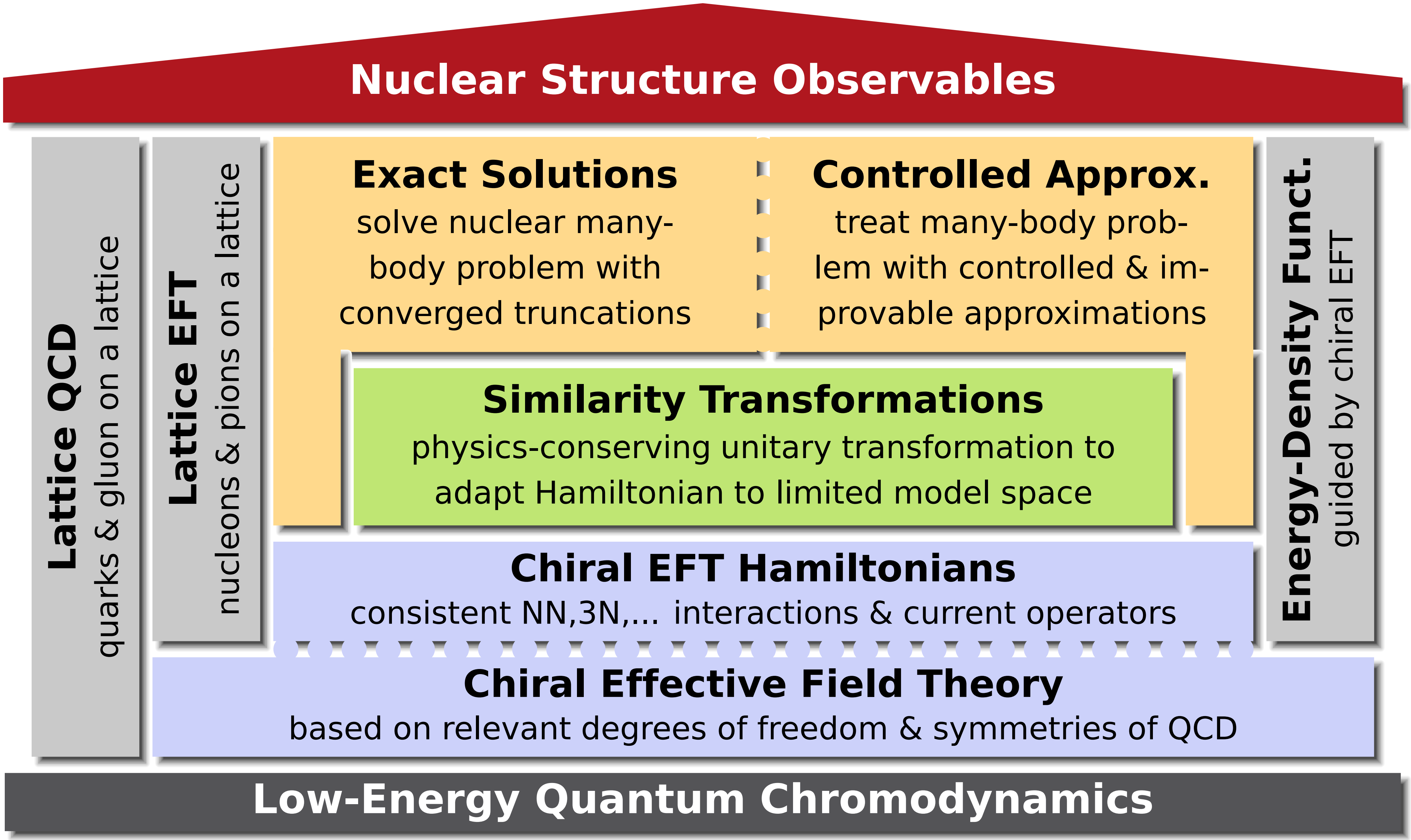
New Horizons in Ab Initio Nuclear Structure Theory

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Nuclear Structure



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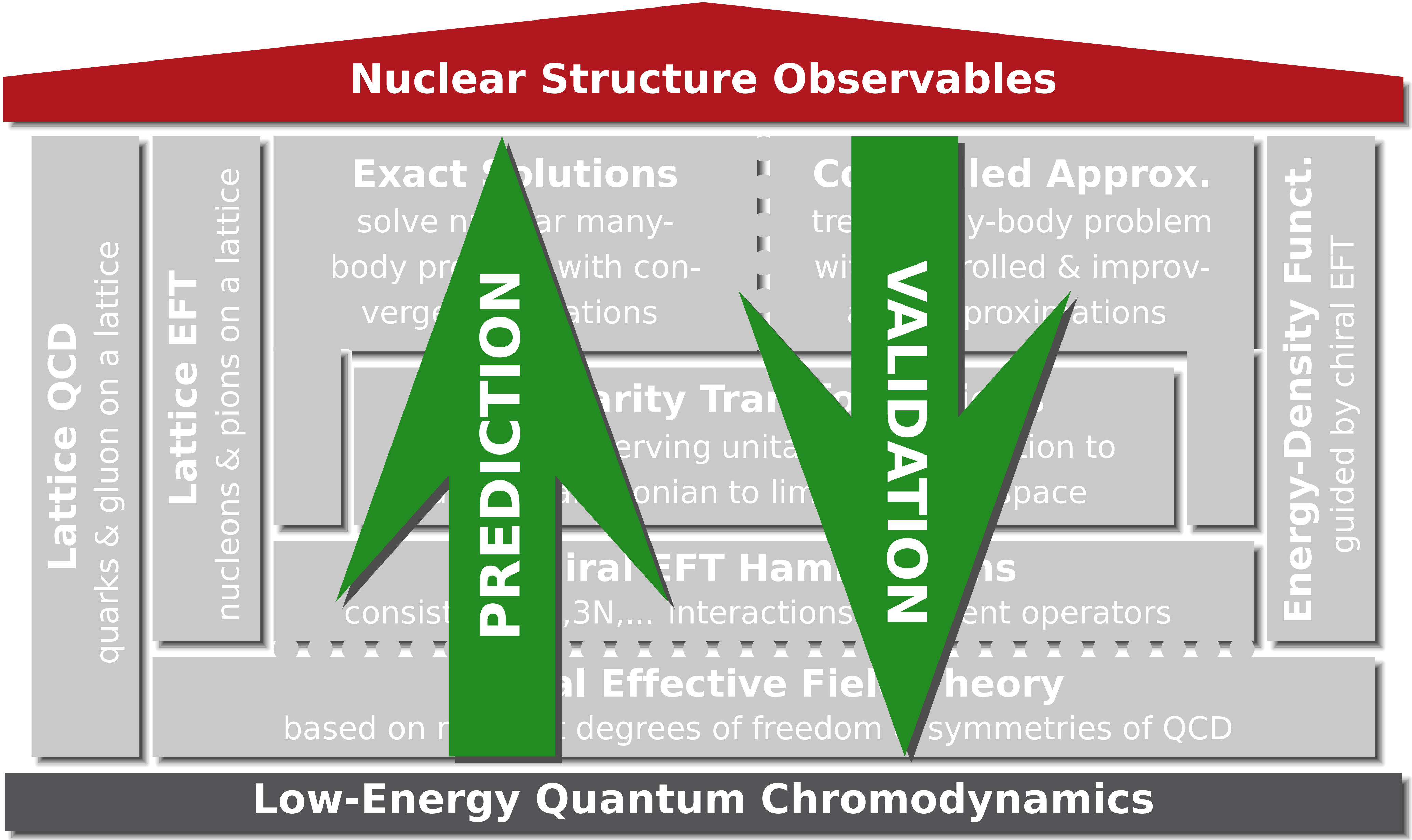

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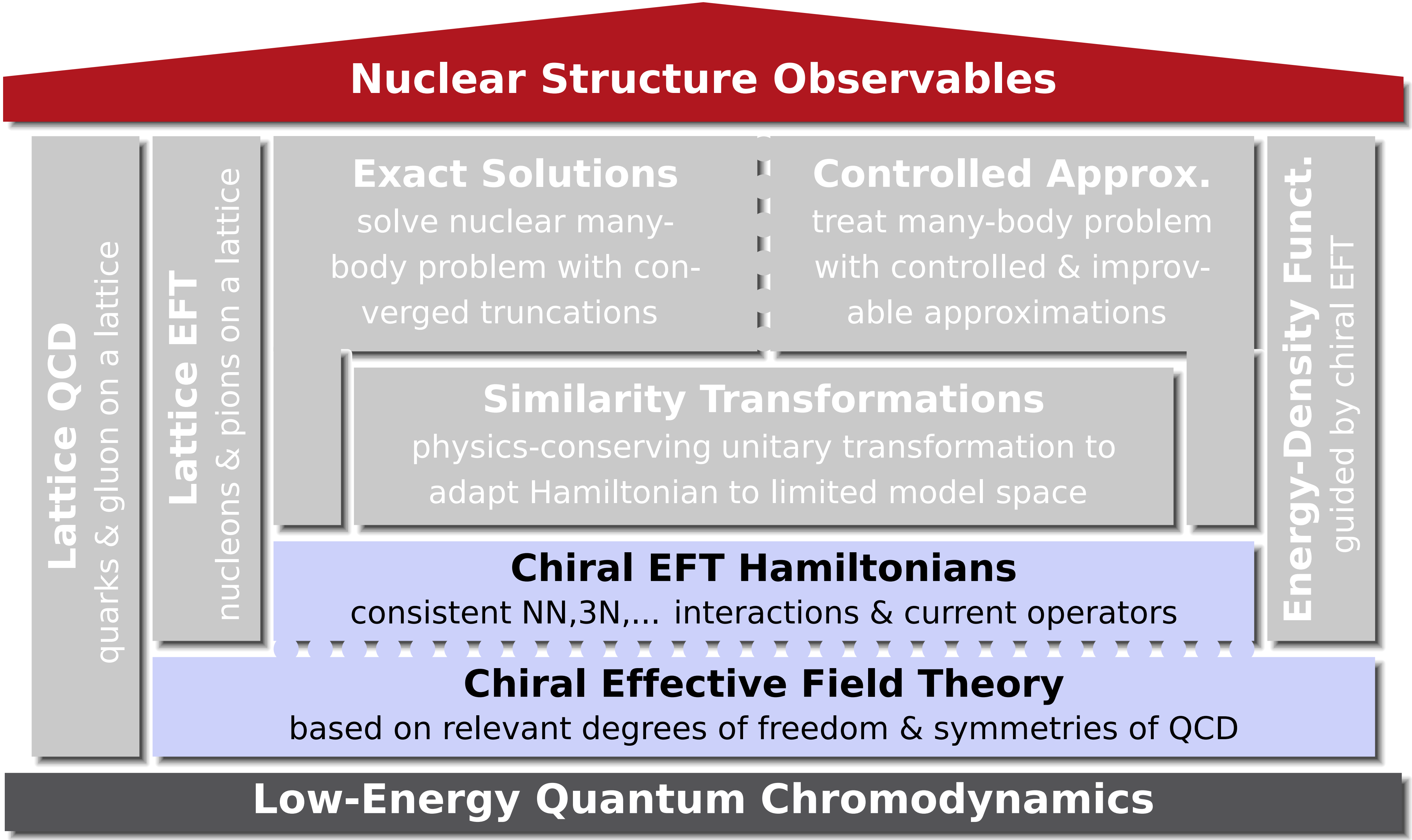
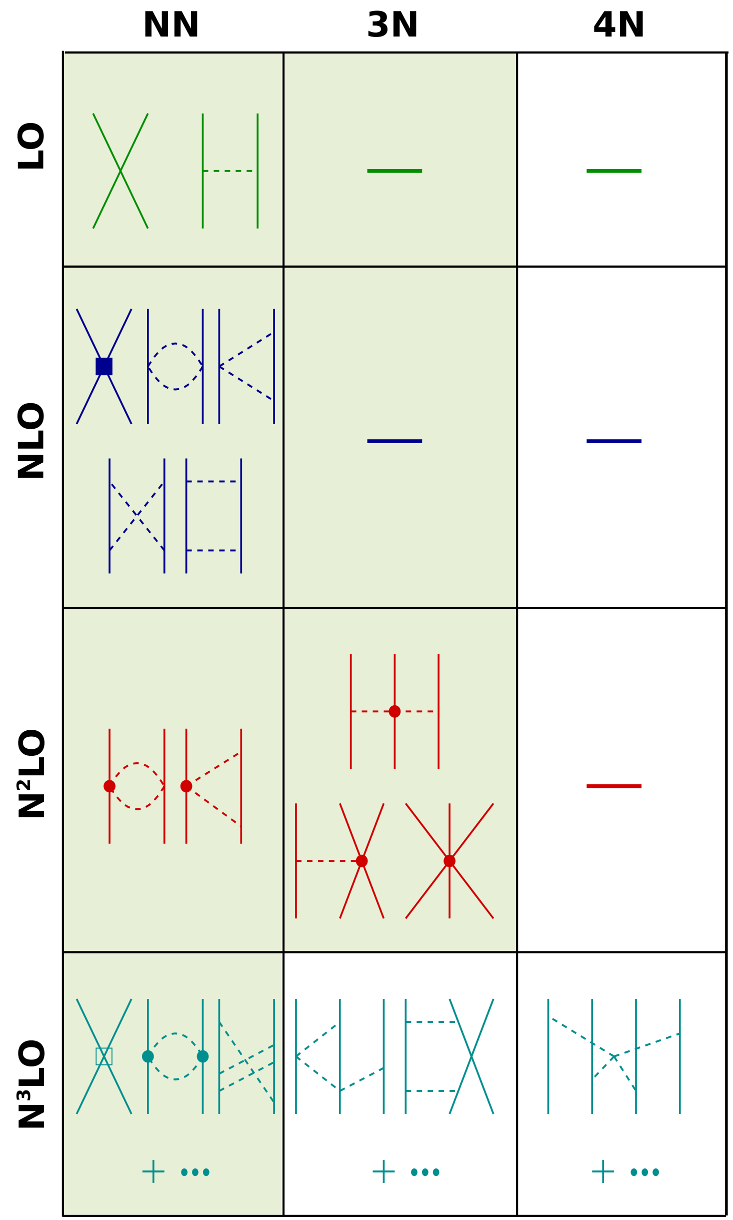


Nuclear Interactions from Chiral EFT

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

- **chiral EFT background**: talks by Machleidt & Epelbaum
- **standard Hamiltonian**:
  - NN at N3LO:
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N2LO:
    Navrátil, A=3 fit, 500 MeV cutoff
- **alternatives**:
  - modified 3N interaction at N2LO (cutoff, LECs)
  - consistent Hamiltonians at N2LO (NN: Epelbaum, POUNDERs-opt.)
  - consistent Hamiltonians at N3LO
  - Δ-full chiral EFT, YN interaction,...



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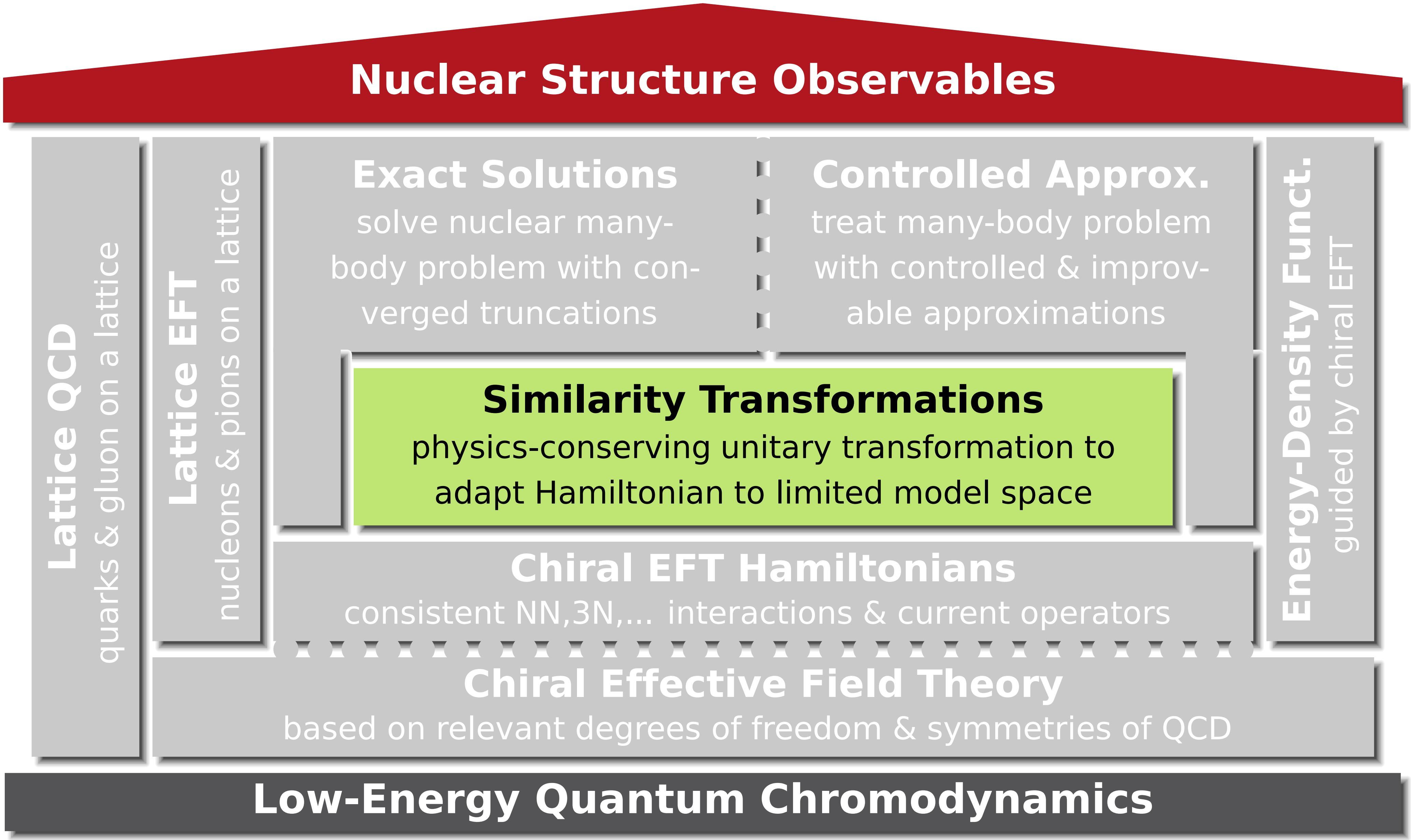


Similarity Renormalization Group

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

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

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hamil

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

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

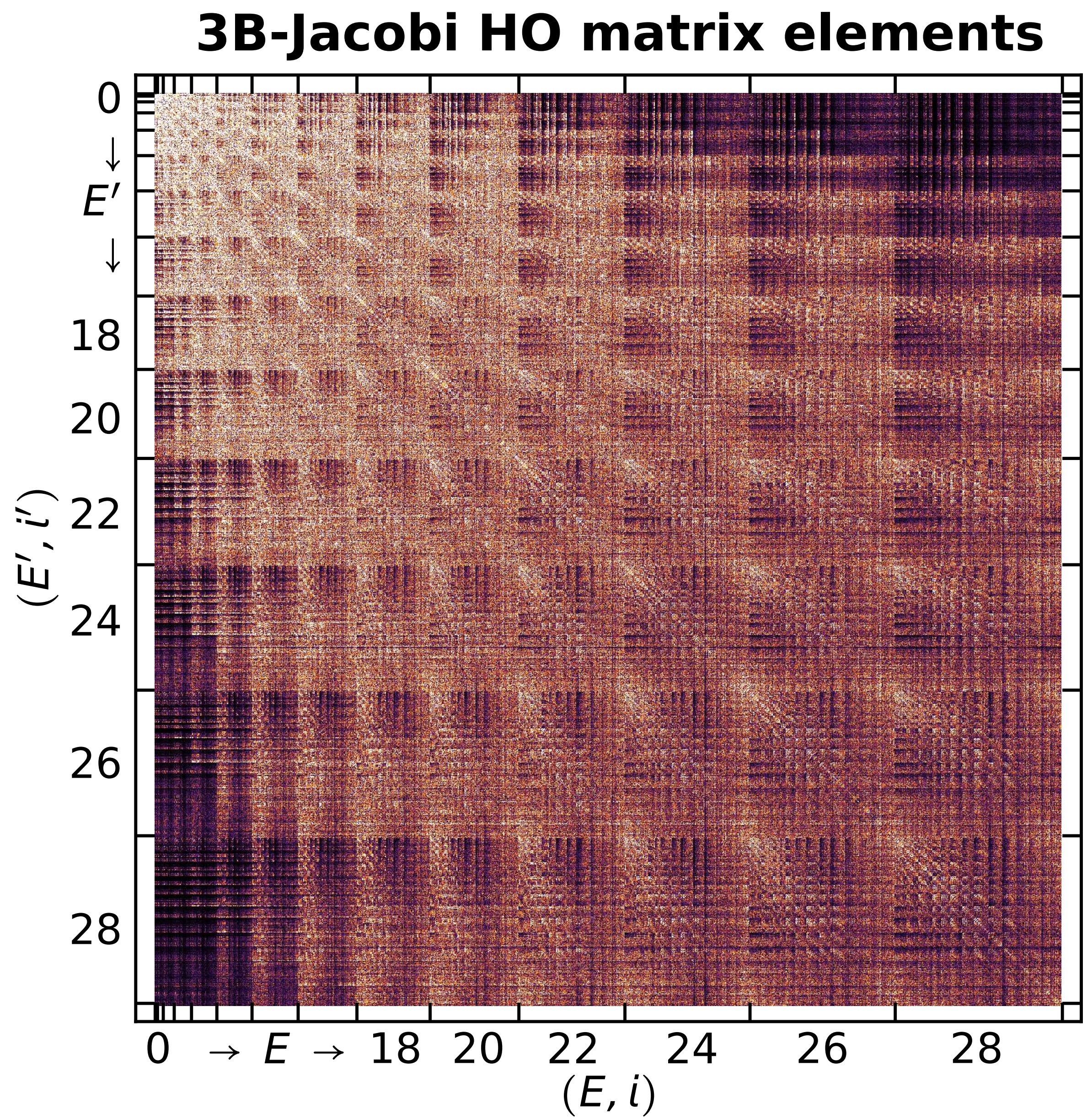
- **evolution equations** for H_α and U

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

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

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

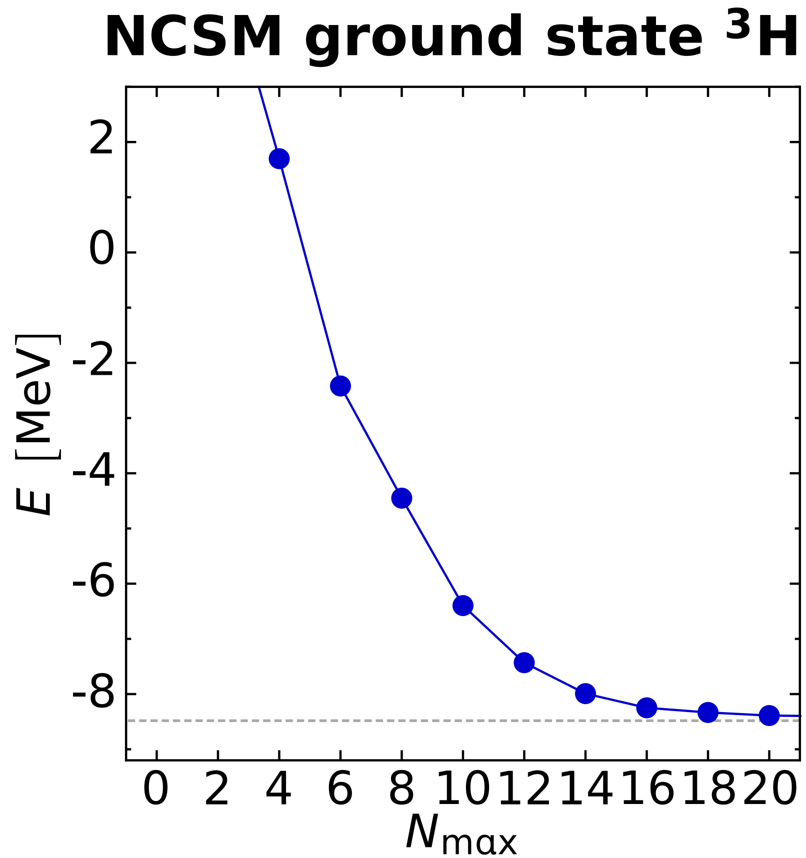
SRG Evolution in Three-Body Space



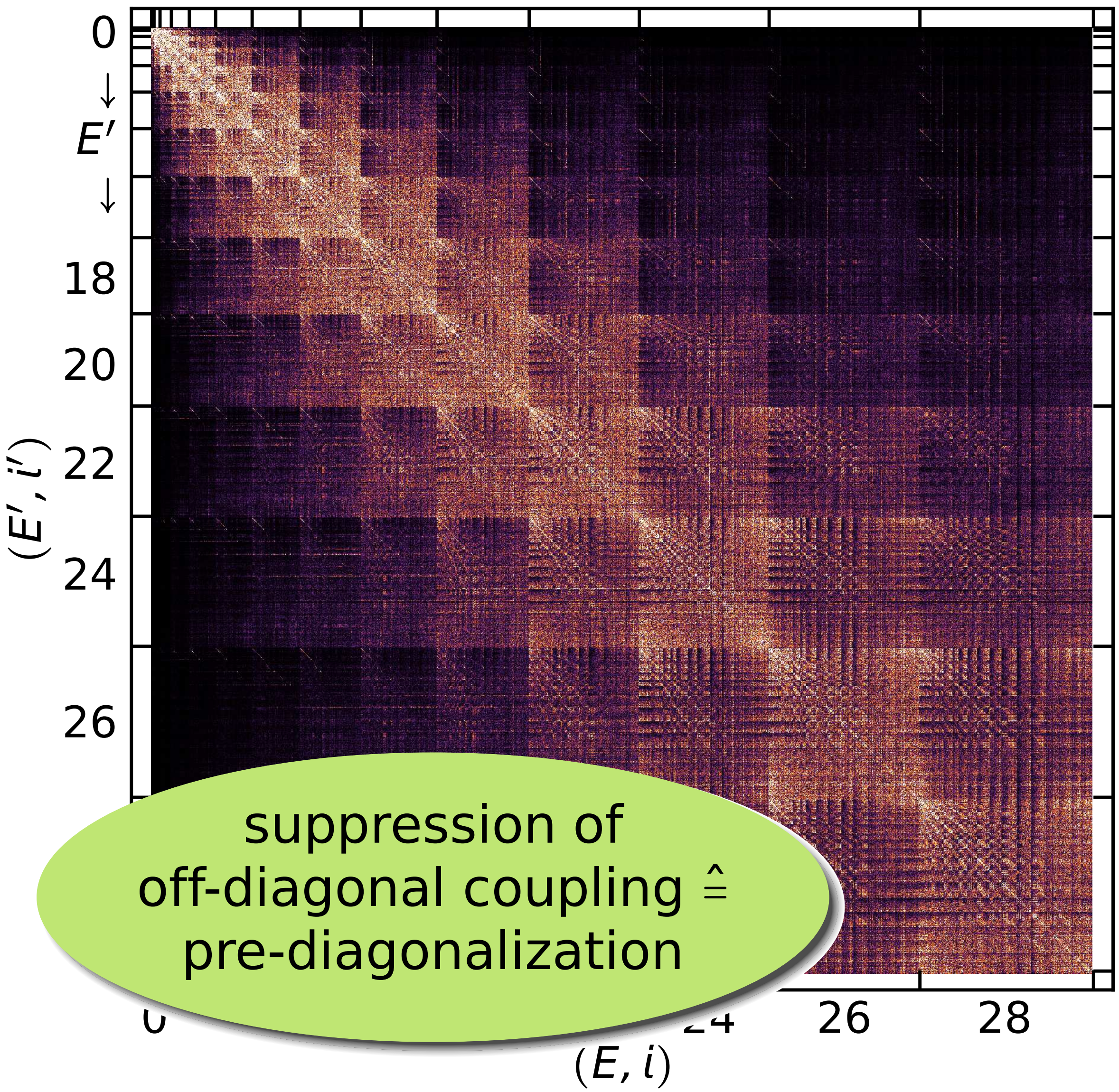
$\alpha = 0.000\,\text{fm}^4$

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

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



SRG Evolution in Three-Body Space

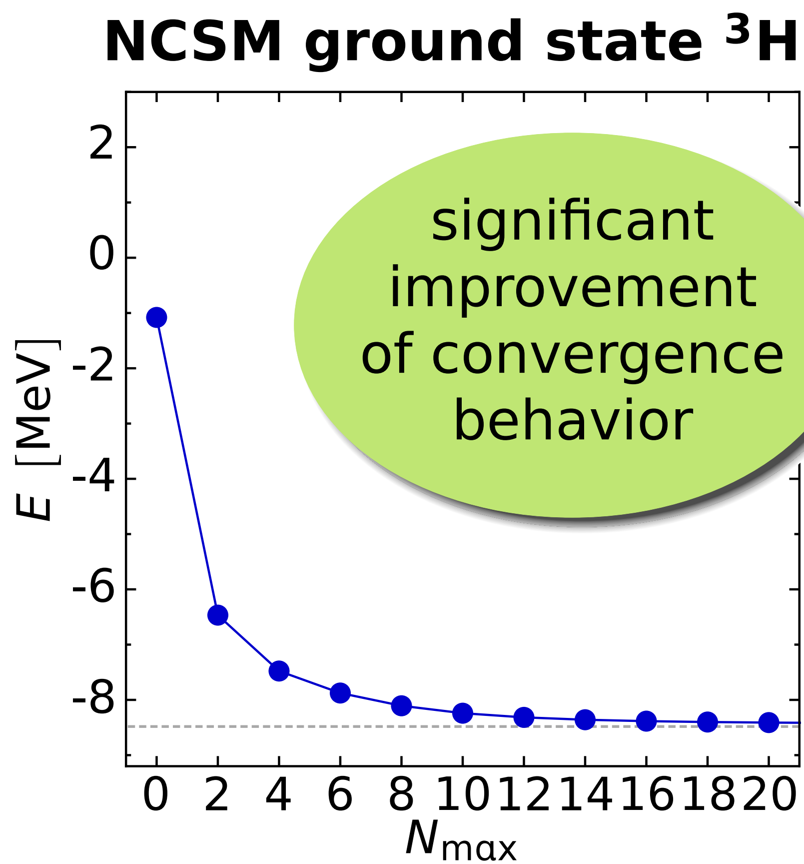


suppression of
off-diagonal coupling ≙
pre-diagonalization

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

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

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



significant
improvement
of convergence
behavior

Hamiltonian in *A*-Body Space

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

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + \dots$$

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

- flow-parameter 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

Nuclear Structure Observables

Lattice QCD
quarks & gluon on a lattice

Lattice EFT
nucleons & pions on a lattice

Exact Solutions
solve nuclear many-body problem with converged truncations

Controlled Approx.
treat many-body problem with controlled & improvable approximations

Energy-Density Funct.
guided by chiral EFT

Similarity Transformations
physics-conserving unitary transformation to adapt Hamiltonian to limited model space

Chiral EFT Hamiltonians
consistent NN,3N,... interactions & current operators

Chiral Effective Field Theory
based on relevant degrees of freedom & symmetries of QCD

Low-Energy Quantum Chromodynamics

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 $N_{\mathrm{max}}\hbar\Omega$
- 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

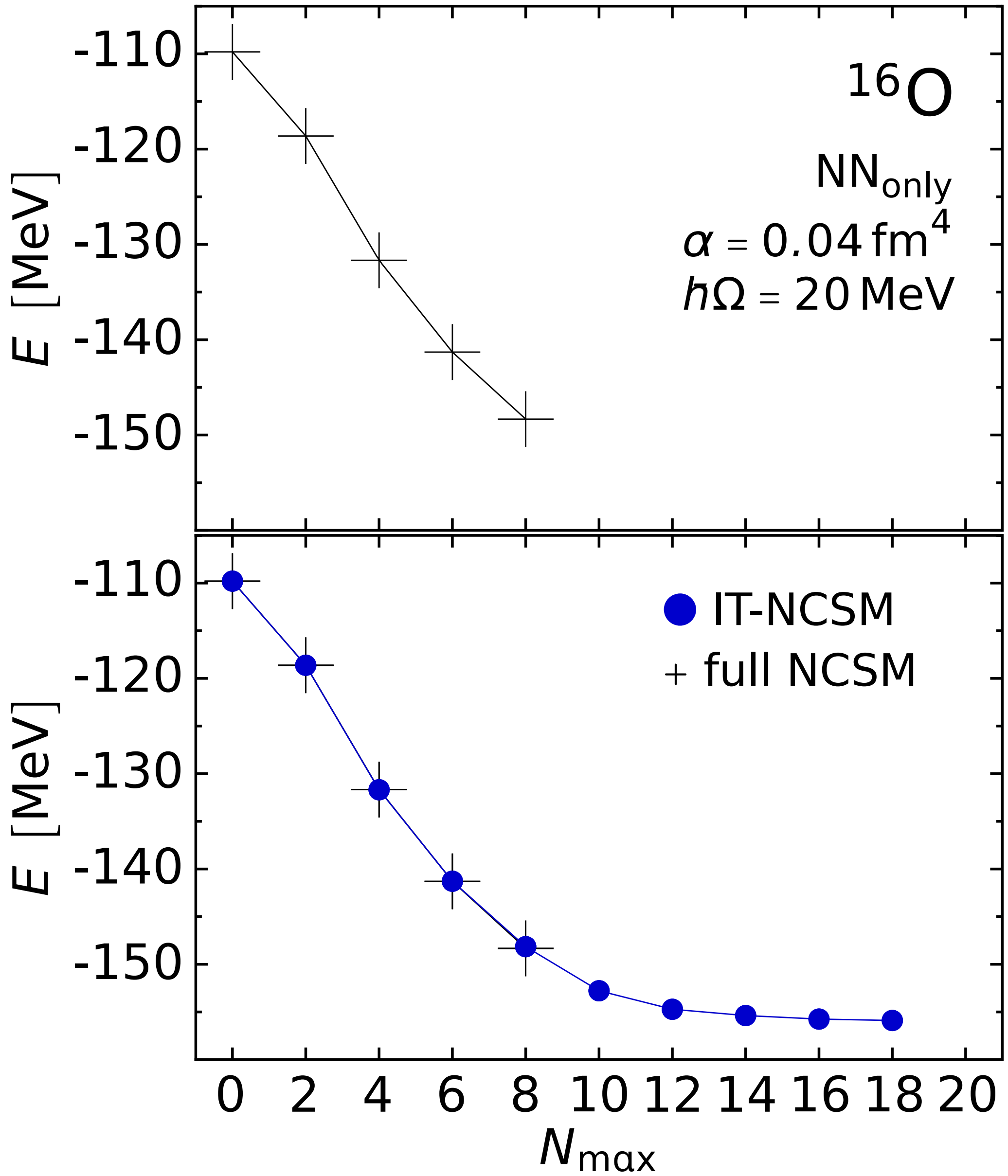
Importance Truncated NCSM

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})

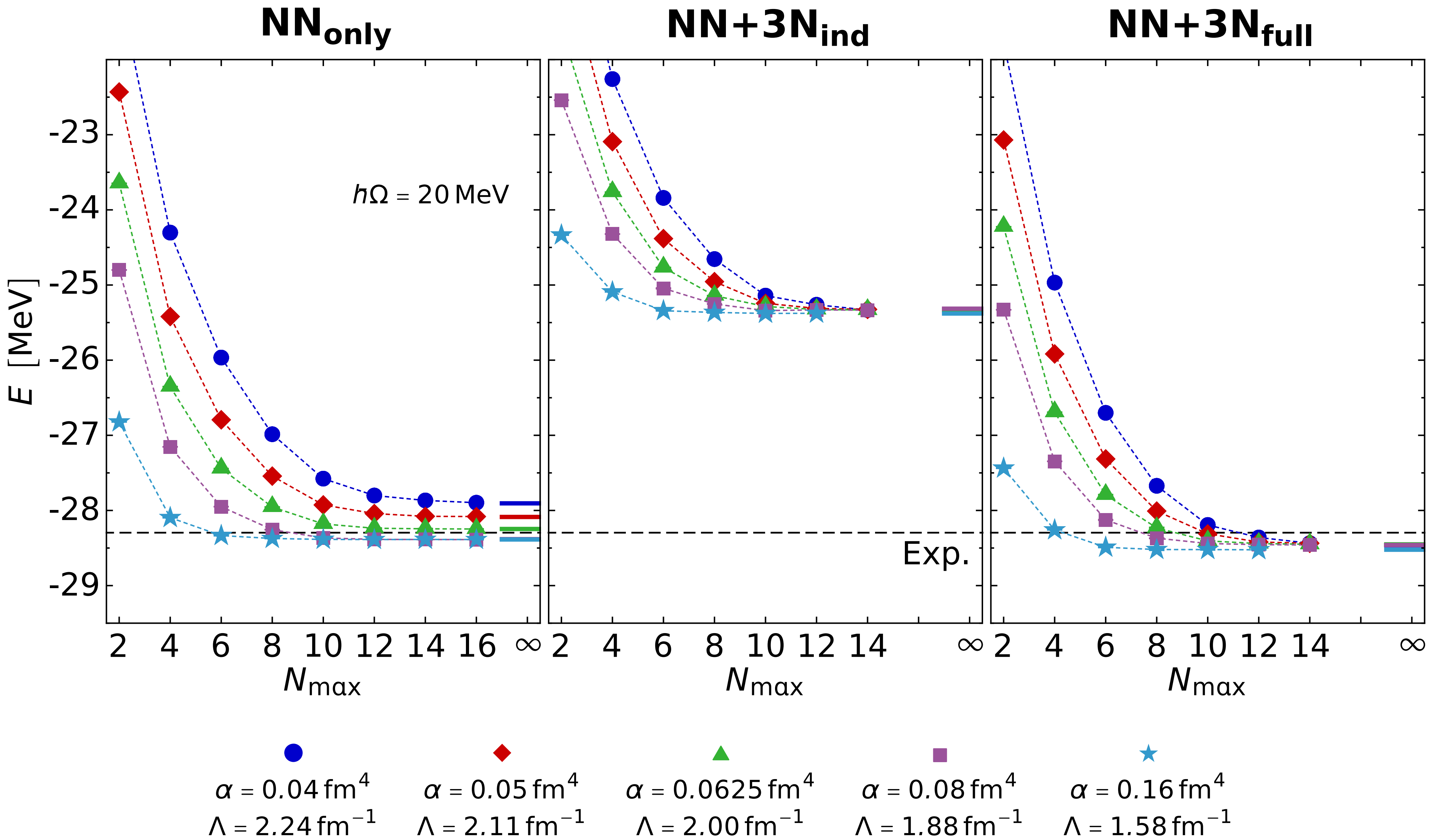
Importance Truncation

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



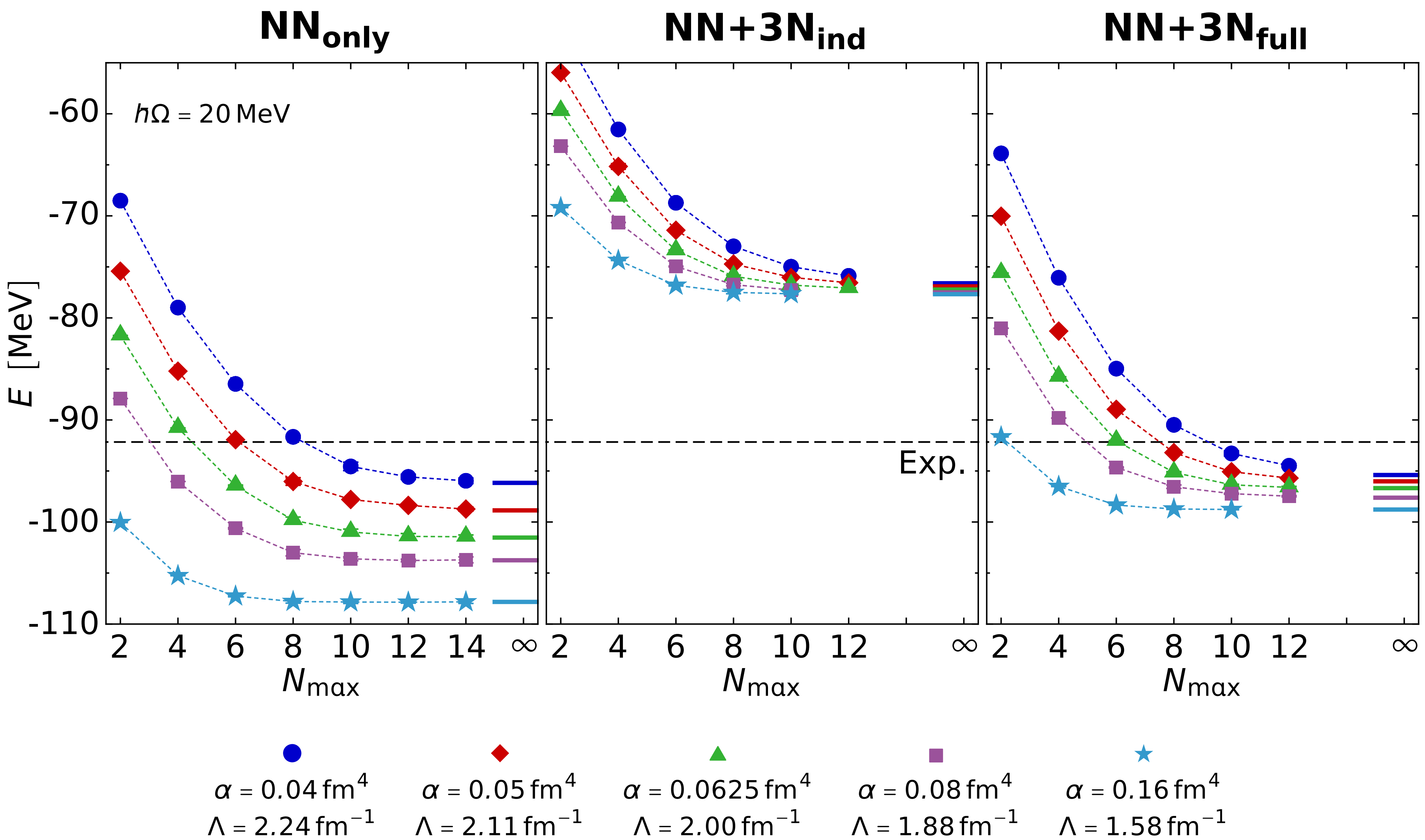
^{4}He: Ground-State Energies

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



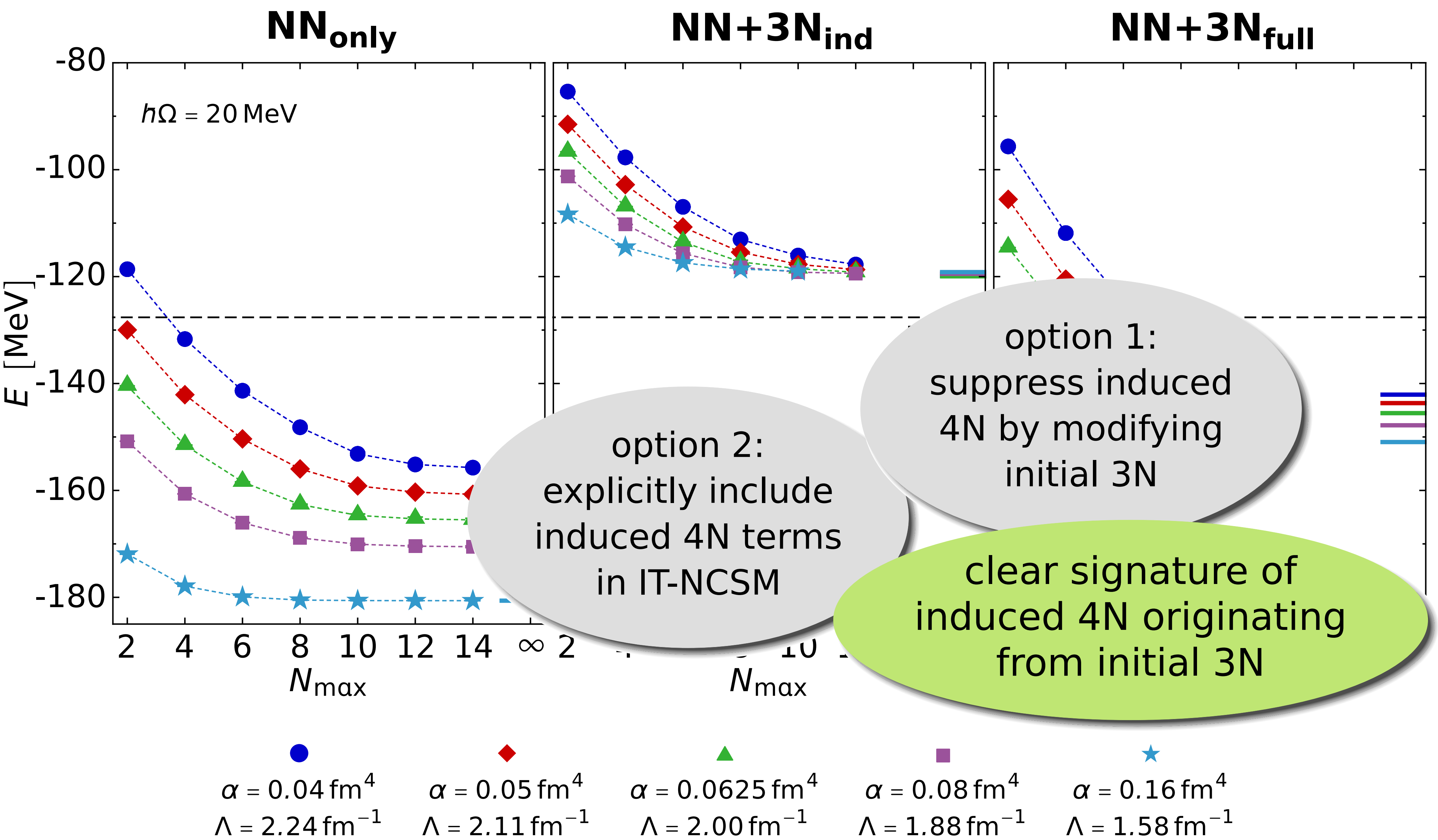
^{12}C: Ground-State Energies

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

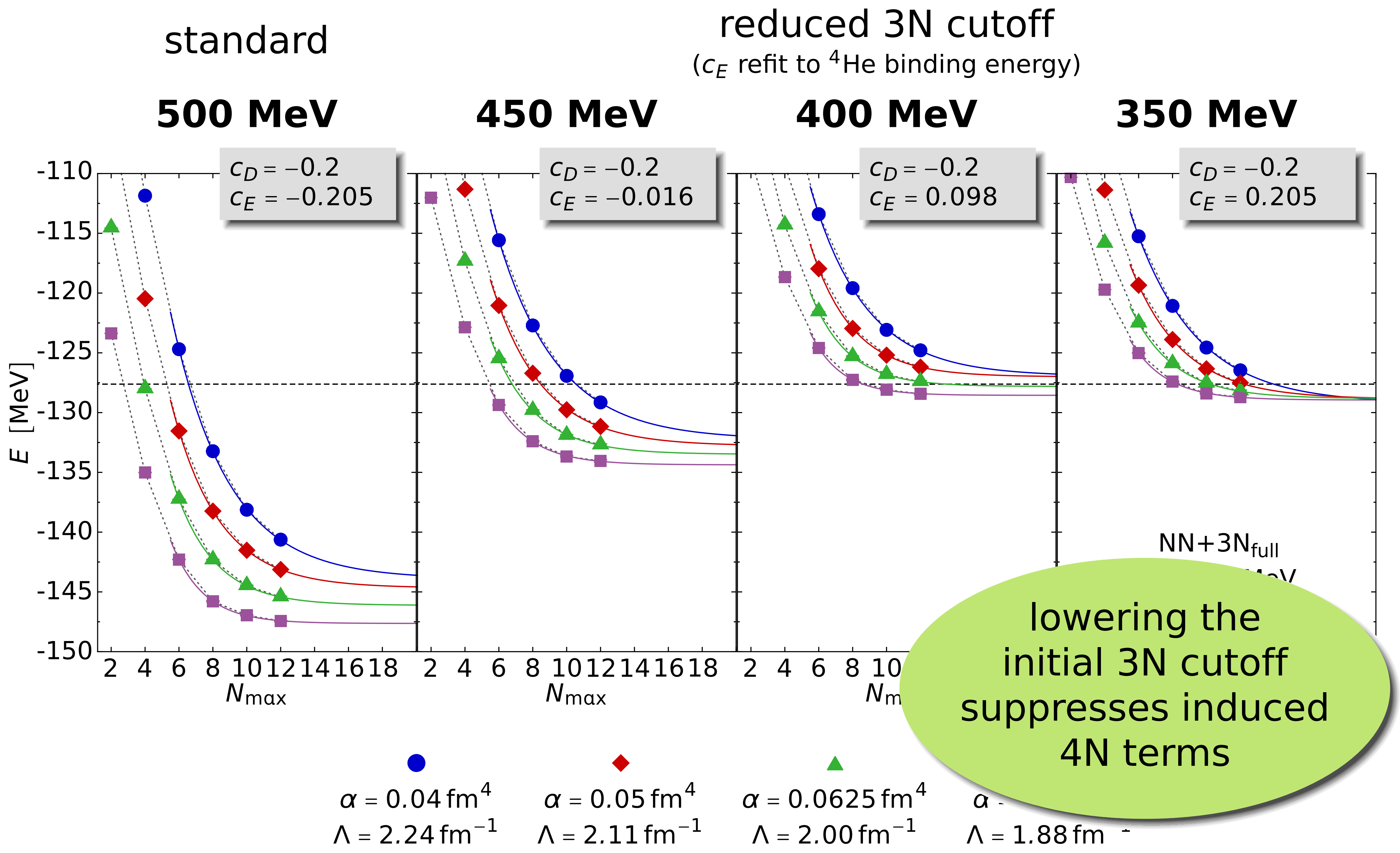


^{16}O: Ground-State Energies

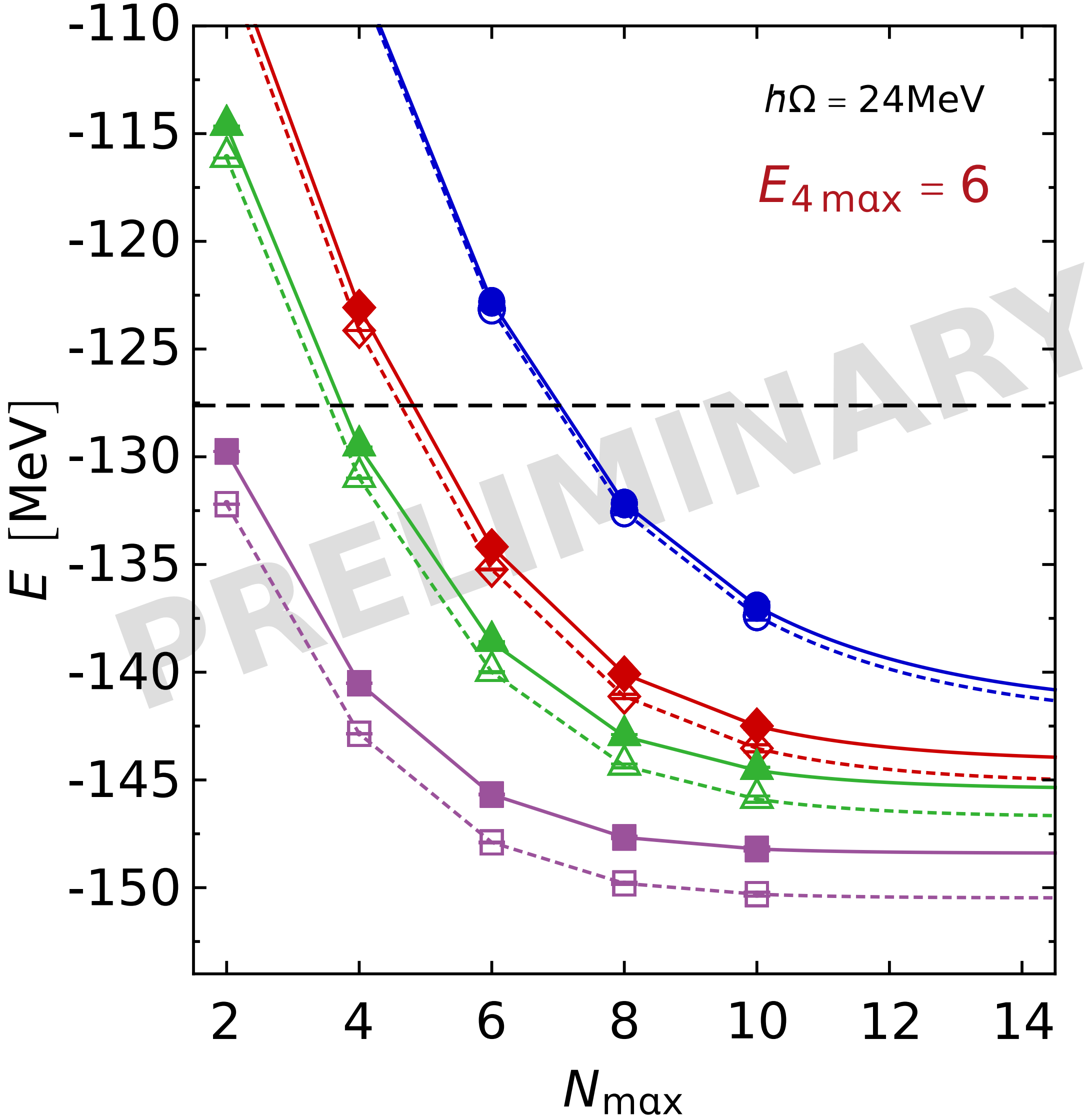
Roth, et al; PRL 107, 072501 (2011)



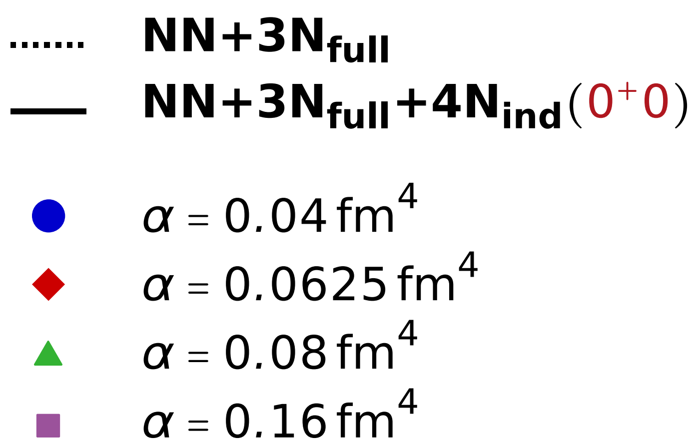
^{16}O: Lowering the Initial 3N Cutoff



^{16}O: Explicit Inclusion of Induced 4N



- induced 4N from SRG evolution in four-body Jacobi-HO
- transformation to *m*- or *JT*-scheme 4N matrix elements
- explicit 4N terms in IT-NCSM



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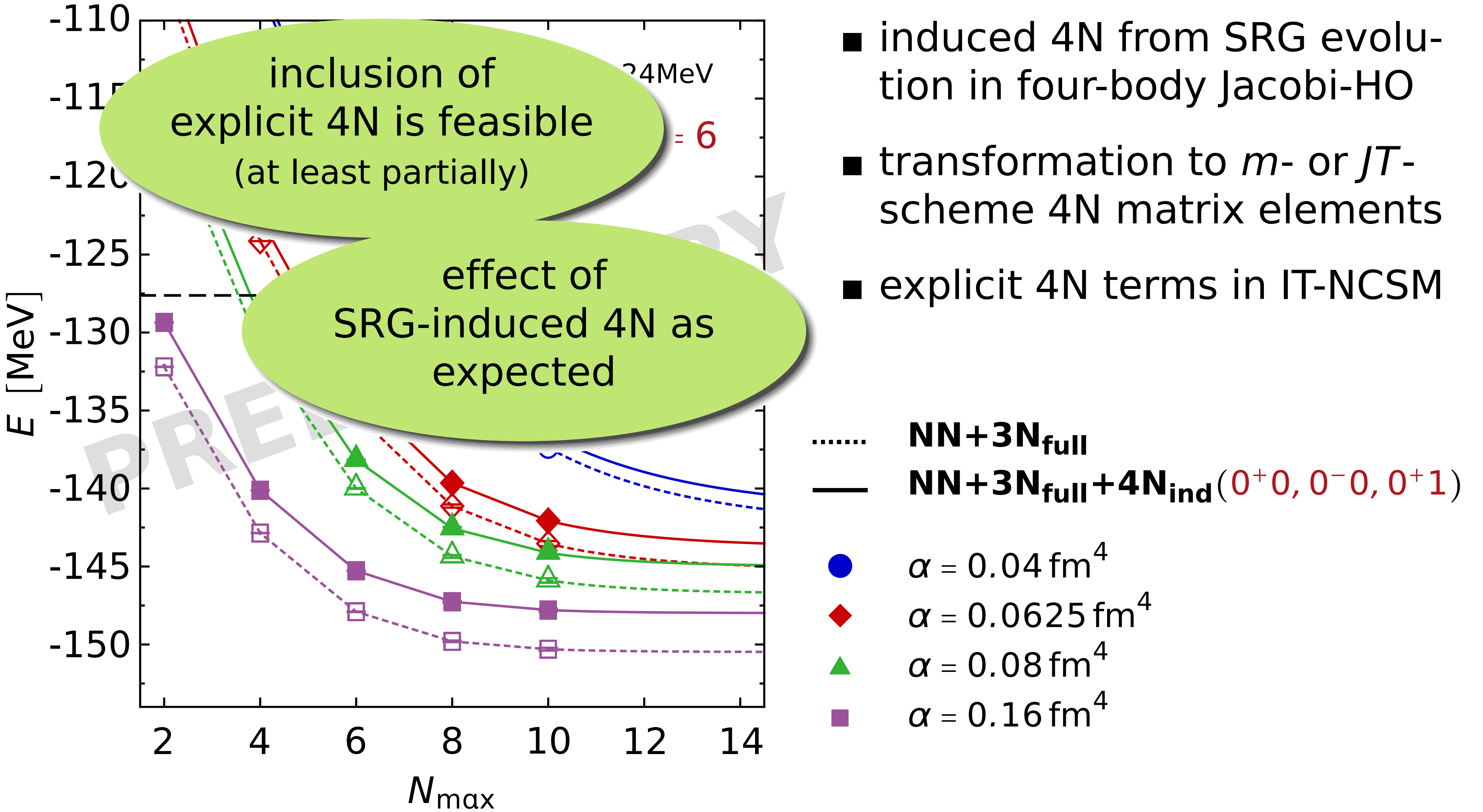

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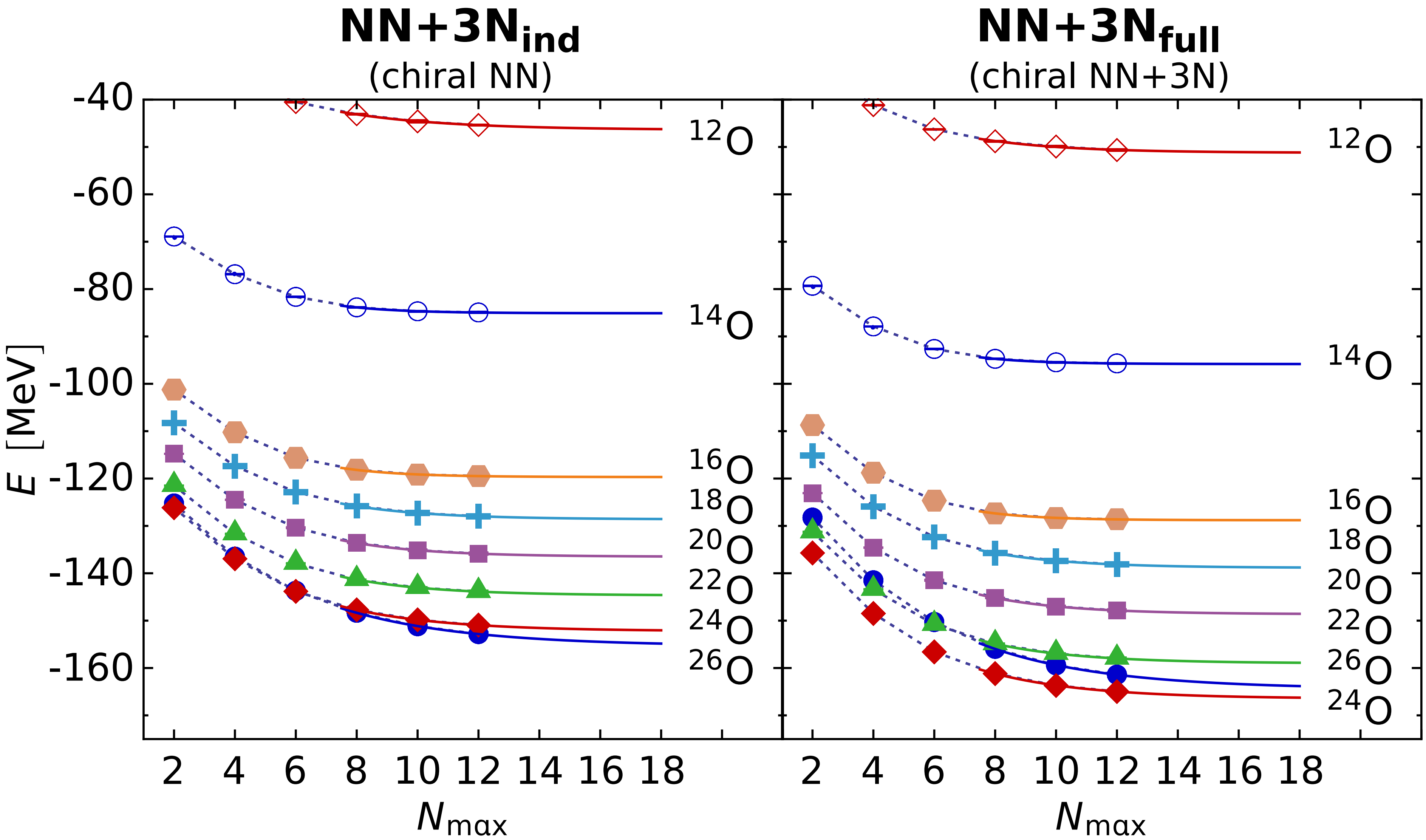
Ground States of Oxygen Isotopes

Hergert et al., PRL (2013); arXiv:1302.7294



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

Ground States of Oxygen Isotopes

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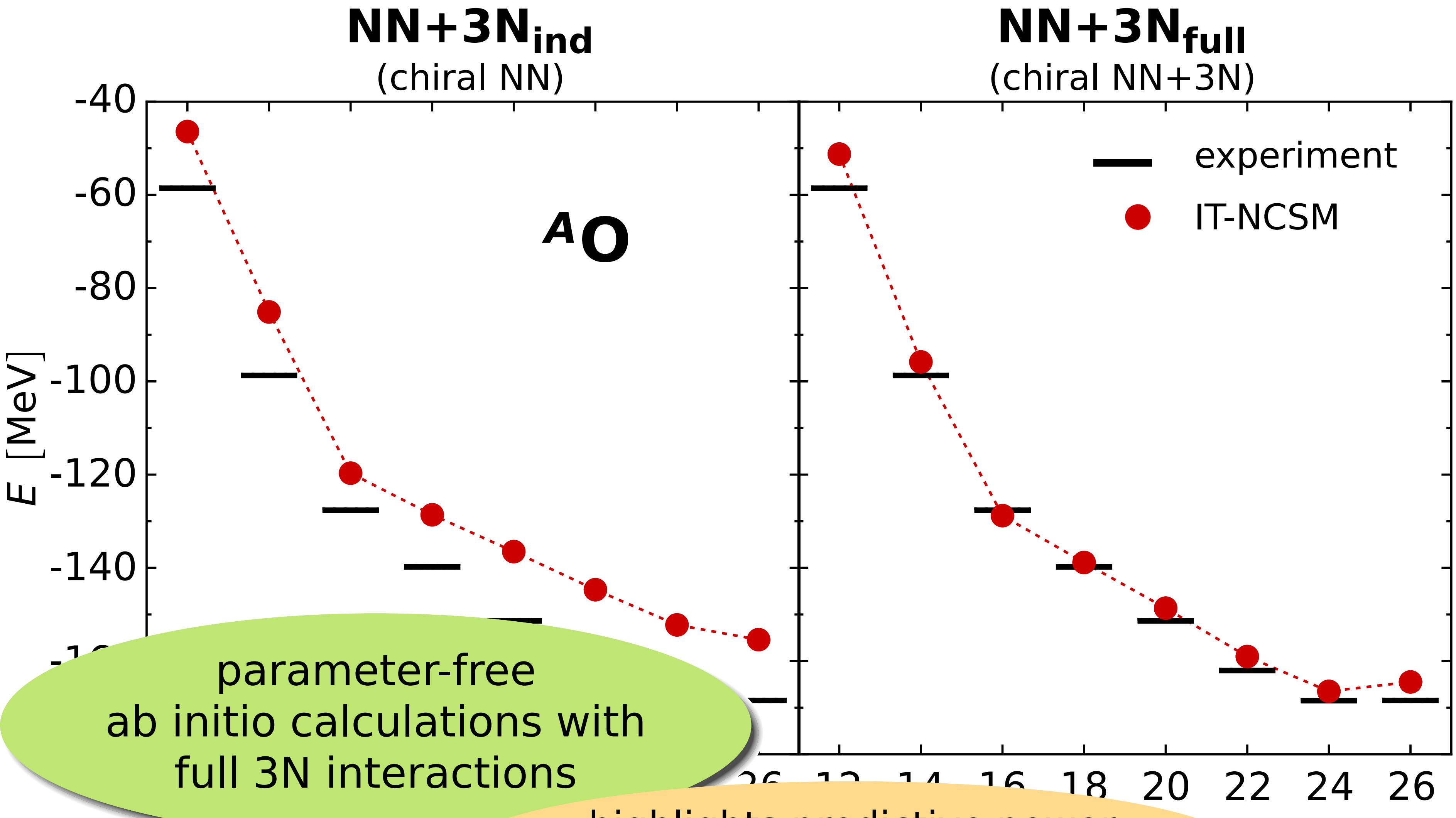


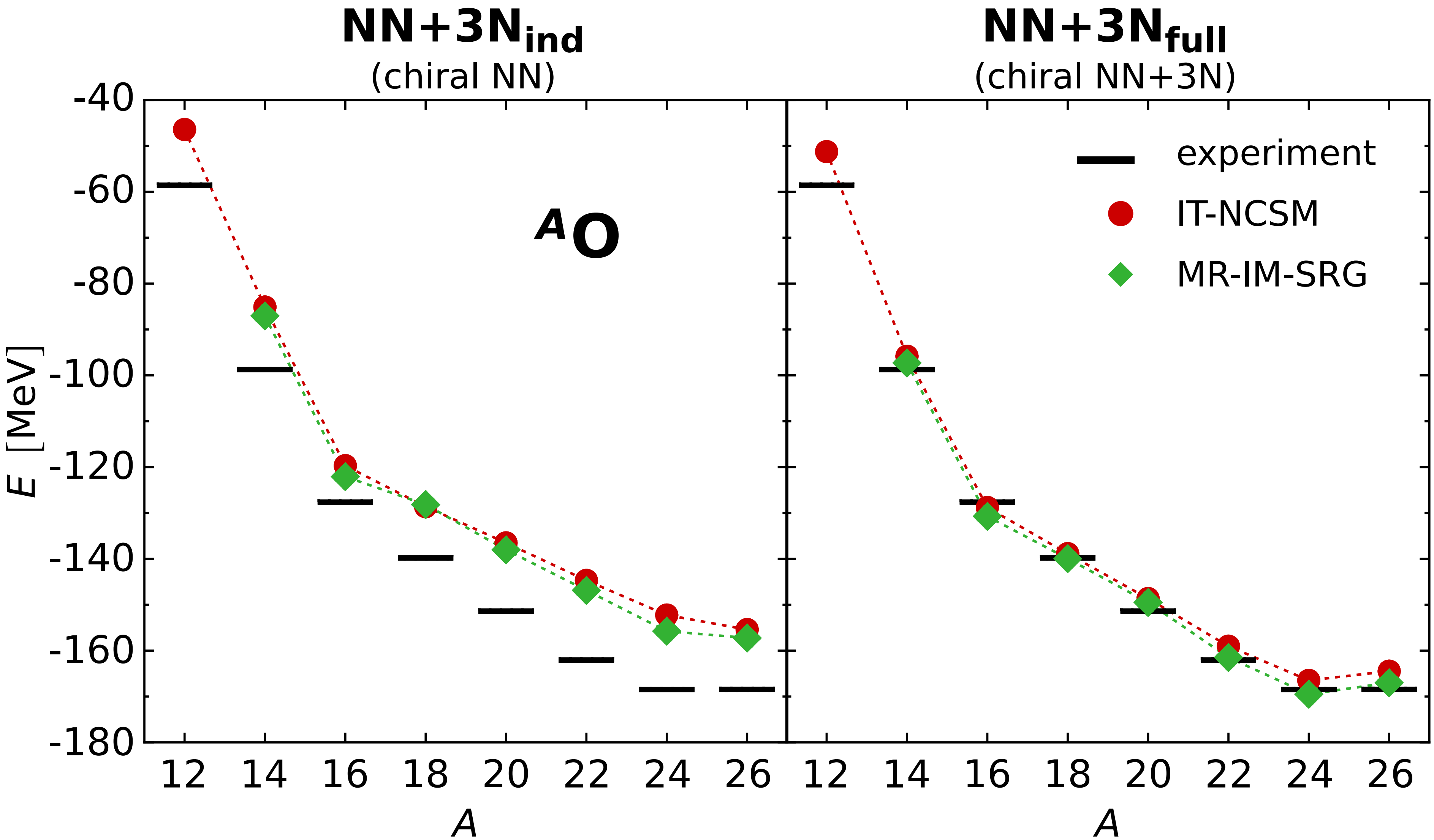
parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

Λ_{3N} = 400 MeV, α = 0… optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

Hergert et al., PRL (2013); arXiv:1302.7294



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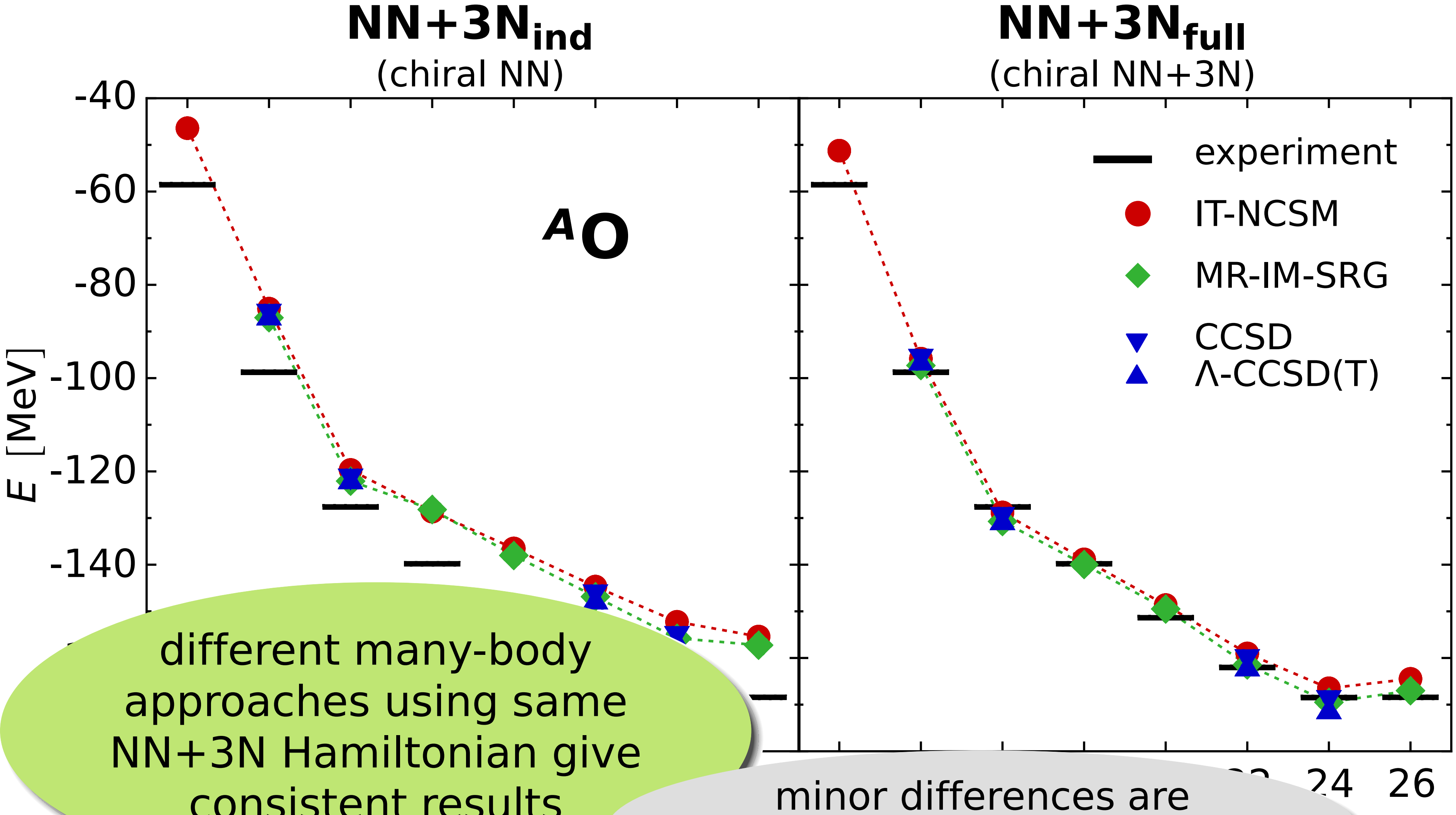

different many-body approaches using same NN+3N Hamiltonian give consistent results

minor differences are understood (NO2B, $E_{3\,\max}$,...)

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Coupled-Cluster Method

Coester, Kuemmel, Bischop, Dean, Piecuch, Walet, Papenbrock, Hagen, Binder,...

CC is one of the most efficient methods for the description of ground states of medium-mass or heavy closed-shell nuclei

- many-body state parametrized as **exponential wave operator** applied to single-determinant **reference state** $|\Phi_{\text{ref}}\rangle$

$$|\Psi_{\text{CC}}\rangle = \Omega \; |\Phi_{\text{ref}}\rangle = \exp\left(\mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3 + \cdots + T_A\right) \; |\Phi_{\text{ref}}\rangle$$

- truncation with respect to *n*-particle-*n*-hole **excitation operators** T_n
- solve **non-linear system** of equations for the amplitudes in T_1, T_2, T_3,...
- extensions to near-closed-shell nuclei and excited states through **equations-of-motion methods**
- we have developed a parallelized CC code for **CCSD and Λ-CCSD(T)**

Inclusion of 3N Interactions

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

- **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)

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

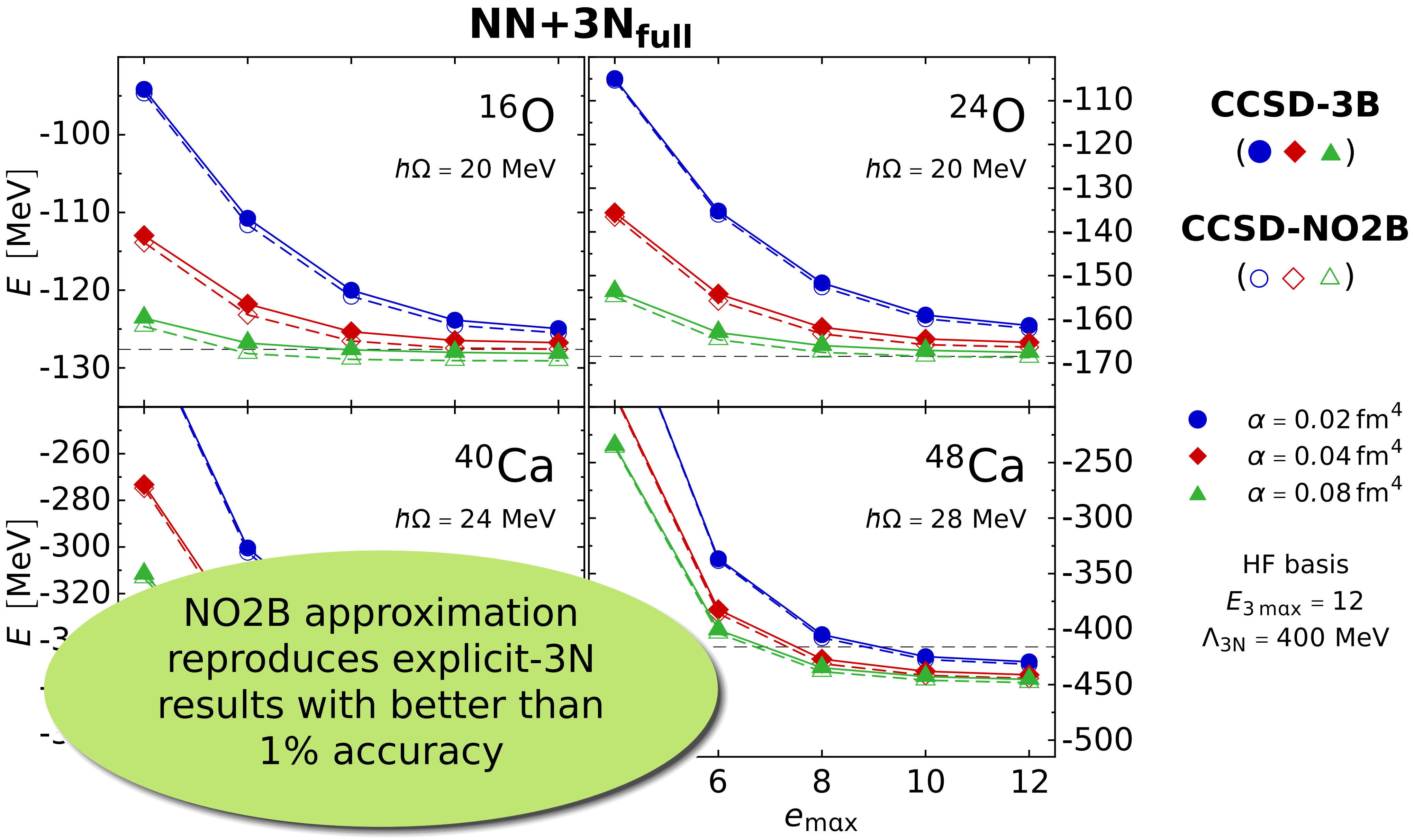
$$= W^{0B} + \sum W^{1B}_{\circ\circ}\, \{a^\dagger_\circ\, a_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ\}$$

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

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

CCSD with Explicit 3N Interactions

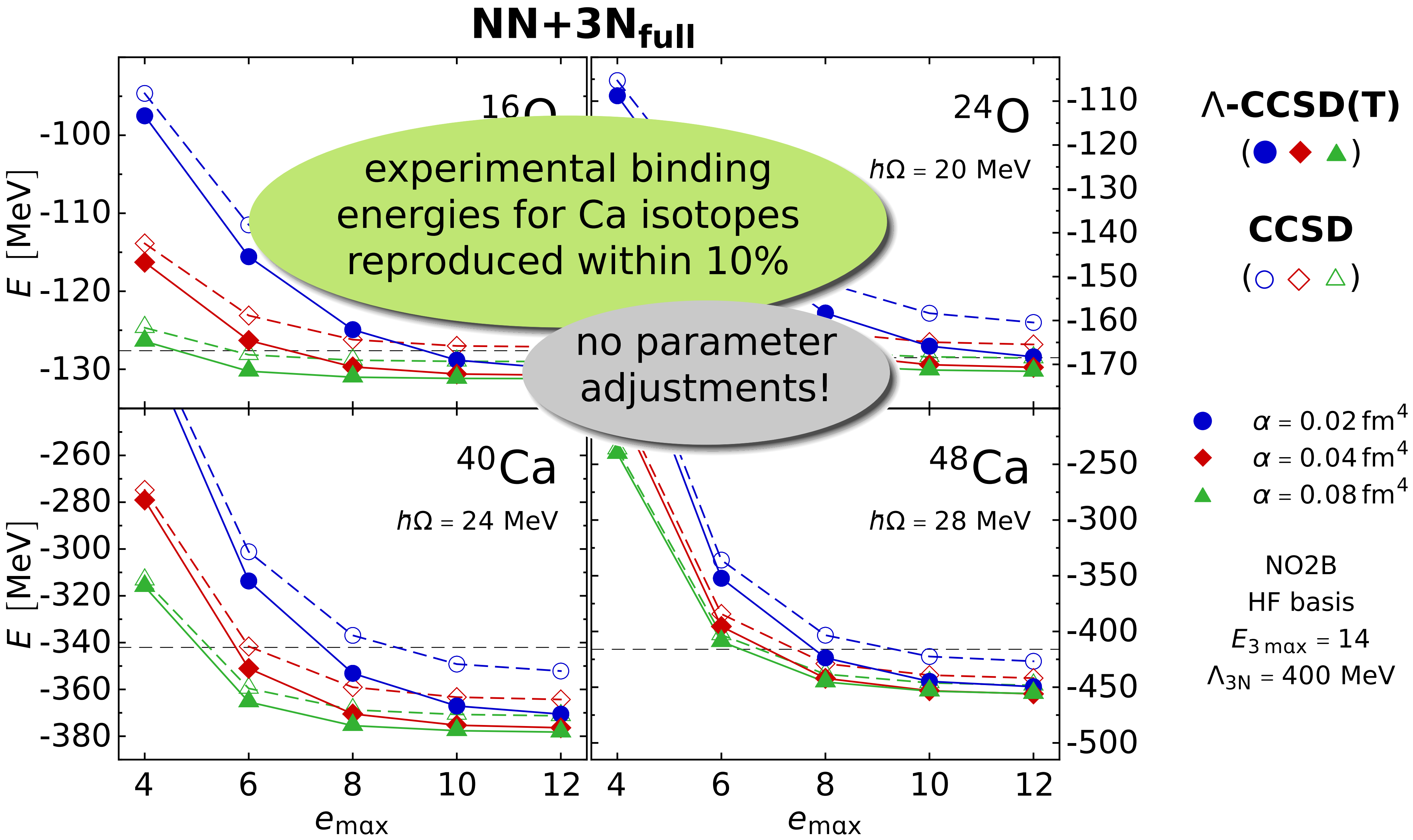
Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)



NO2B approximation reproduces explicit-3N results with better than 1% accuracy

Λ-CCSD(T) with NO2B Approximation

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



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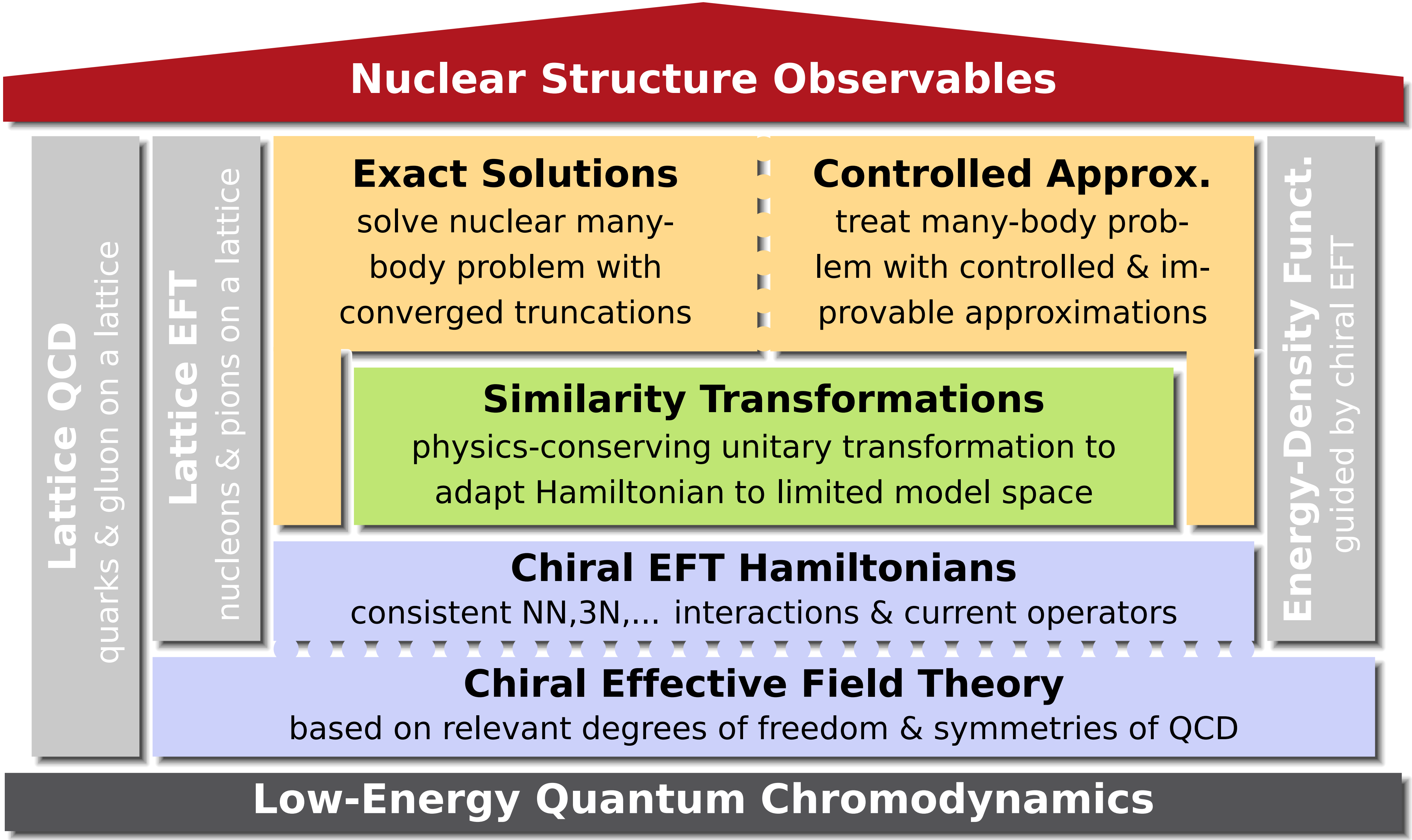
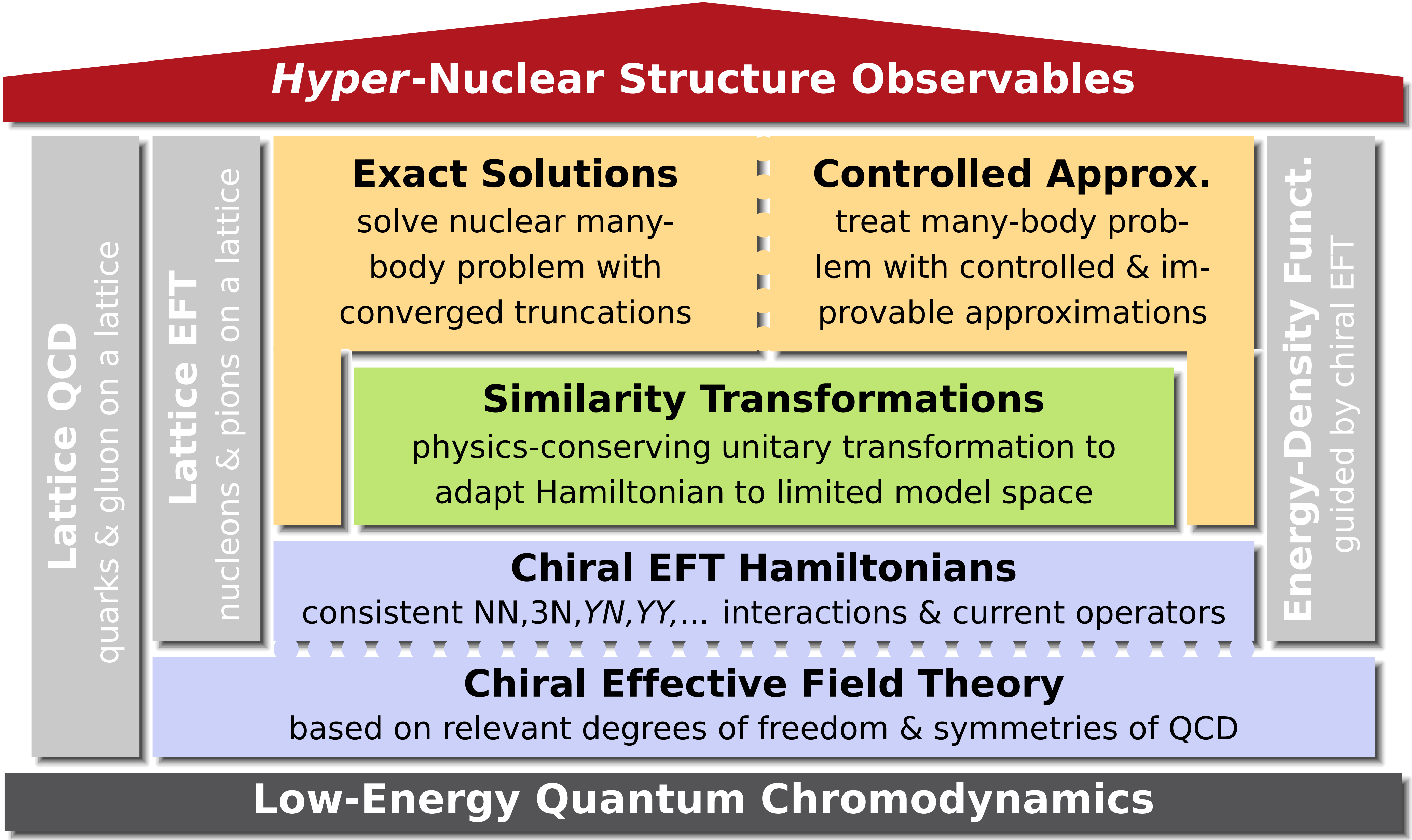
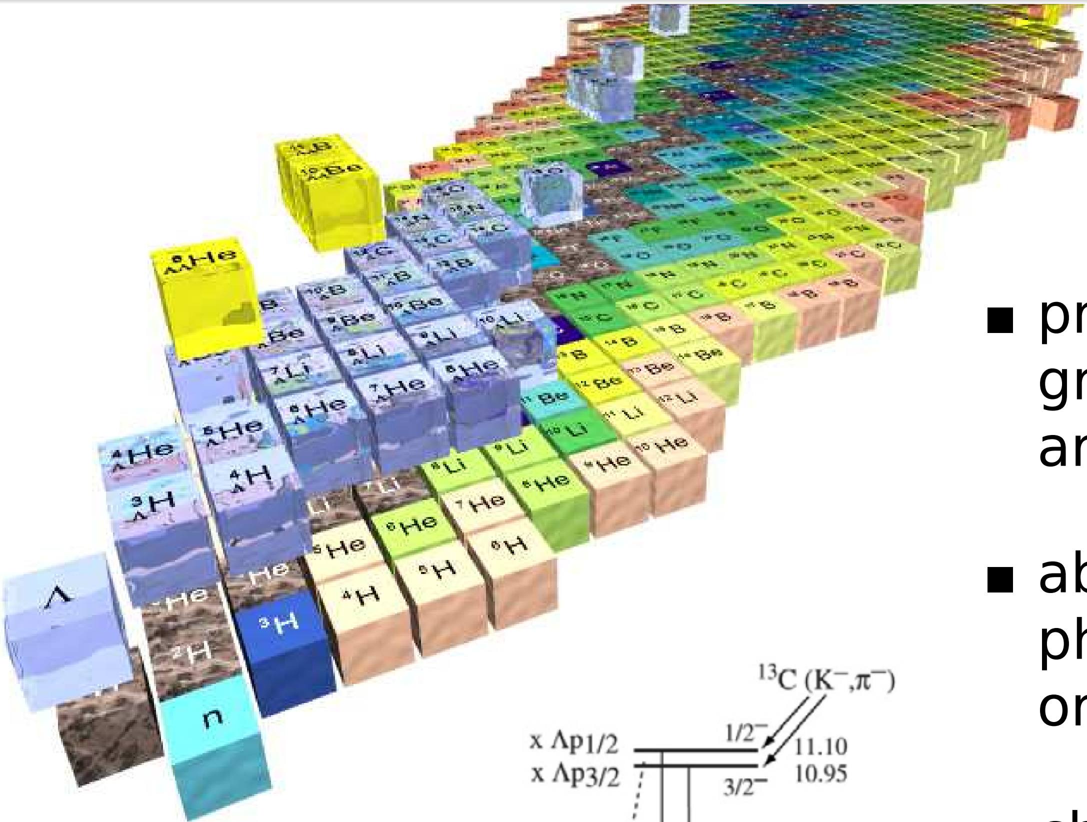
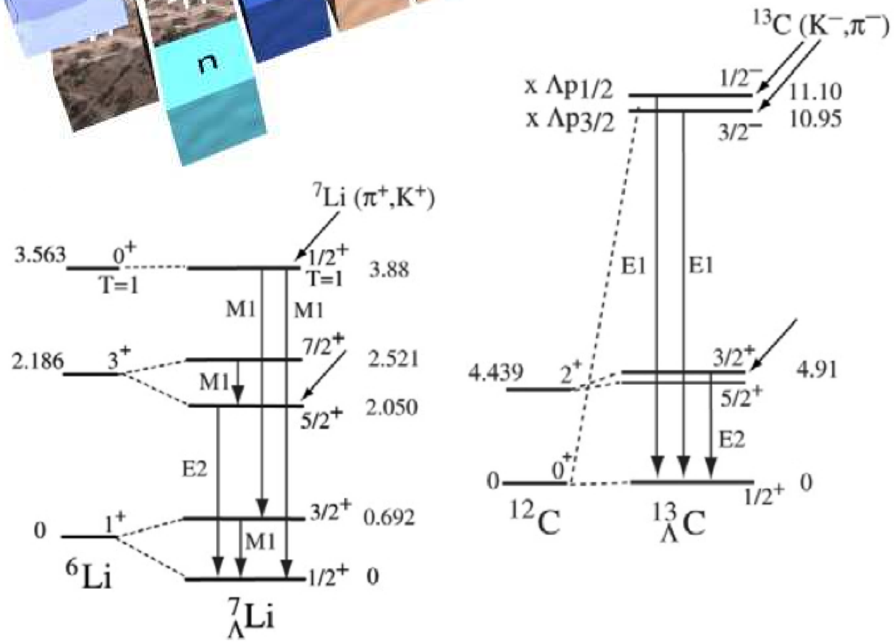


Ab Initio *Hyper*-Nuclear Structure



Motivation: Hypernuclear Structure



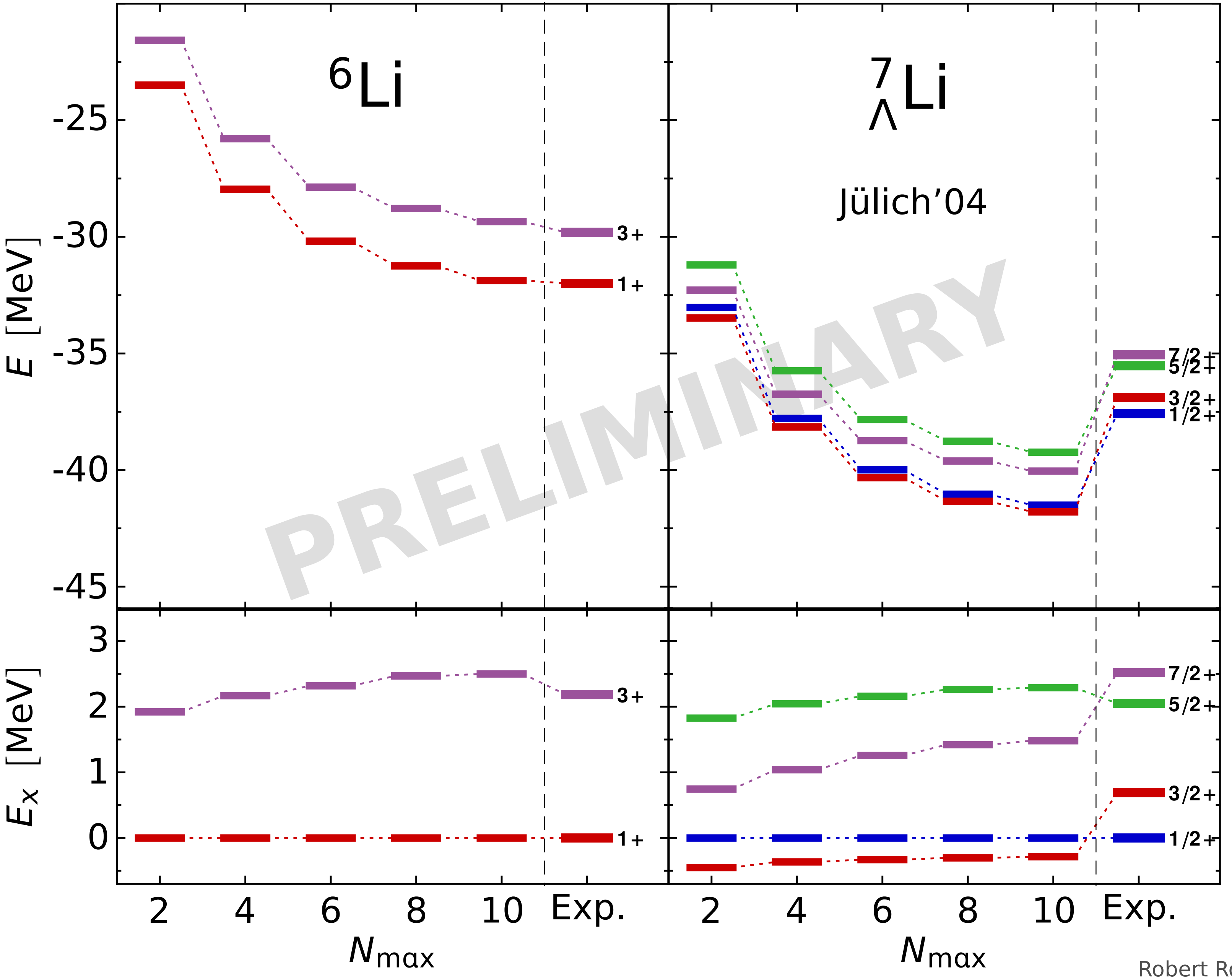


- precision data on hypernuclear ground states and spectroscopy are available
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations so far
- chiral EFT interactions including hyperons are being constructed
- constrain YN & YY interaction by ab initio hypernuclear structure calculations

Ab Initio Toolbox

- **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: $^{7}_{\Lambda}\mathrm{Li}$



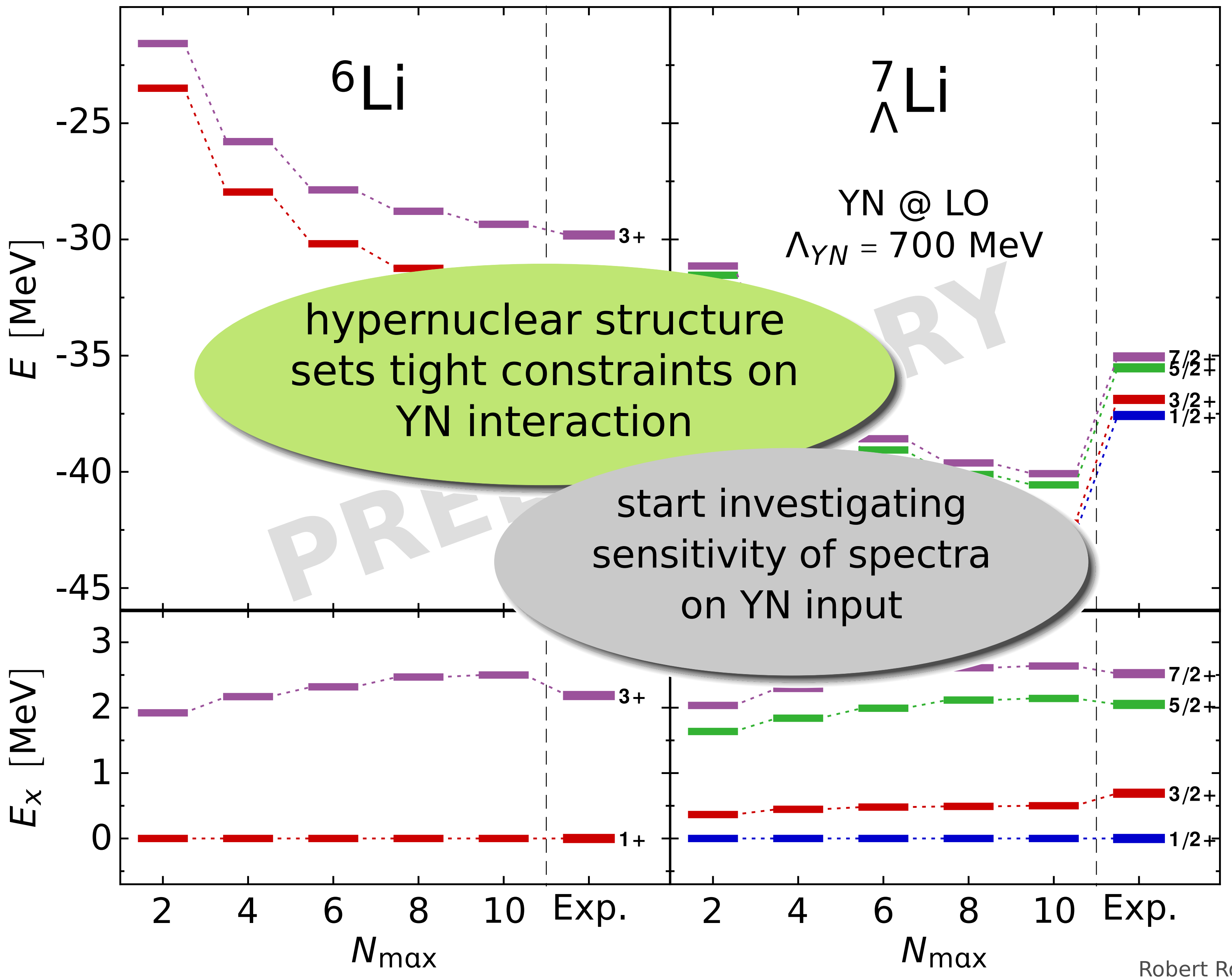
NN @ N3LO
Entem&Machleidt
$\Lambda_{NN} = 500$ MeV

3N @ N2LO
Navratil
$\Lambda_{3N} = 500$ MeV
triton fit

Jülich'04
Haidenbauer et al.
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

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



NN @ N3LO
Entem&Machleidt
Λ_{NN} = 500 MeV

3N @ N2LO
Navratil
Λ_{3N} = 500 MeV
triton fit

YN @ LO
Haidenbauer et al.
Λ_{YN} = 700 MeV
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

Conclusions

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... propagate uncertainties & provide feedback
- consistent **inclusion of 3N & 4N interactions** in similarity transformations & many-body calculations
  - breakthrough in treatment of 3N & 4N matrix elements
- **innovations in many-body theory**: extended reach of exact methods & improved control over approximations
  - versatile toolbox for different observables & mass ranges
- many **exciting applications** ahead...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, E. Gebrerufael, H. Krutsch, **J. Langhammer**, S. Reinhardt, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth
    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
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    Ohio State University, USA
  - P. Papakonstantinou
    IPN Orsay, F
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

SFB 634

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HIC for FAIR
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Exzellente Forschung für Hessens Zukunft

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JUROPA — JÜLICH FORSCHUNGSZENTRUM
LOEWE-CSC — CSC Center for Scientific Computing Frankfurt
HOPPER — NERSC

COMPUTING TIME

Happy Birthday James !!!

...and many more happy & productive visits to Darmstadt