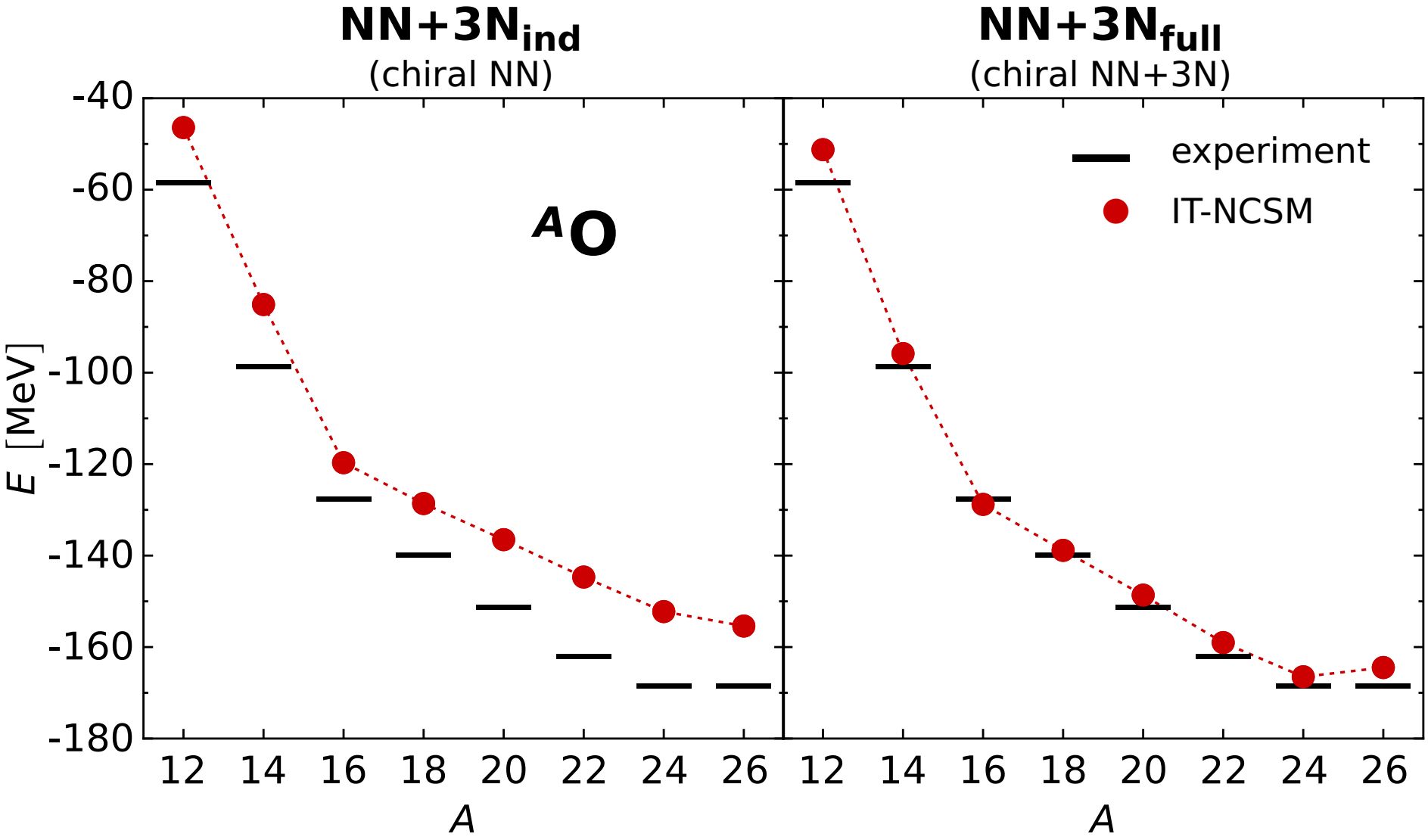
Λ-CCSD(T) with NO2B Approximation

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)



Ground States of Oxygen Isotopes

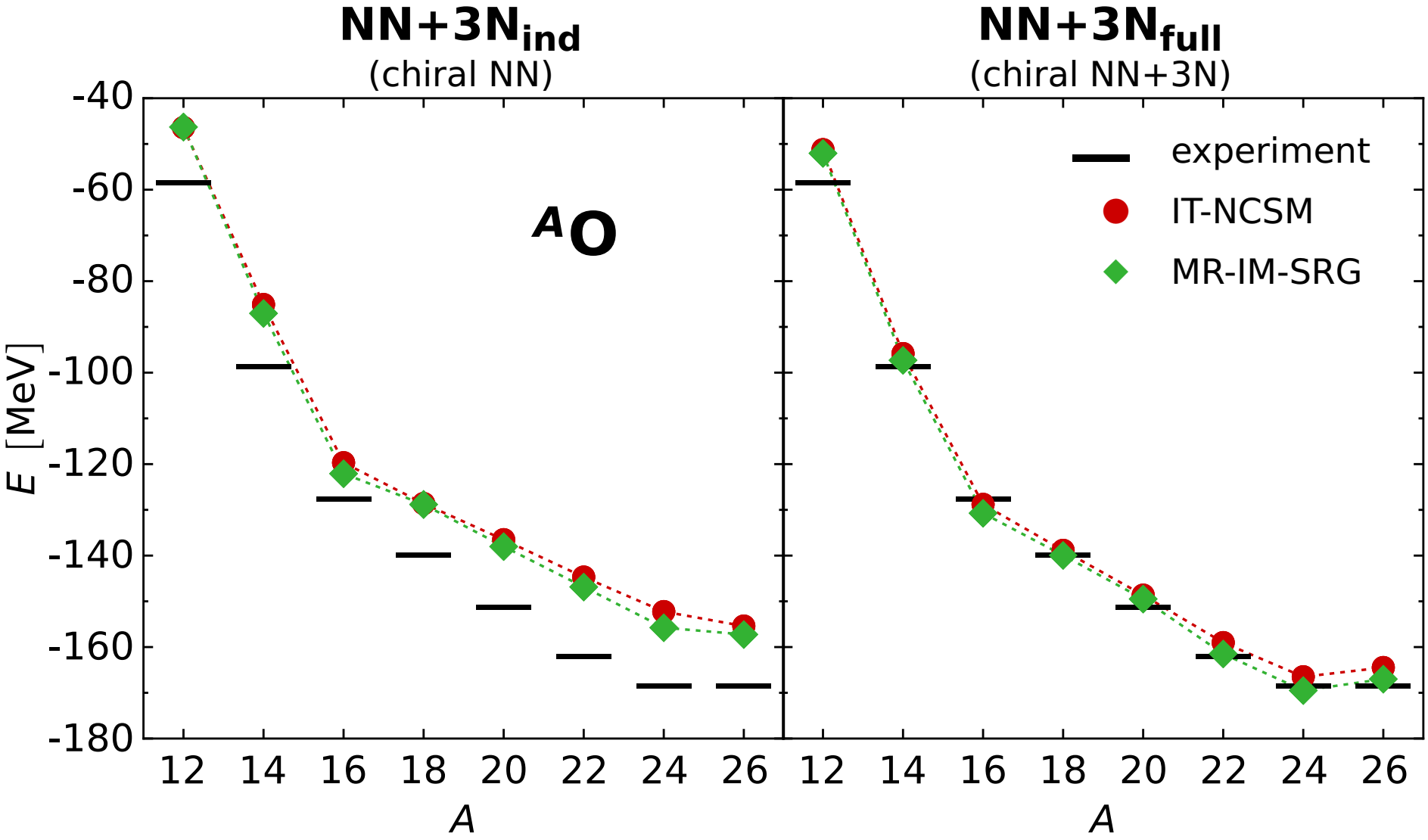
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

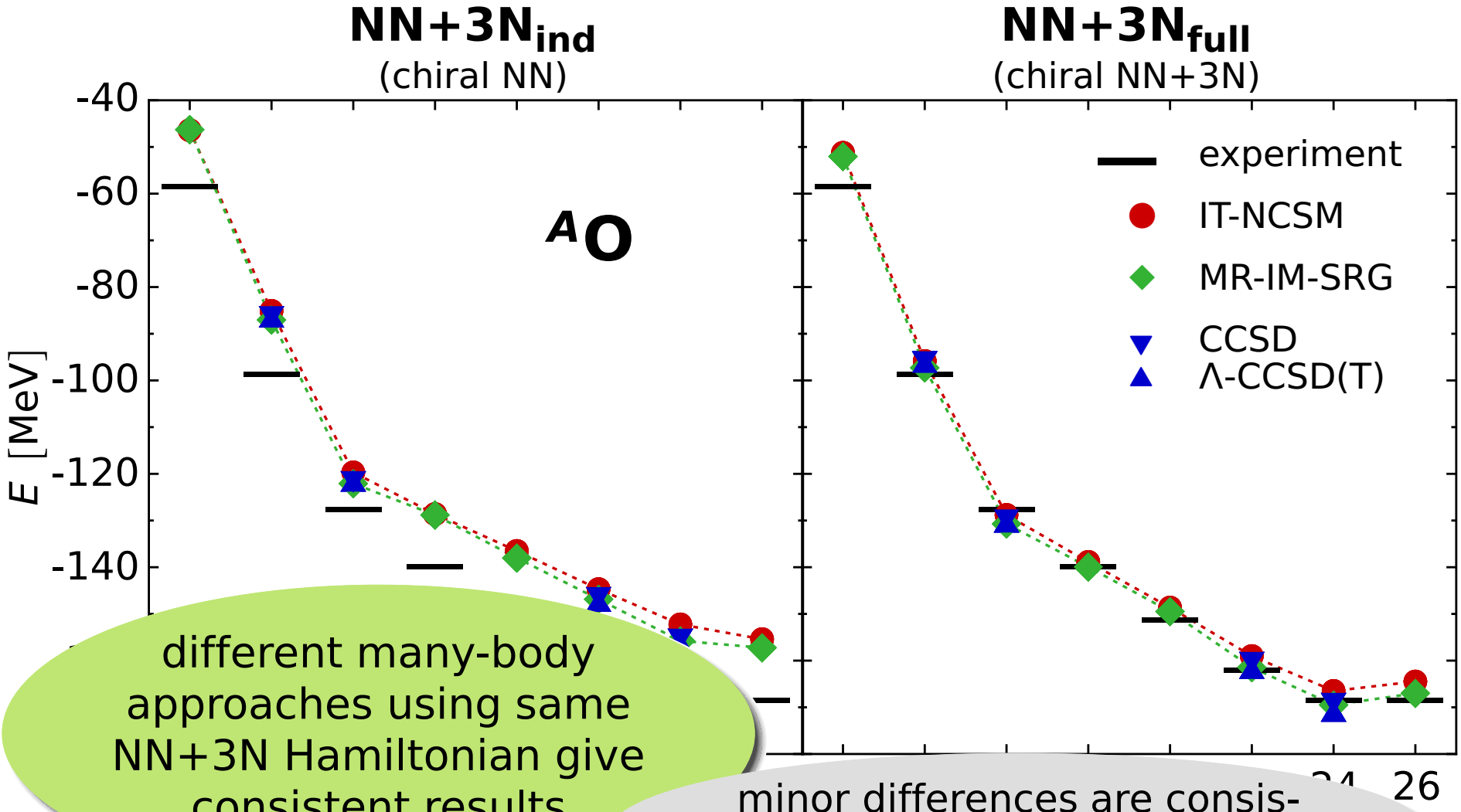
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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)

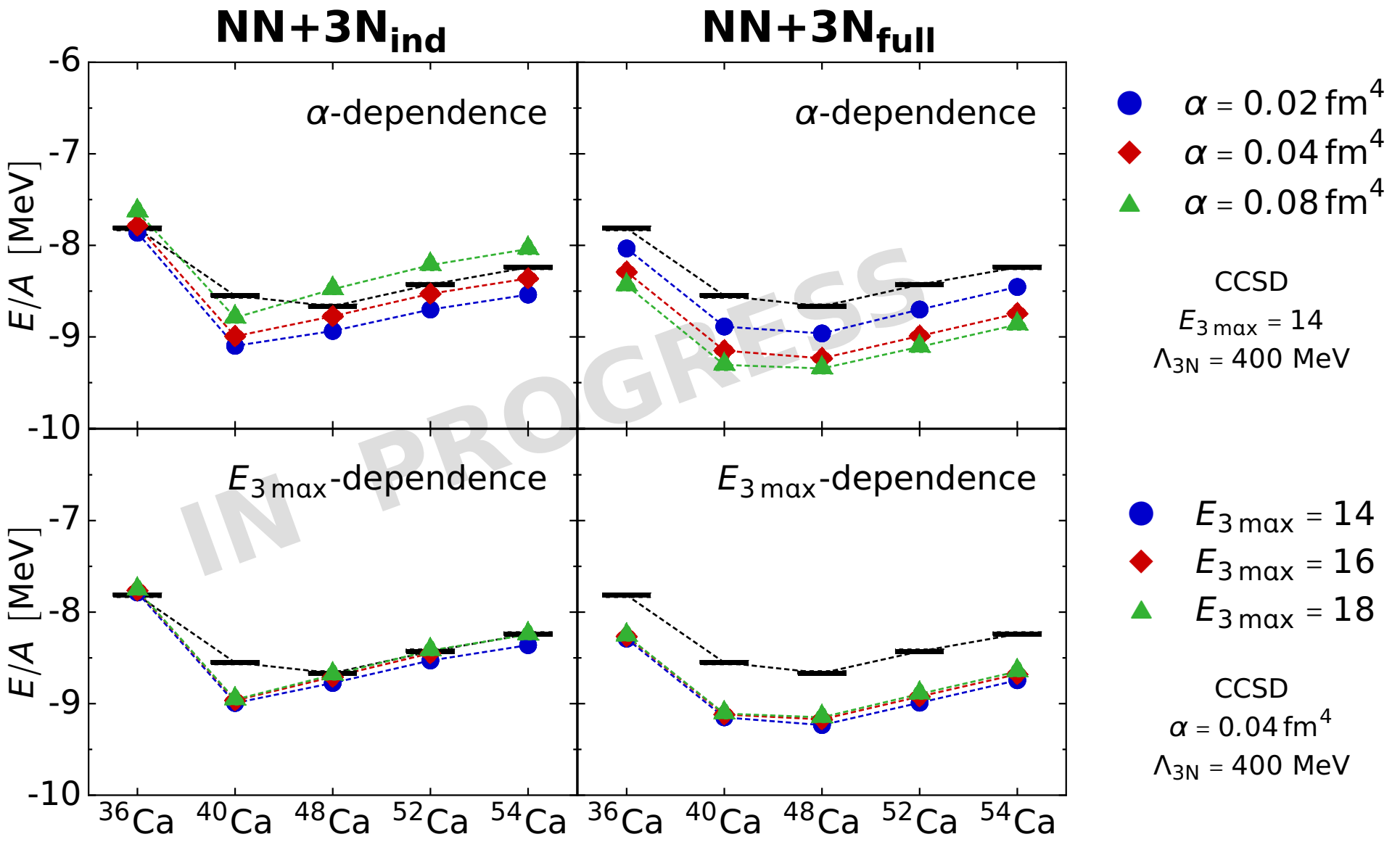


different many-body approaches using same NN+3N Hamiltonian give consistent results

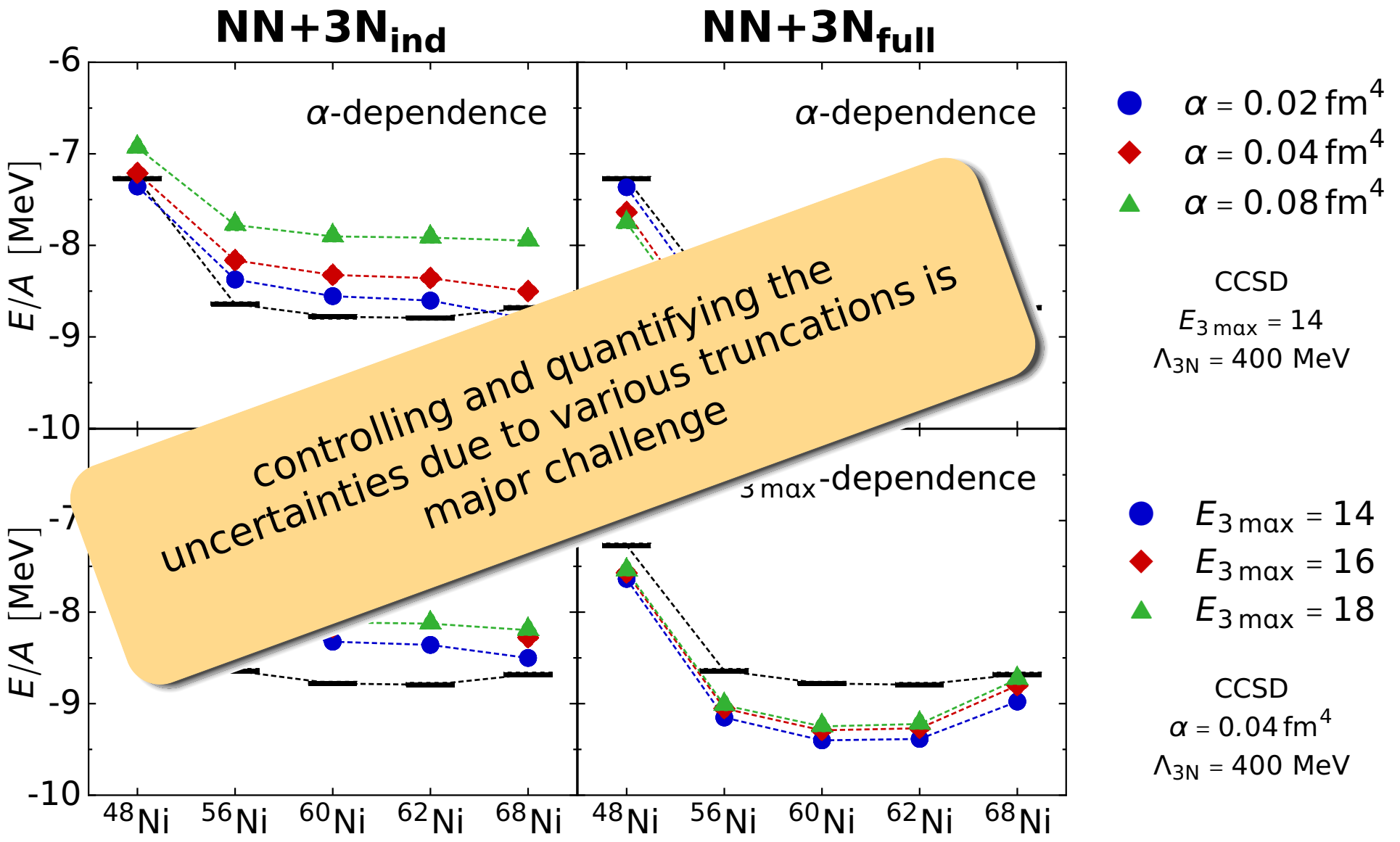
minor differences are consistent with uncertainty analysis

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^{4}$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

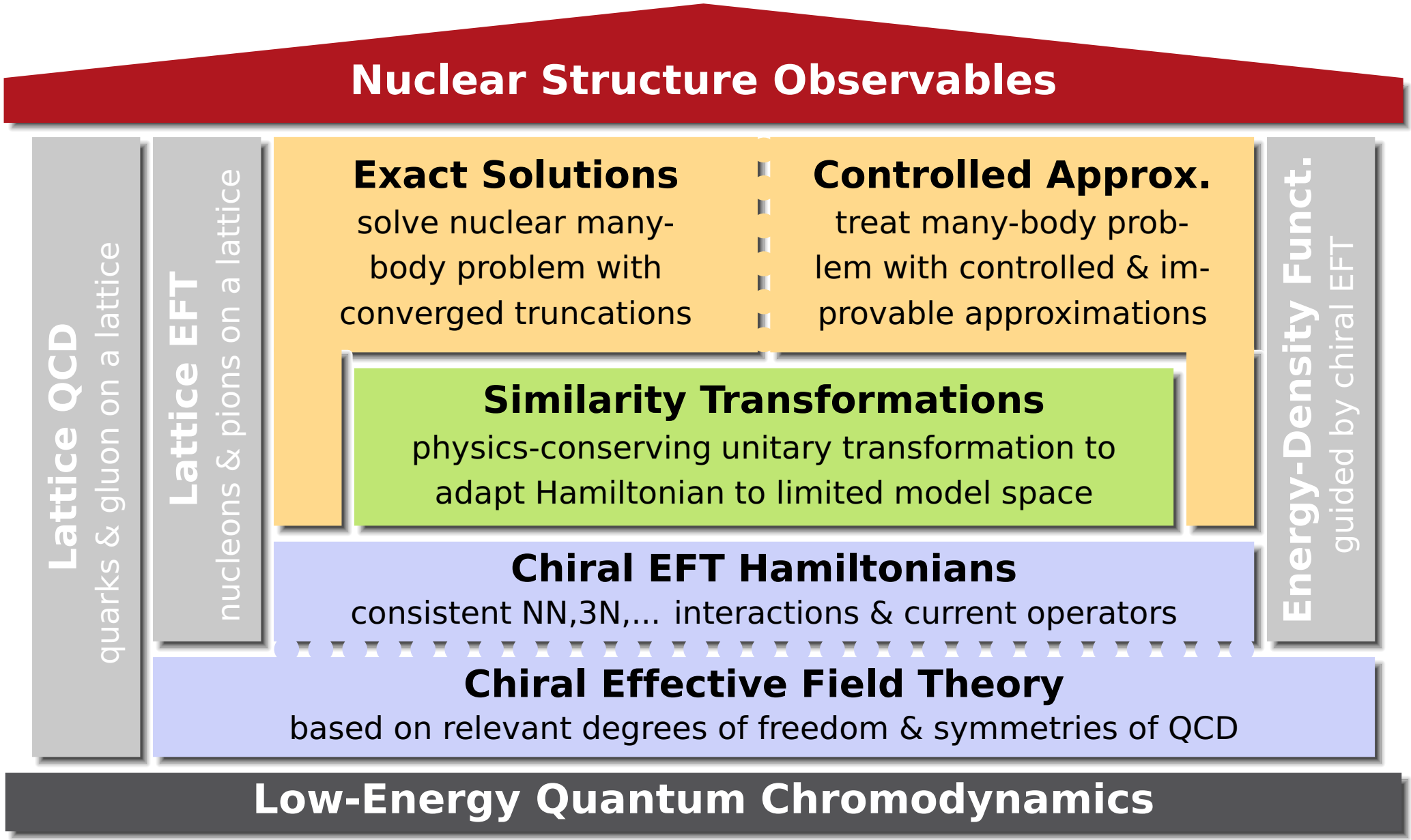
Next Step: Calcium Isotopes



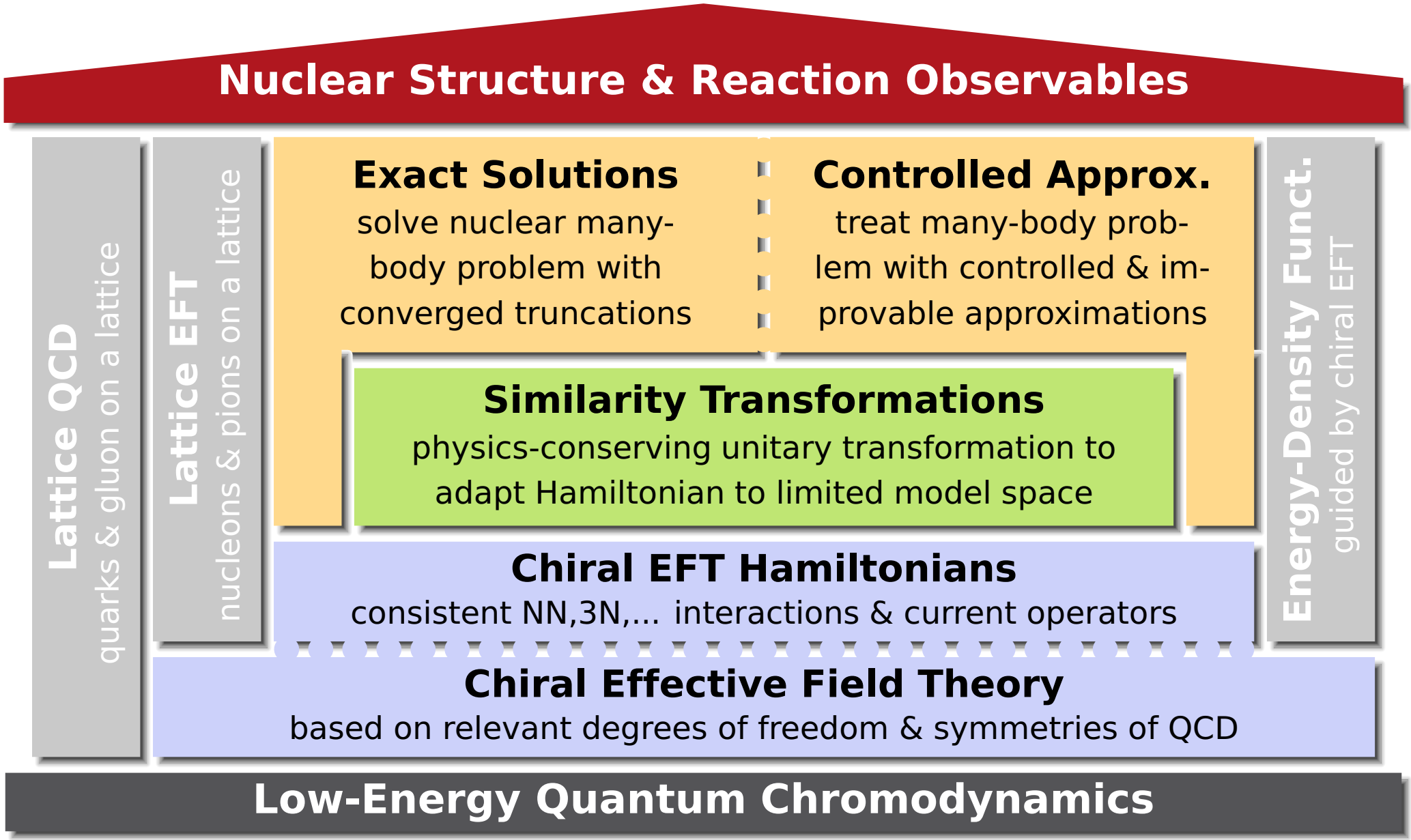
Next Step: Nickel Isotopes



Ab Initio Nuclear Structure



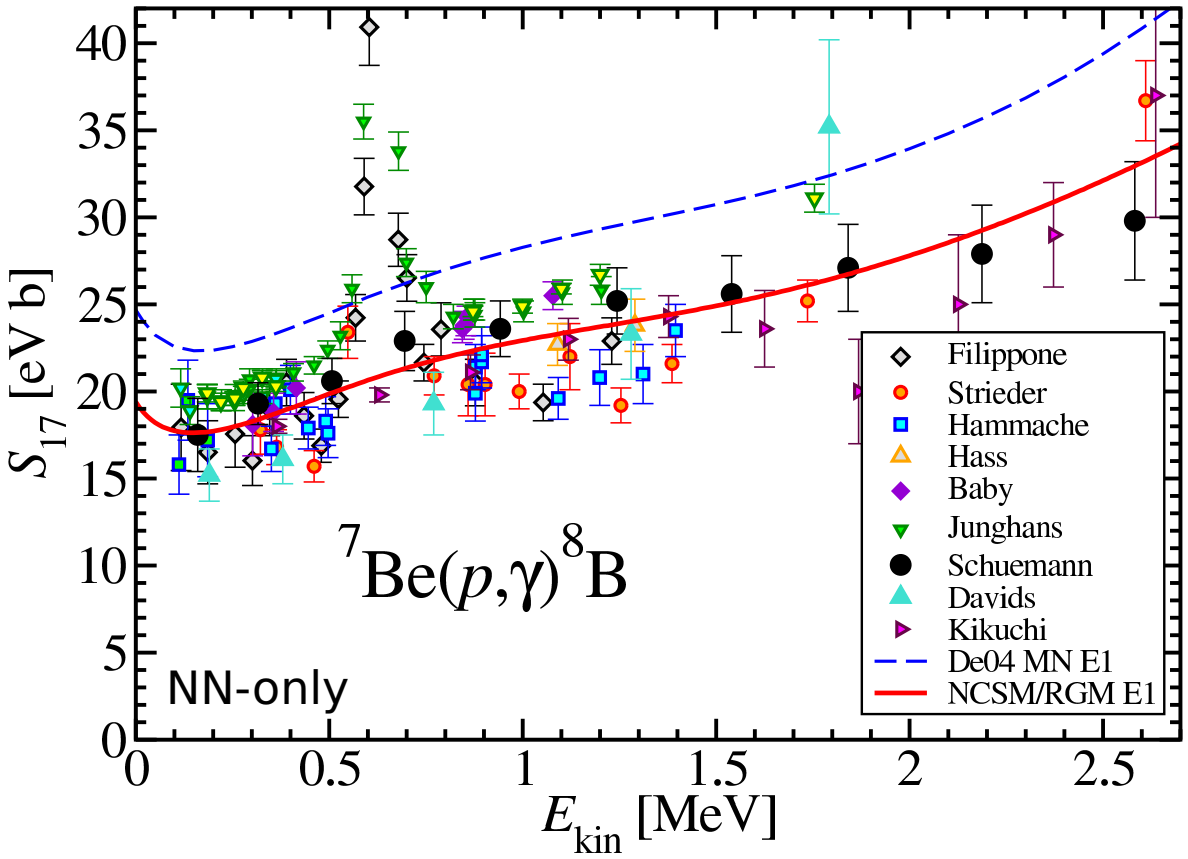
Ab Initio Nuclear Structure & Reactions



Bridge to Reaction Theory

Navratil, Quaglioni, Roth, Langhammer, Hupin

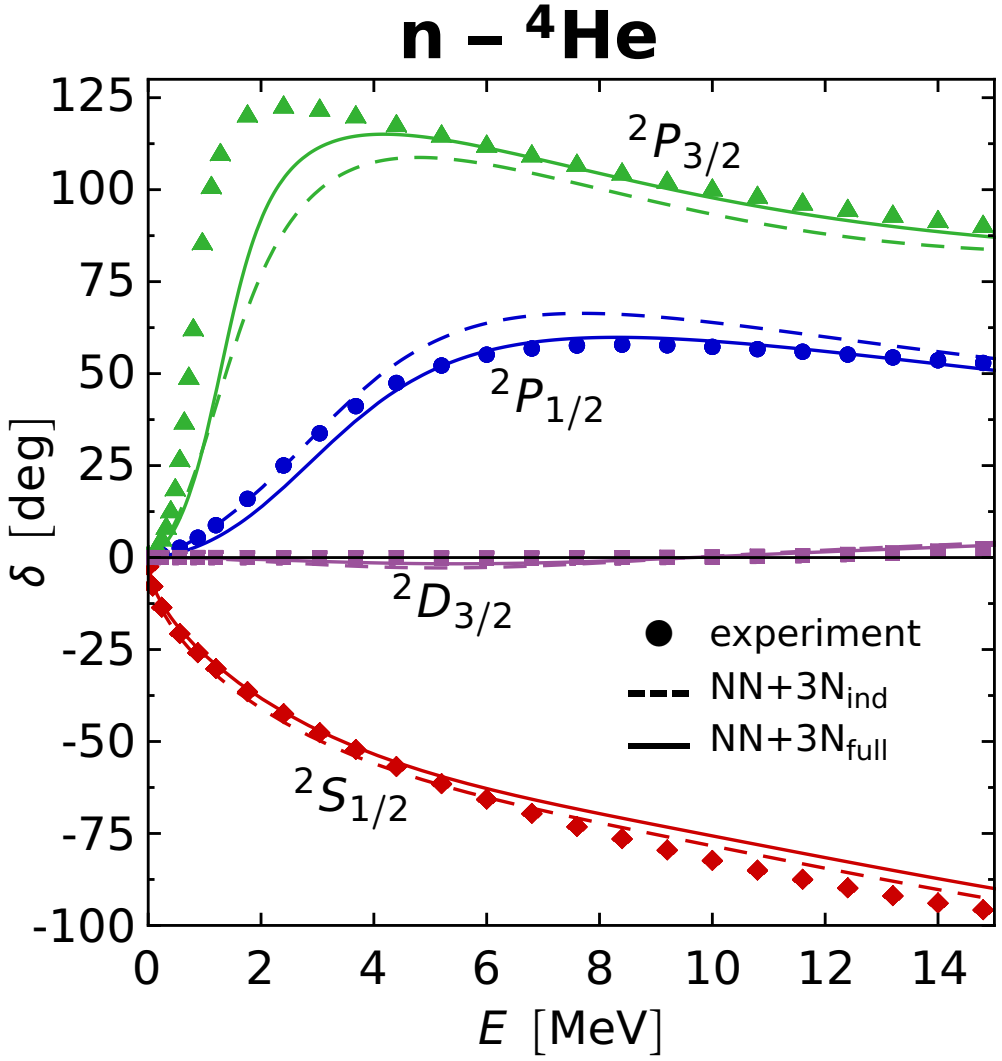
combine NCSM for bound states with Resonating Group Method for relative motion of sub-clusters



- astrophysical S-factor for proton capture on ^{7}Be
- IT-NCSM wave functions for ^{7}Be for up to 8 eigenstates
- solution of the RGM with kernels involving the full many-body information
- SRG-evolved chiral NN interaction with α adjusted to reproduce ^{8}B energy relative to threshold

Ab Initio Reactions with Chiral 3N

Hupin, Langhammer, Navratil, Quaglioni, Calci, Roth, arXiv:1308.2700



$N_{max} = 13$, $E_{3\,max} = 14$, $\hbar\Omega = 20$ MeV
including 6 excited states of ^{4}He

- inclusion of **full 3N interactions** into NCSM/RGM
- new computational scheme for evaluating 3N kernels
- phase shifts for n-^{4}He show **increase of spin-orbit splittings** by initial 3N
- ready for scattering calculations for **p-shell nuclei** and **NCSM with Continuum**

New Horizons...

- **nuclear structure theory connected to QCD via chiral EFT**
  - chiral EFT as universal, controlled and improvable starting point
  - consistent and optimized interactions at N2LO, N3LO,...
  - consistent similarity transformation of Hamiltonian and observables

- **innovations in ab initio many-body theory**
  - consistent inclusion of 3N (and 4N) interactions
  - precision structure and spectroscopy in p- and sd-shell (IT-NCSM,...)
  - access to the medium-mass regime (CC, IM-SRG,...)
  - extension to ab initio hyper-nuclear structure
  - bridge to reaction theory (NCSM/RGM, NCSMC)
  - uncertainty quantification, error propagation, feedback cycle

- **many exciting applications ahead...**

Epilogue

thanks to my group & my collaborators

- **S. Binder**, **A. Calci**, S. Fischer, E. Gebrerufael, H. Spiess, **J. Langhammer**, S. Reinhardt, 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
  IPN Orsay, F
- C. Forssén
  Chalmers University, Sweden
- H. Feldmeier, T. Neff
  GSI Helmholtzzentrum

JUROPA — JÜLICH FORSCHUNGSZENTRUM
LOEWE-CSC — 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