# New Horizons in Ab Initio Nuclear Structure Theory

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# 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

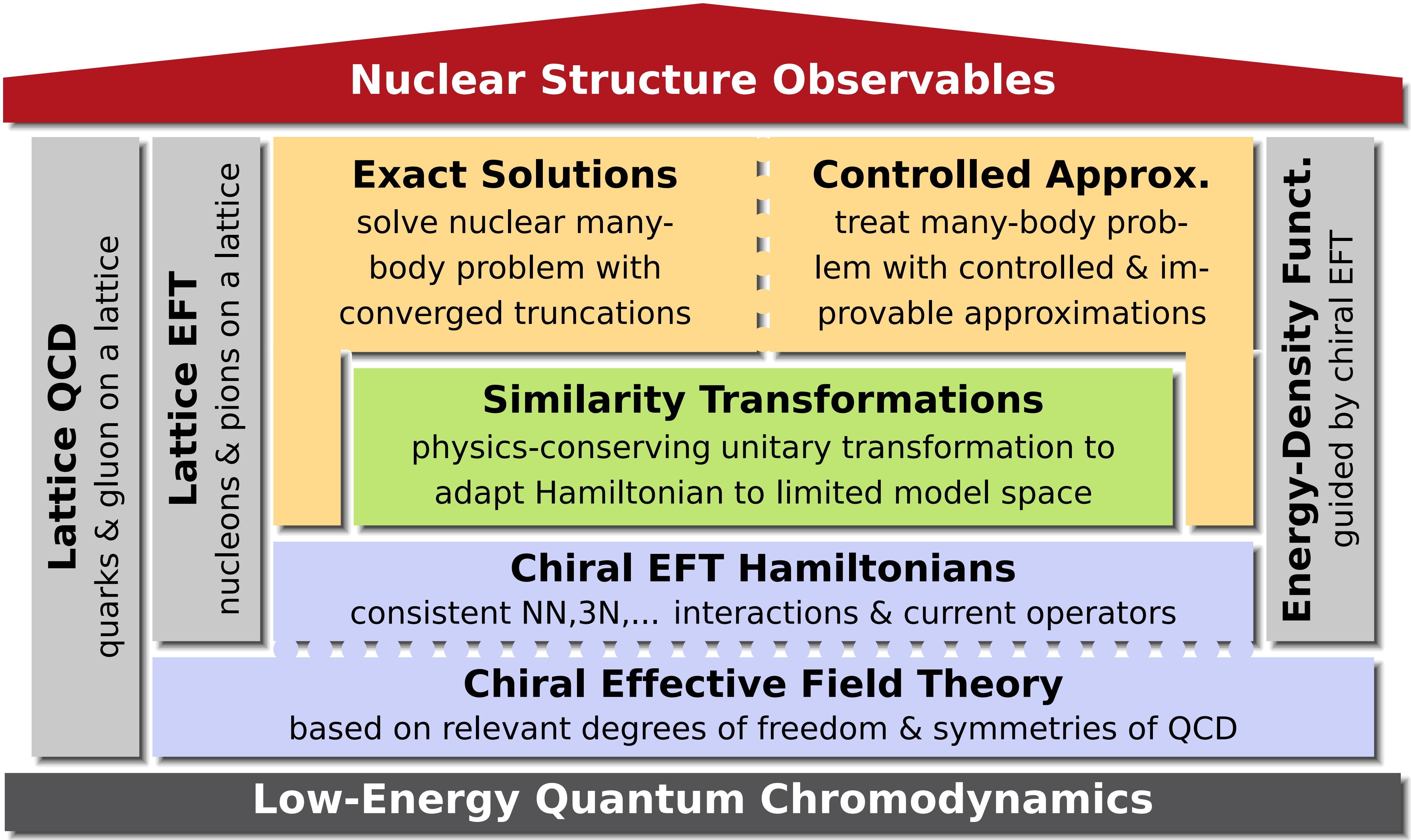
- **computing & algorithms**

  increase of computational resources & improved algorithms

- **experimental facilities**

  amazing perspectives for the study of nuclei far-off stability

# Ab Initio Nuclear Structure



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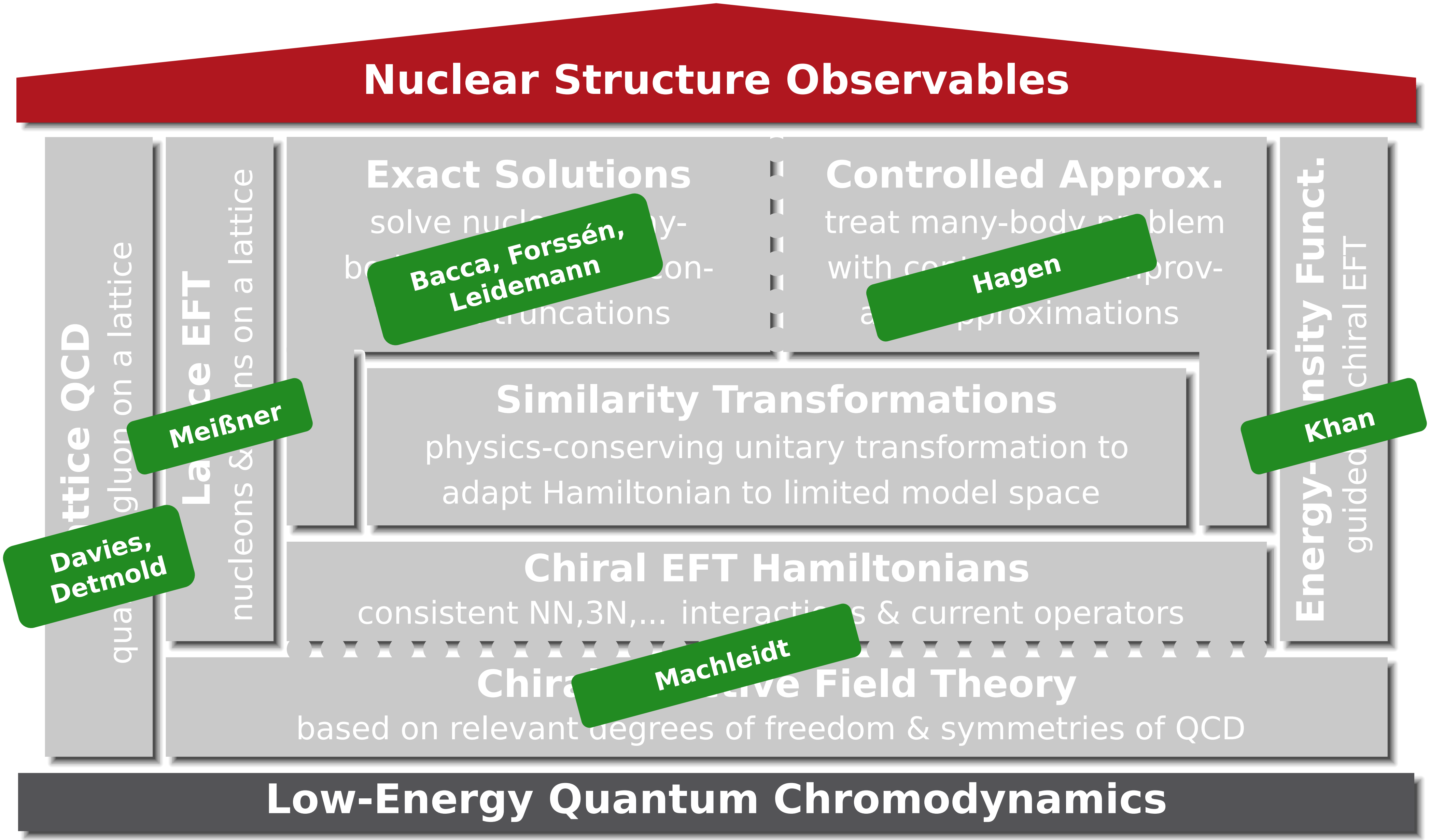

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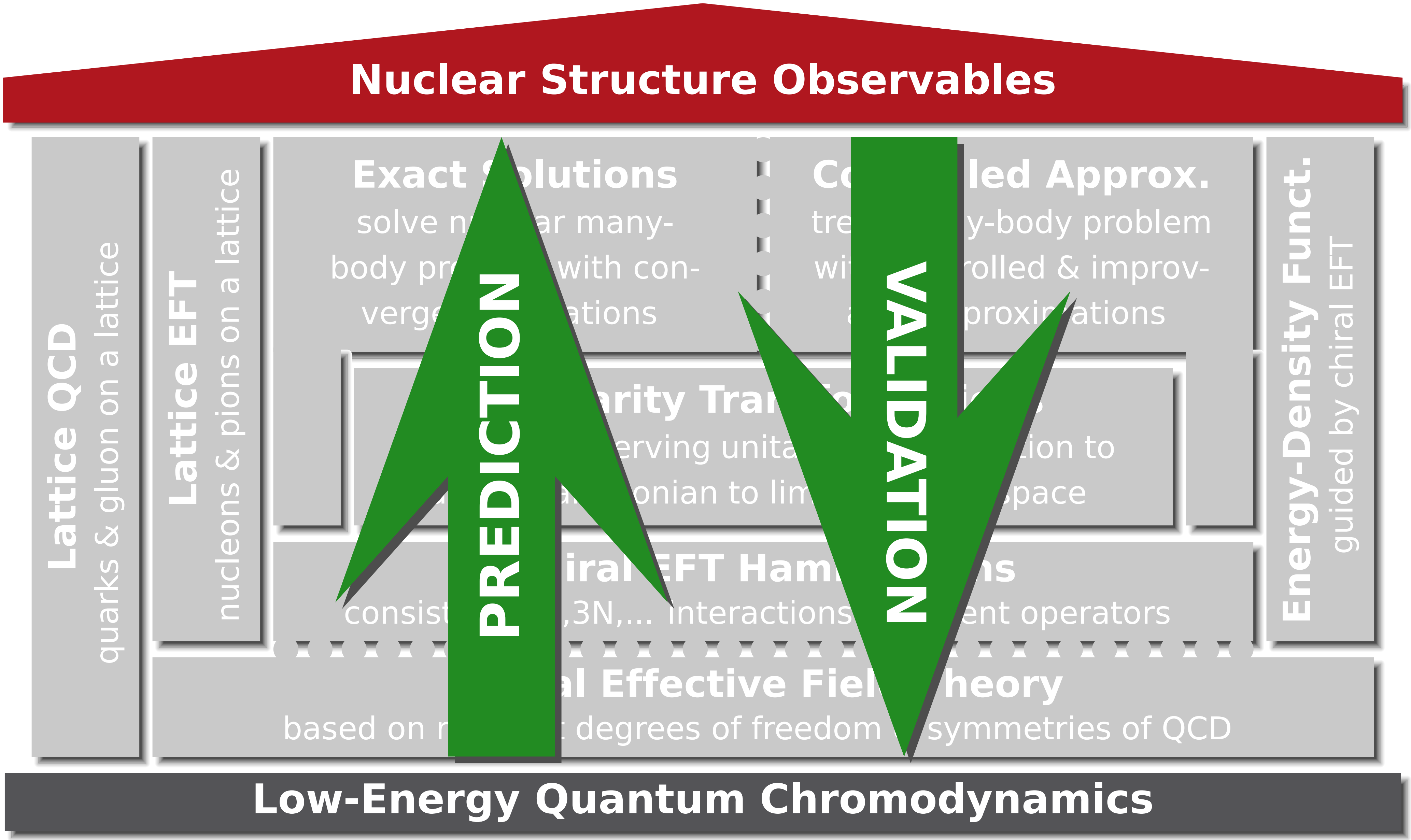

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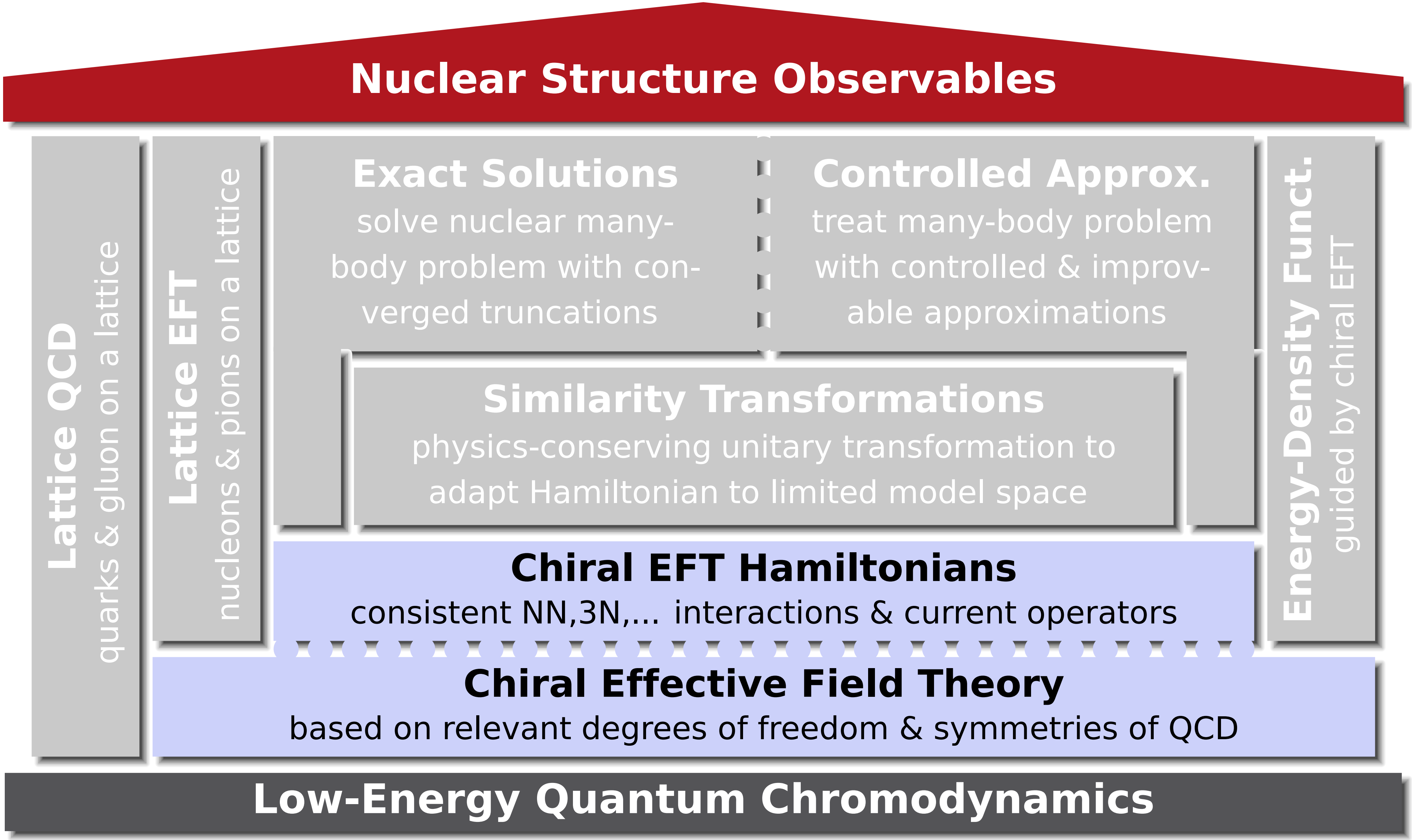
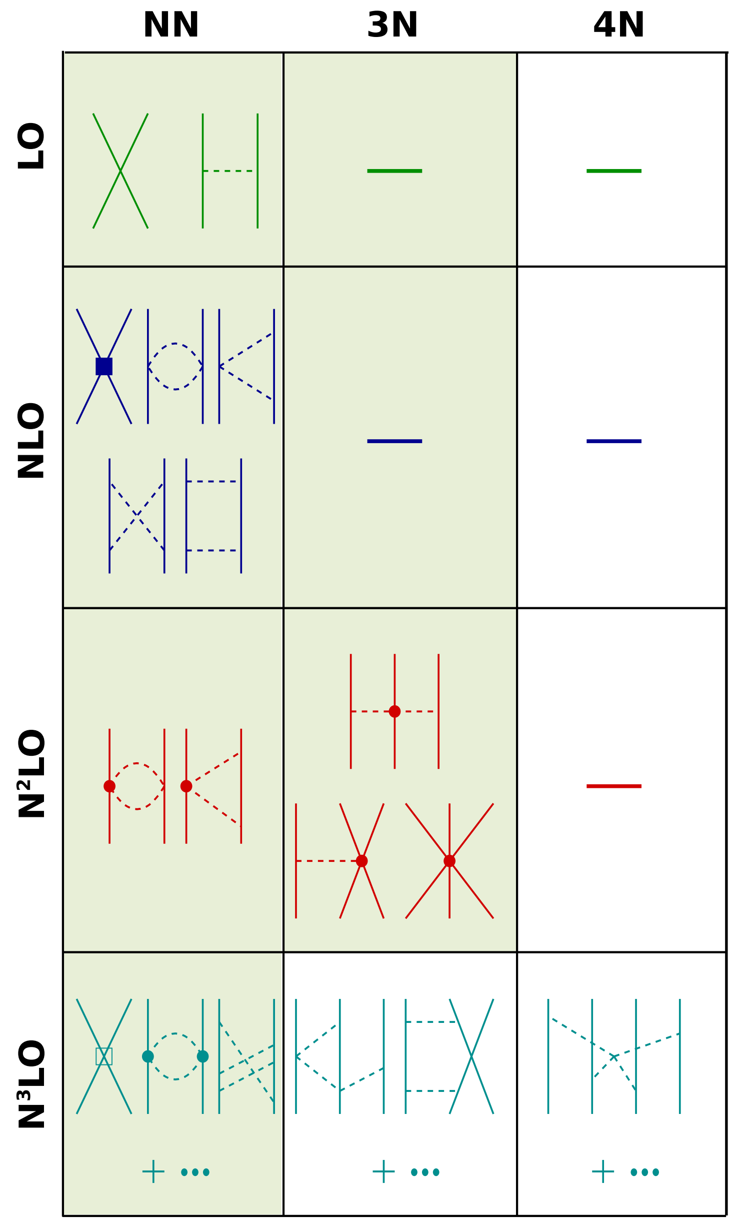


# Nuclear Interactions from Chiral EFT

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

- talks by Machleidt & Meißner
- low-energy **effective field theory** for relevant degrees of freedom ($\pi$,$N$) based on symmetries of QCD
- long-range **pion dynamics** explicitly, short-range physics absorbed in **contact terms** fitted to data ($NN$, $\pi N$,...)
- hierarchy of **consistent NN, 3N,... interactions** plus currents
- **standard Hamiltonian**:
  - NN at N3LO:
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N2LO:
    Navrátil, A=3 fit, 500 MeV cutoff



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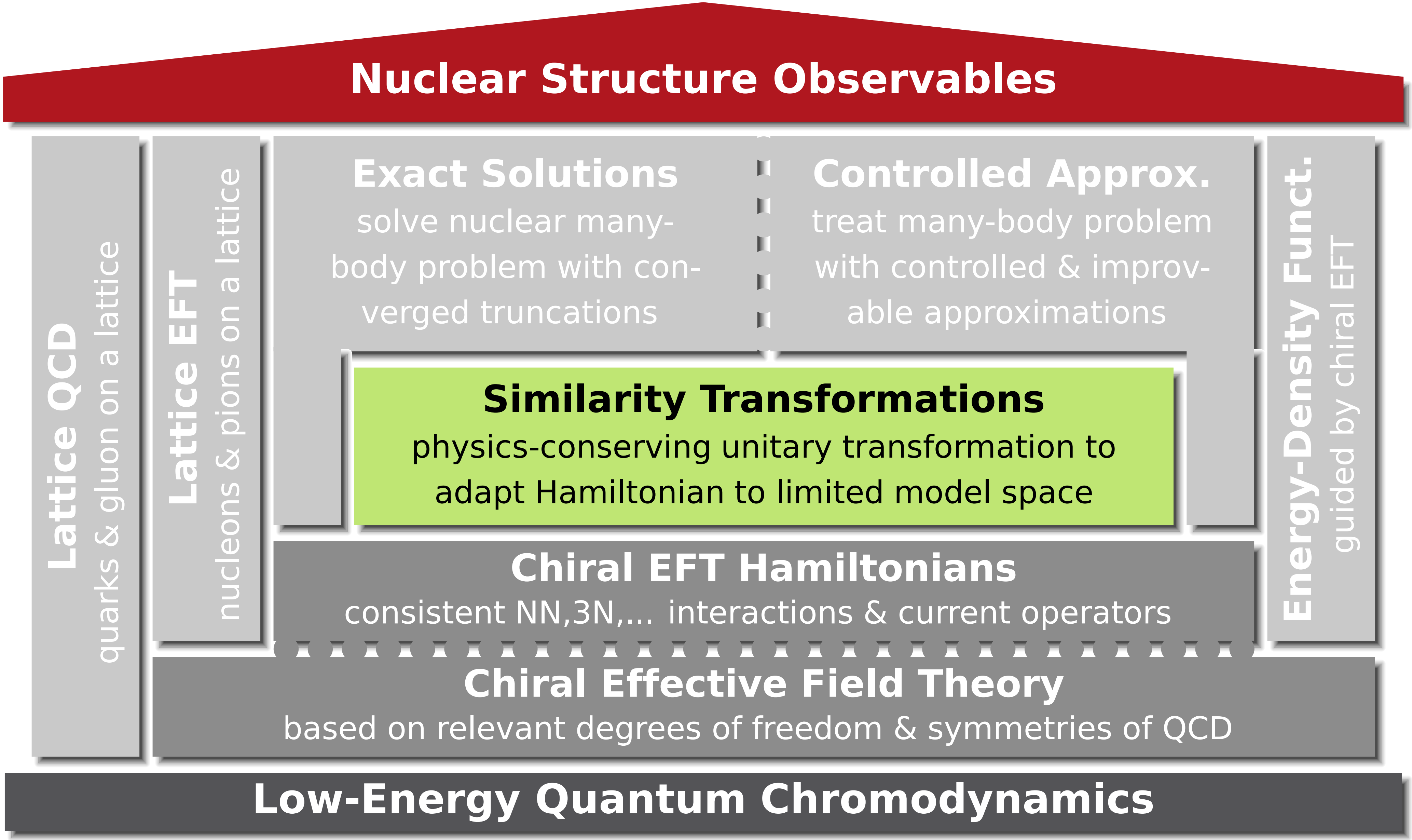


# Similarity Renormalization Group

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

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

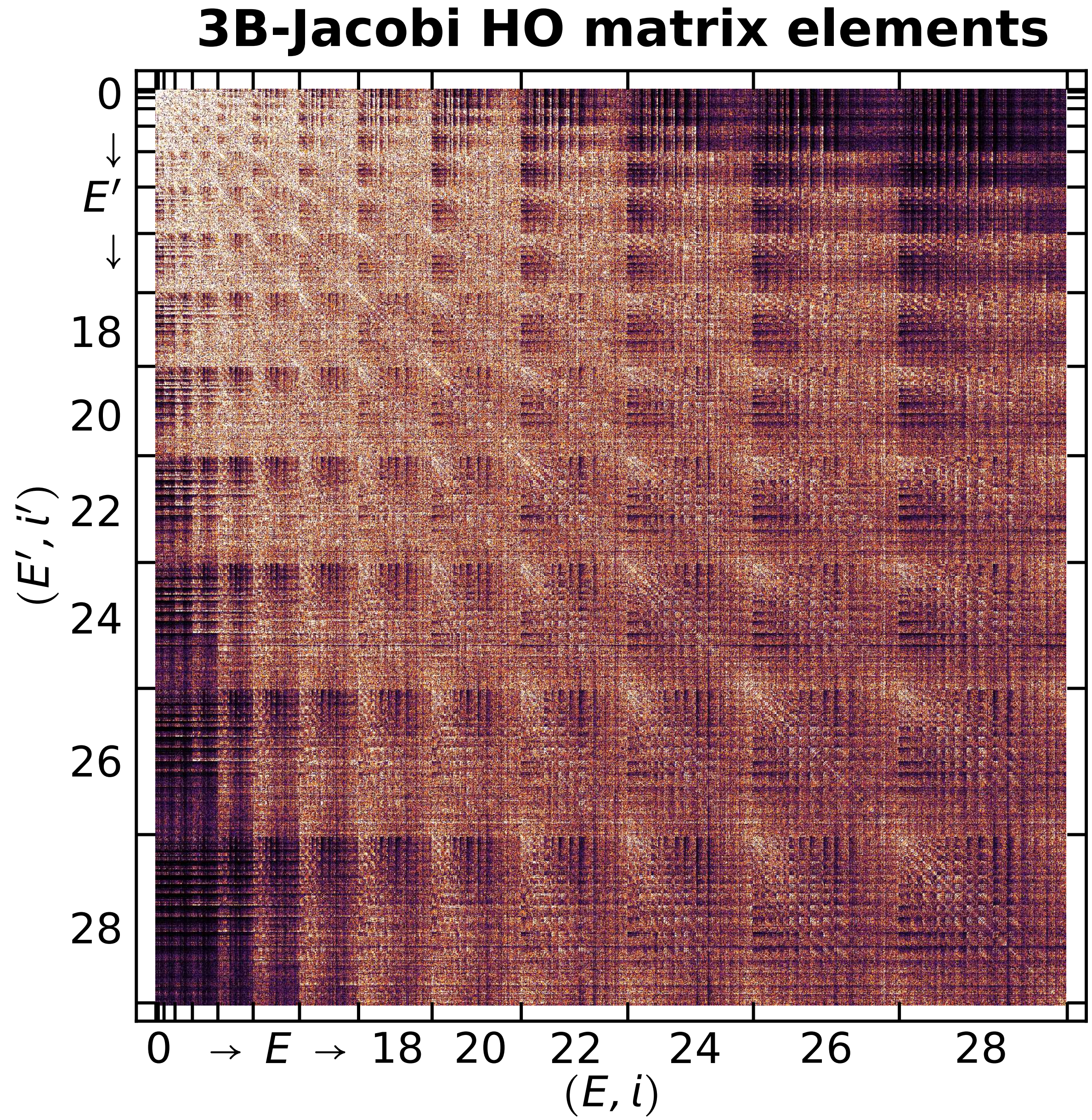
- **evolution equations** for $H_\alpha$ and U

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

- **dynamic generator**: commutator with the operator in whose eigenbasis $H_\alpha$ shall be diagonalized

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

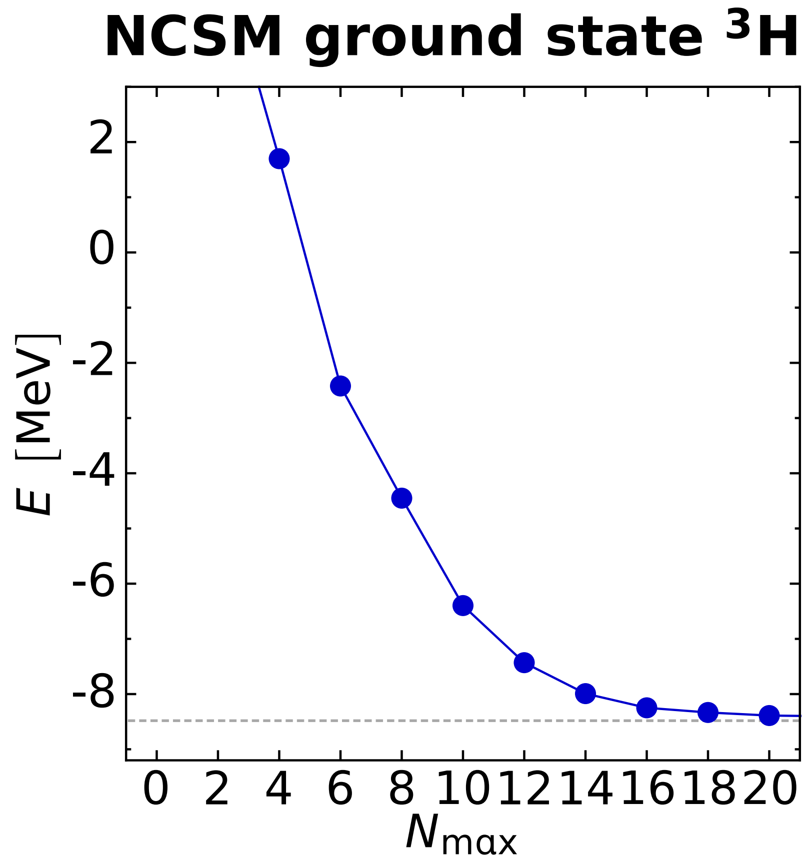
# SRG Evolution in Three-Body Space




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

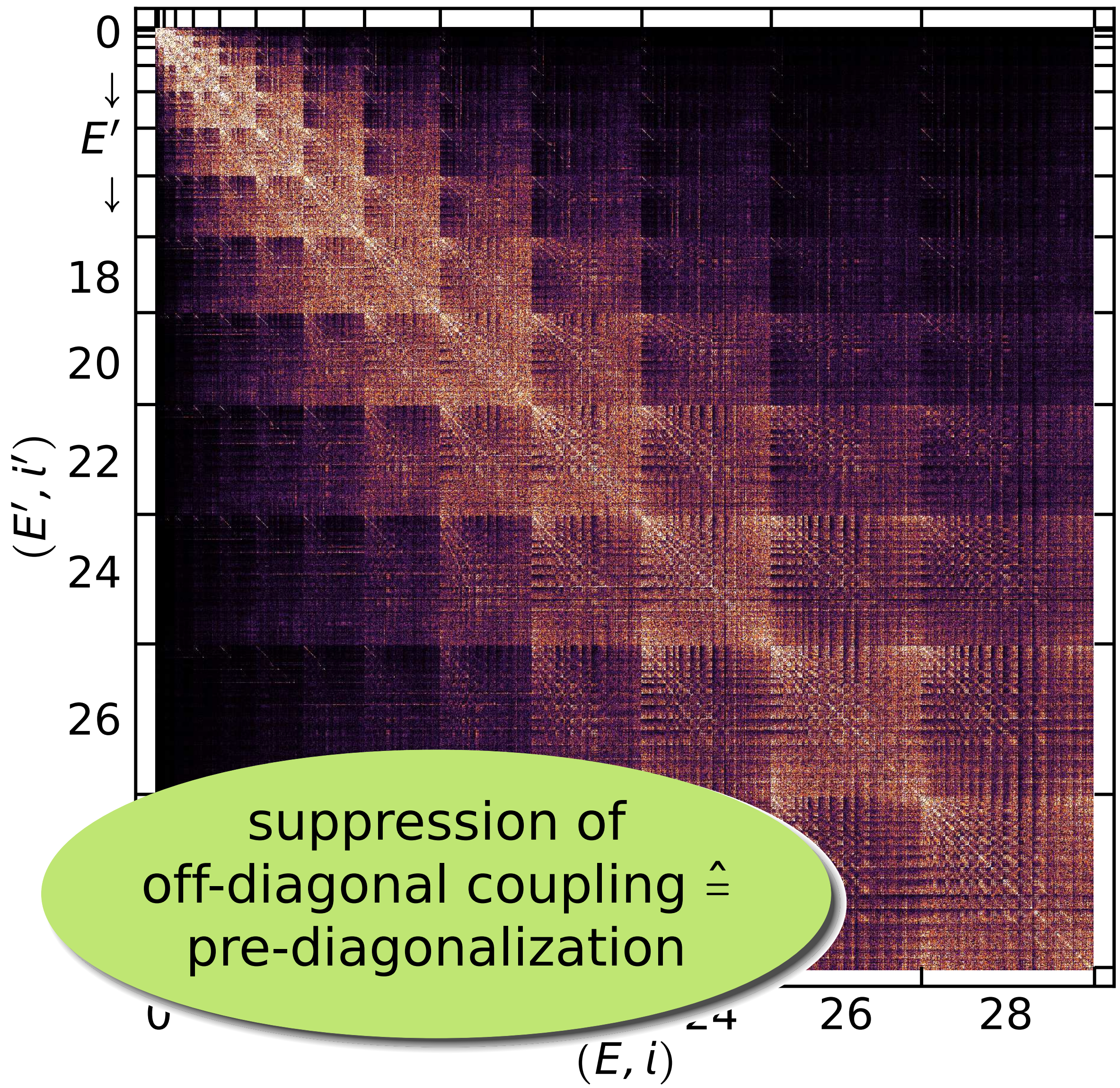
$\Lambda = \infty\,\mathrm{fm}^{-1}$

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



# SRG Evolution in Three-Body Space

**3B-Jacobi HO matrix elements**

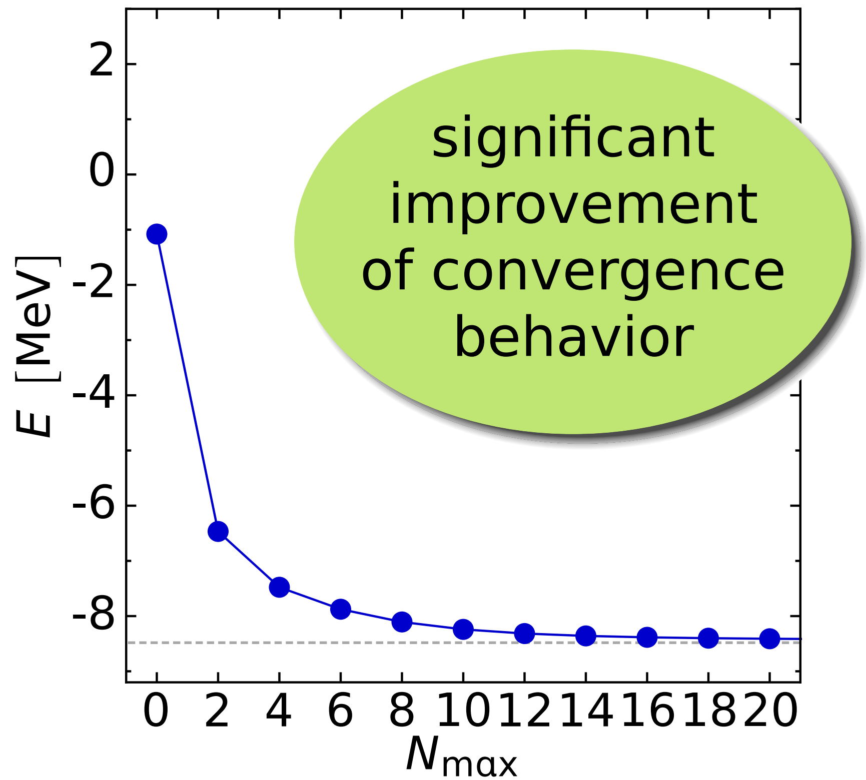



$\alpha = 0.320\,\mathrm{fm}^4$

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

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

**NCSM ground state $^3$H**



# Hamiltonian in $A$-Body Space

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

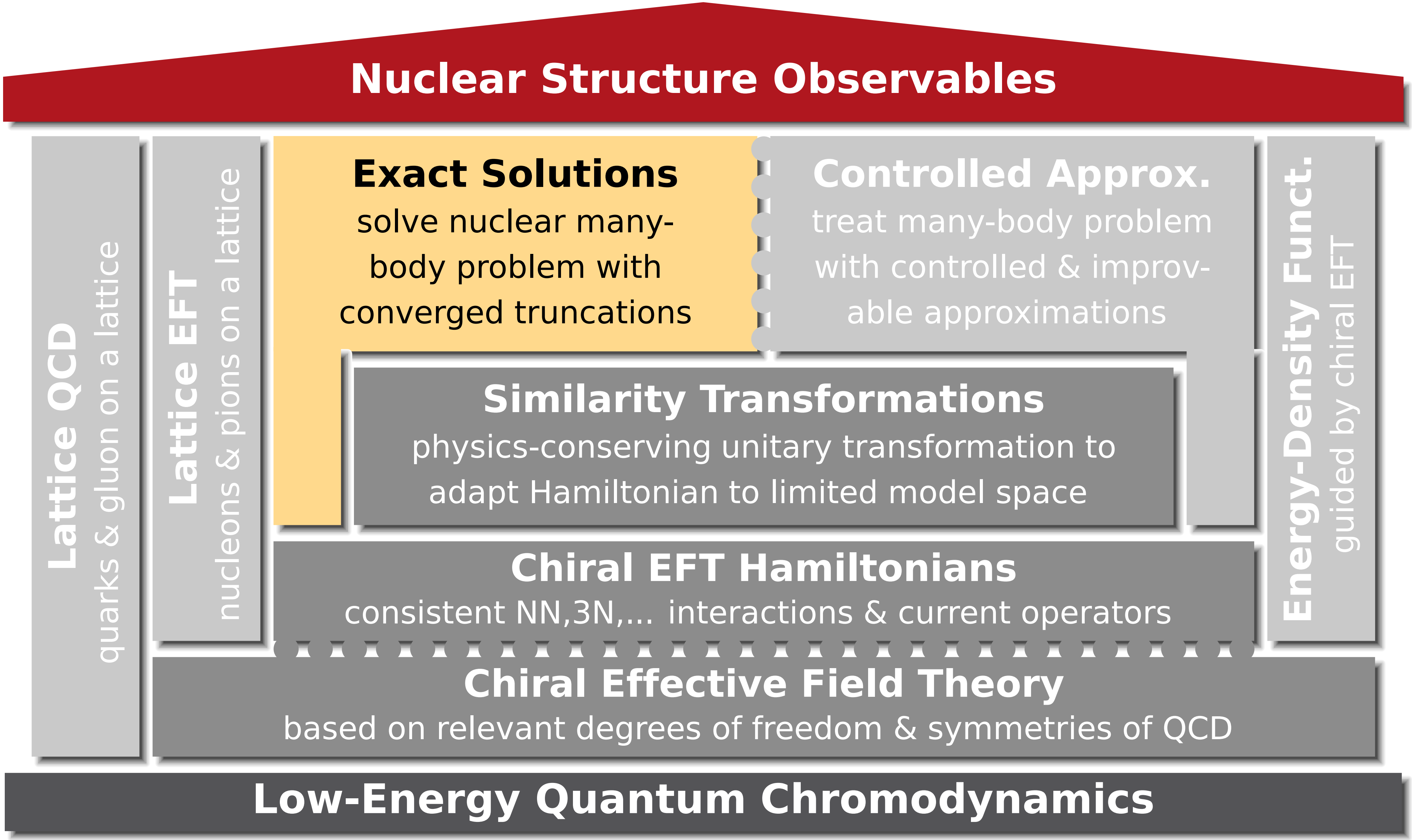
$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + H_\alpha^{[5]} + \ldots$$

- **truncation of cluster series** formally destroys unitarity and invariance of energy eigenvalues (independence of $\alpha$)
- flow-parameter $\alpha$ 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, Forssen, 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 $N_{\max}$ & $A$

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

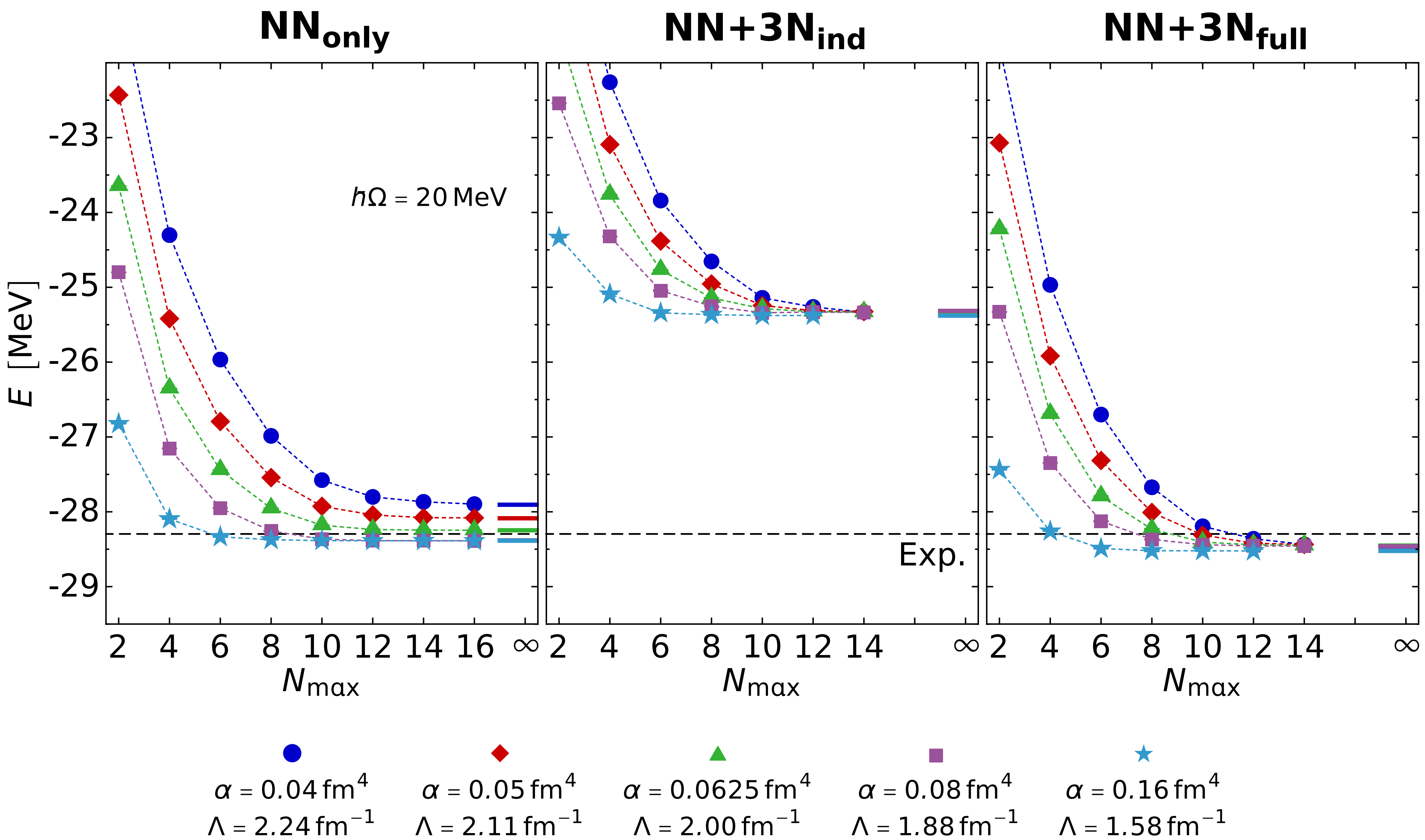
- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states

*Otsuka, Abe, Draayer, Dytrych,...*

- Monte-Carlo NCSM and symmetry-adapted NCSM employ analogous strategies to reduce model-space dimension

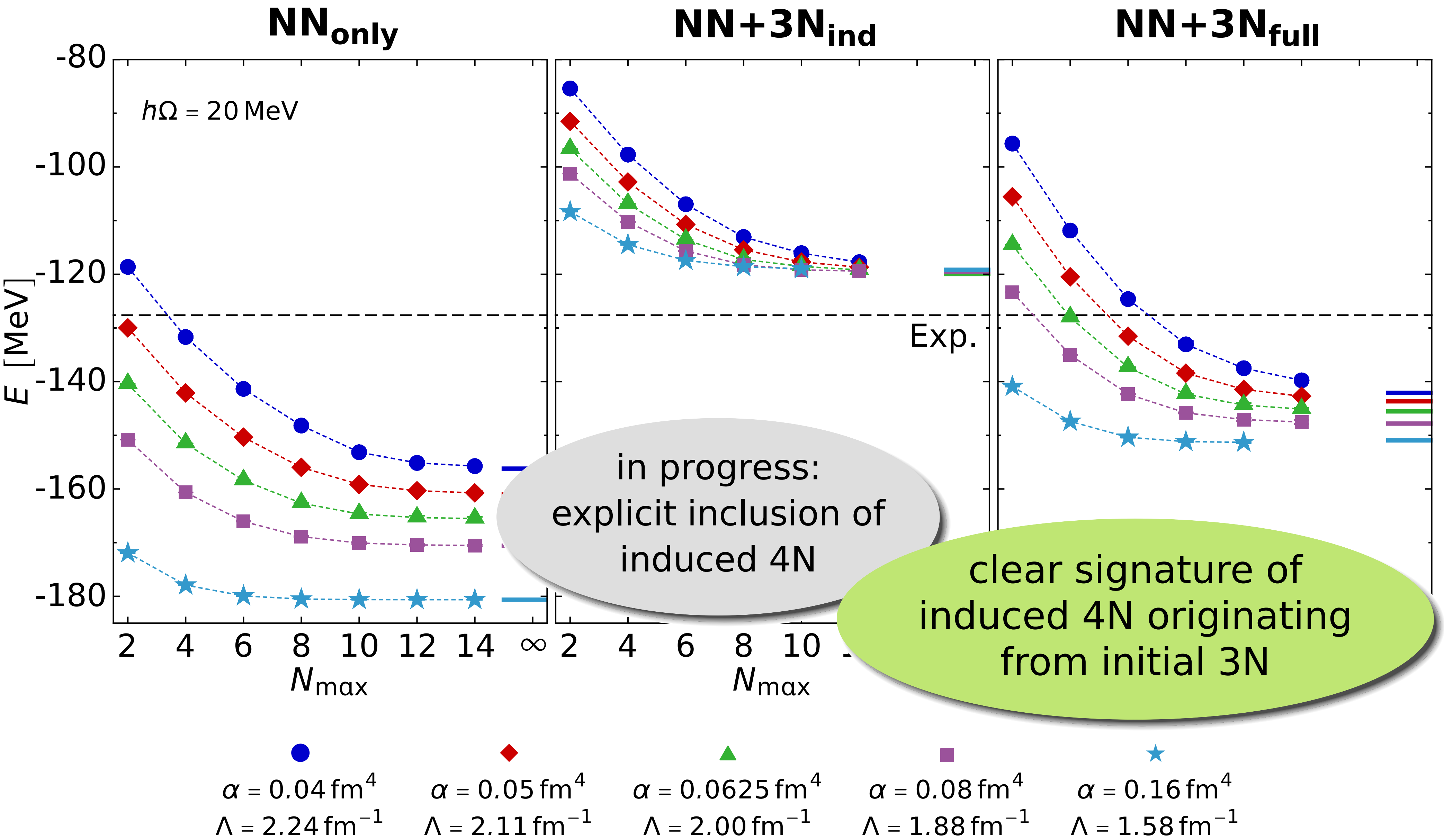
# $^4$He: Ground-State Energies

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



# $^{16}$O: Ground-State Energies

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




in progress: explicit inclusion of induced 4N

clear signature of induced 4N originating from initial 3N

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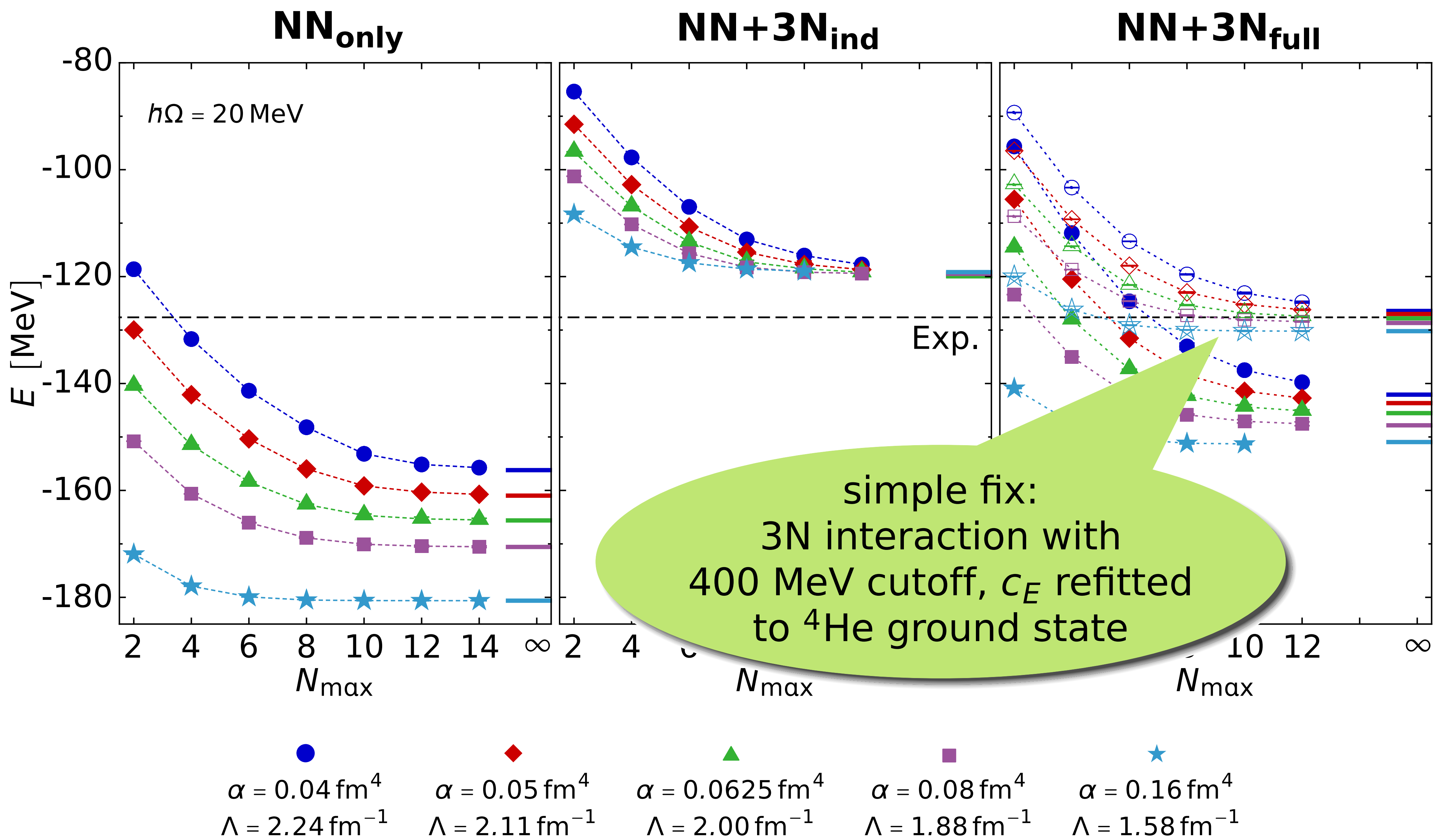
Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



# 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)*

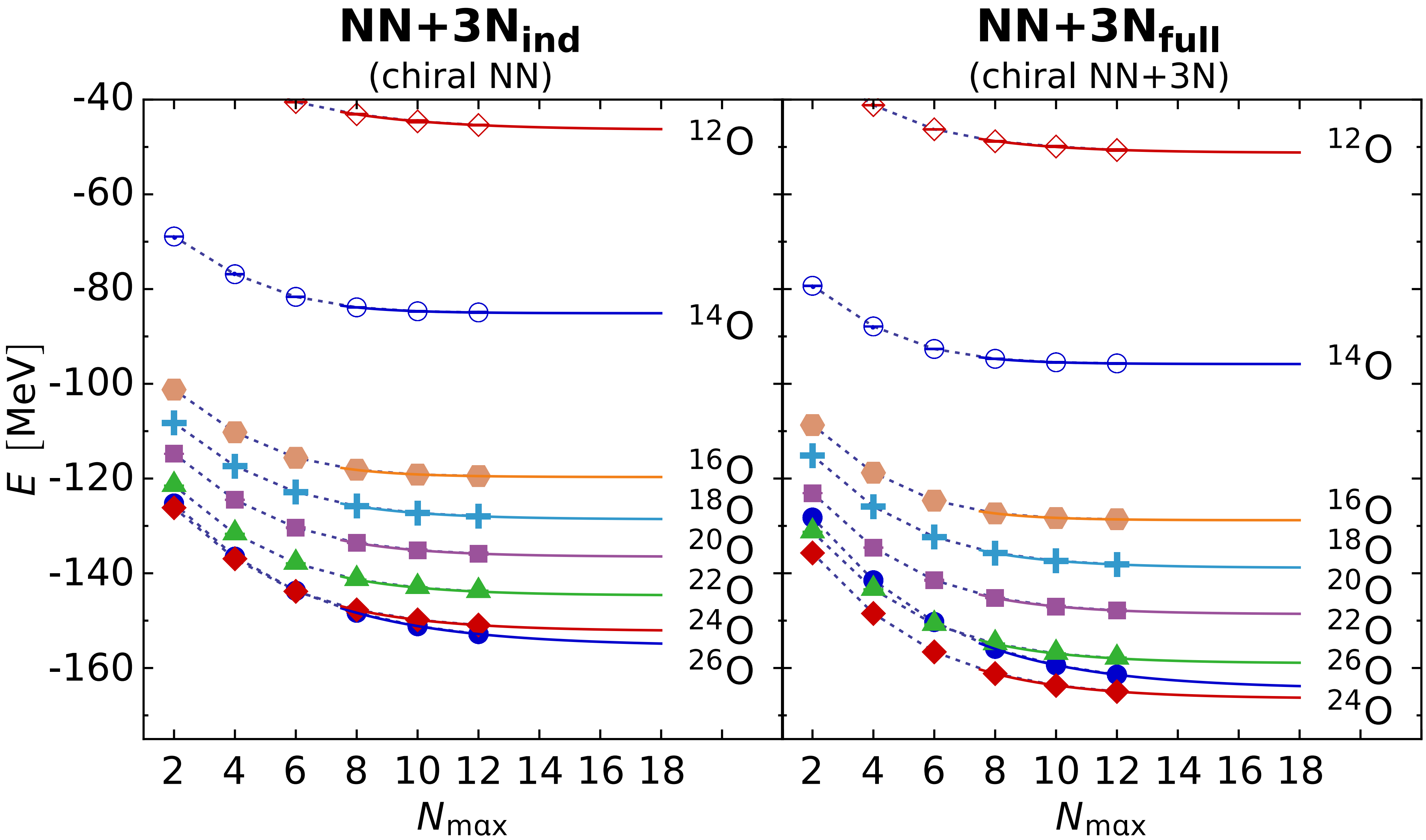
- 2012: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

*Hergert, Binder, Calci, Langhammer, Roth, PRL 110, in print (2013)*

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

# Ground States of Oxygen Isotopes

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




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

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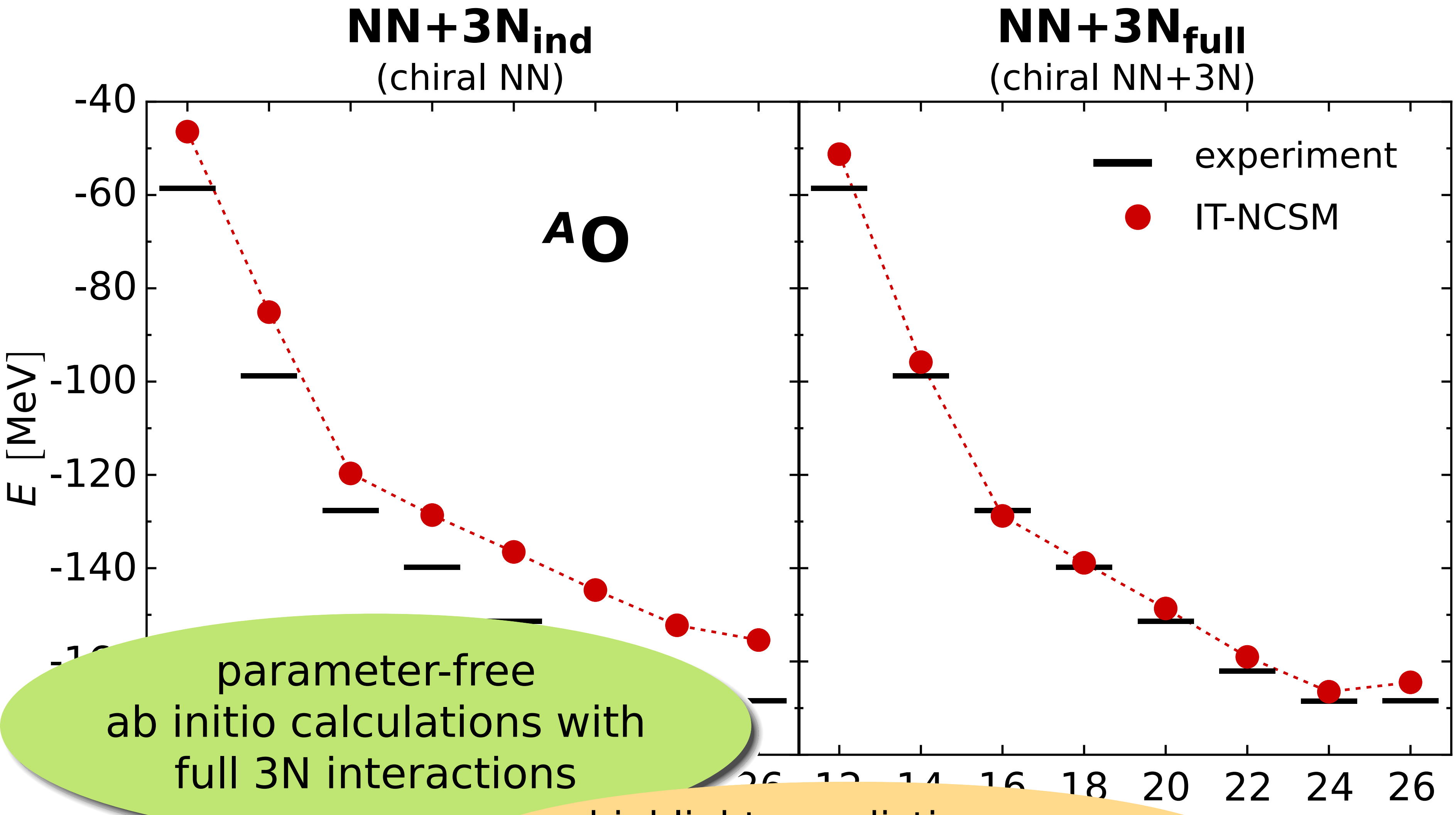


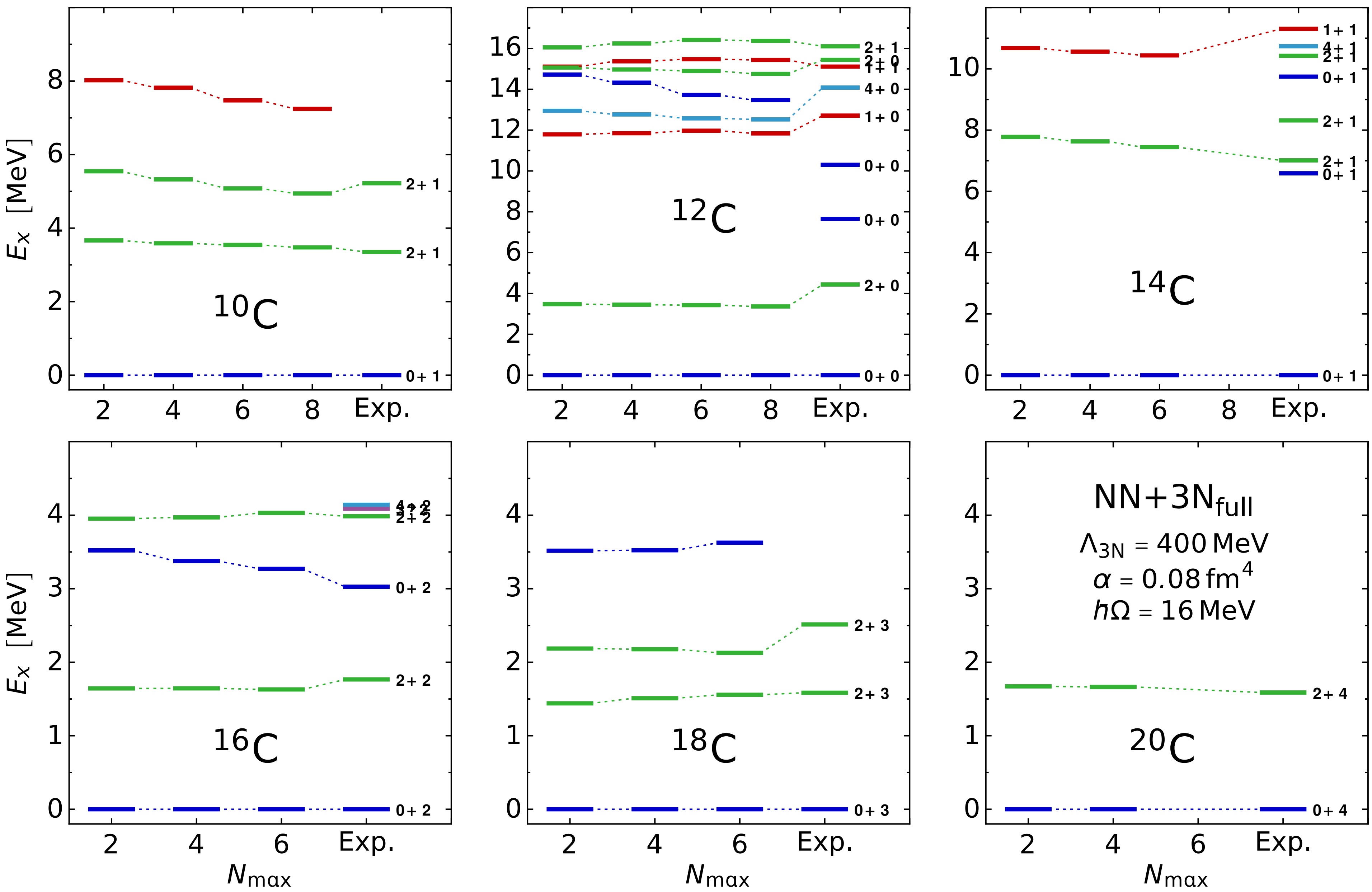

parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

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

# Spectroscopy of Carbon Isotopes

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



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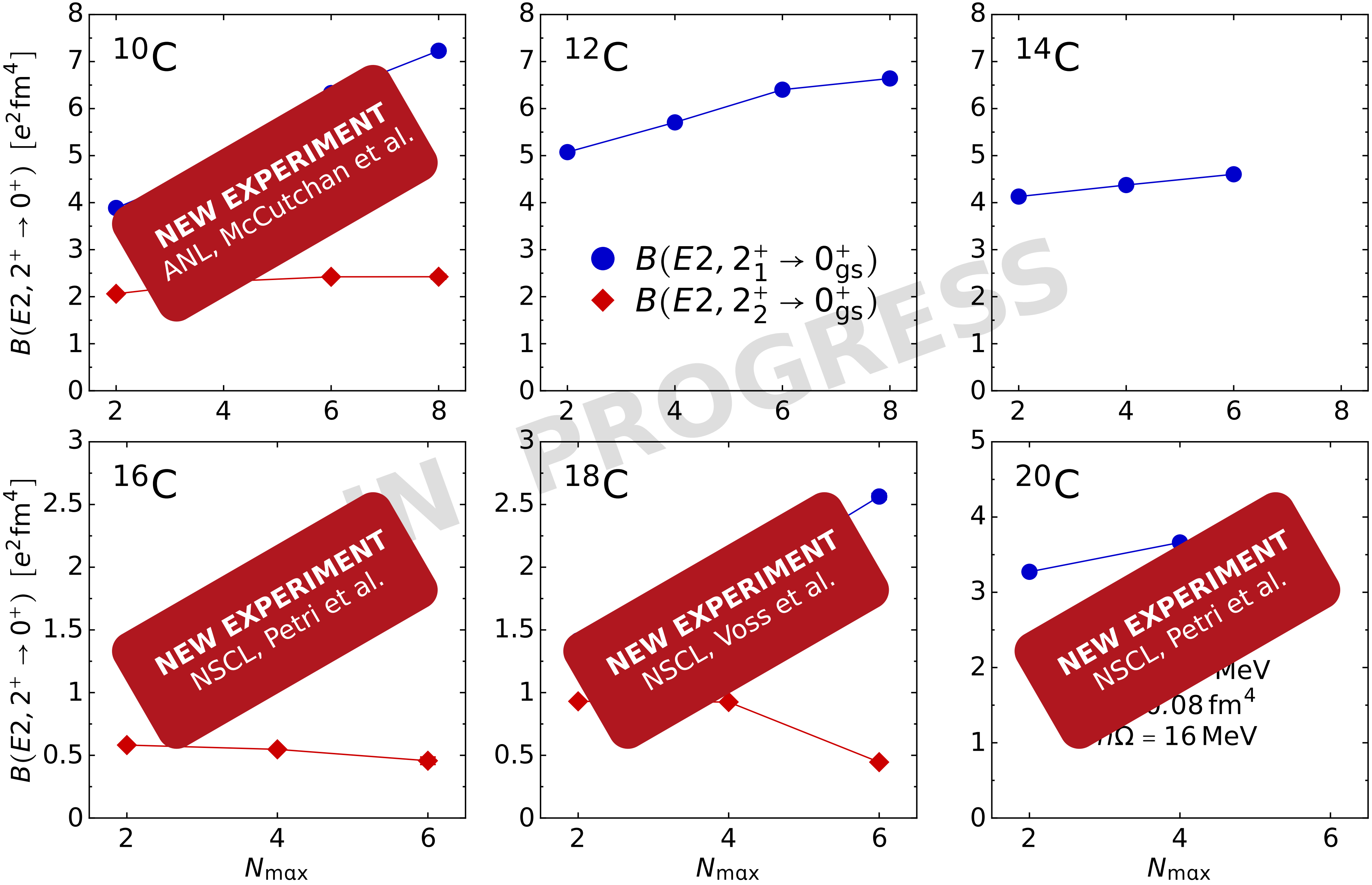

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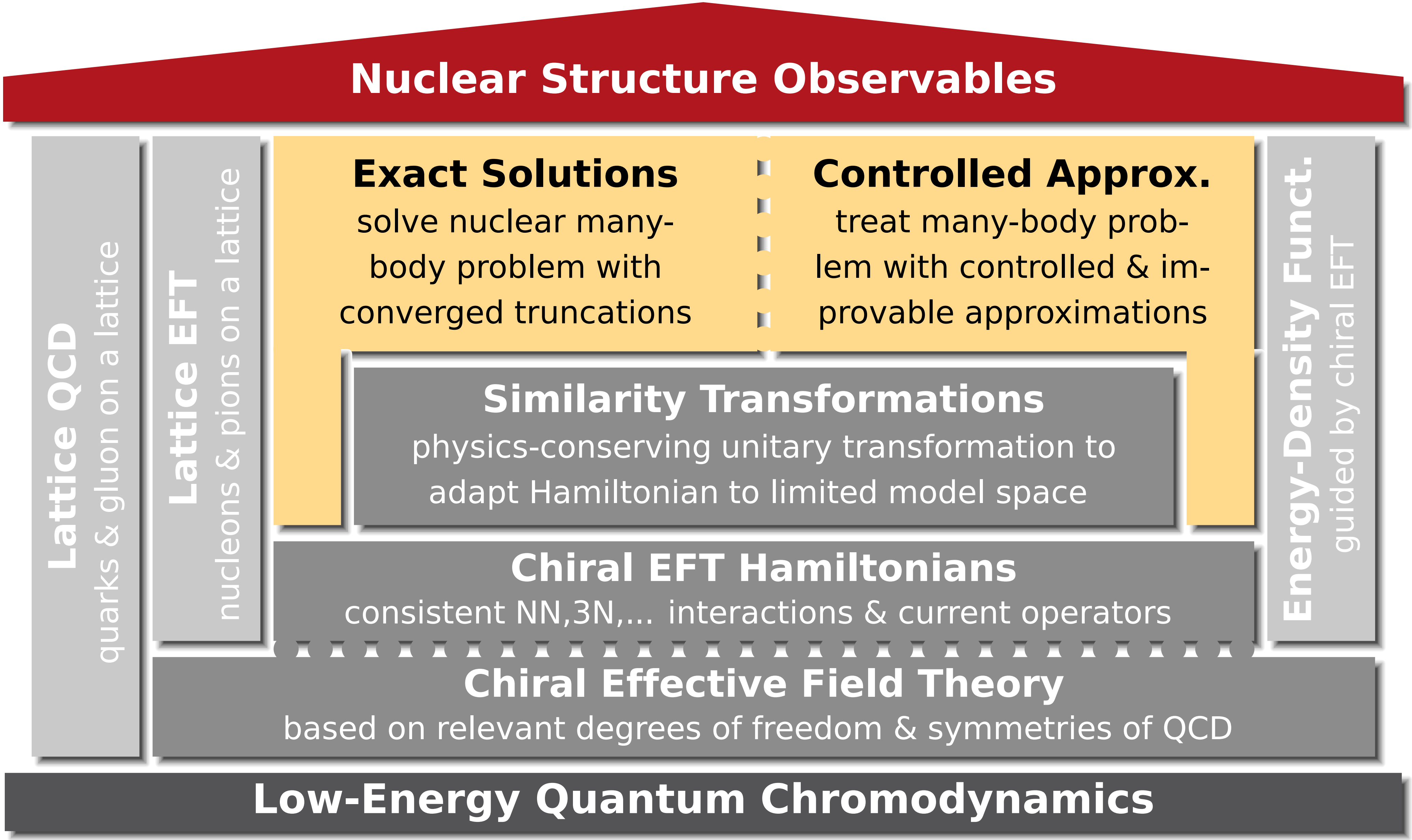


# Frontier: Medium-Mass Nuclei

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 … xponential wave operator applied to single-determinant refer…
  - truncation at doubles level (CCSD) plus tri… …D(T))
  - equations of motion for excited st… …

*…iyama, Schwenk, Hergert,...*

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

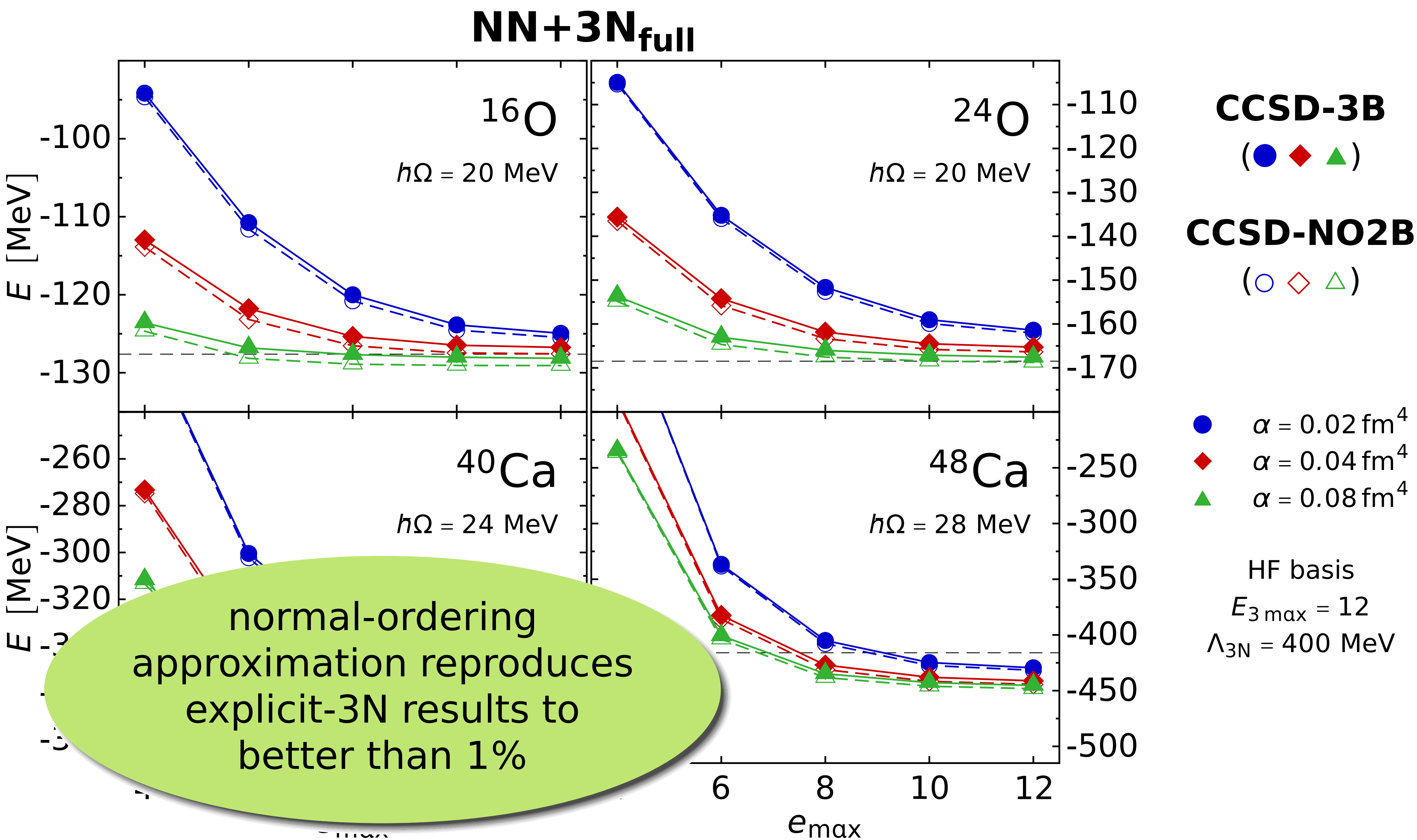
controlling and quantifying the
uncertainties due to various truncations is
major challenge

*Barbieri, Soma, Duguet,...*

- self-consistent Green's function approaches and others...

# CCSD with Explicit 3N Interactions

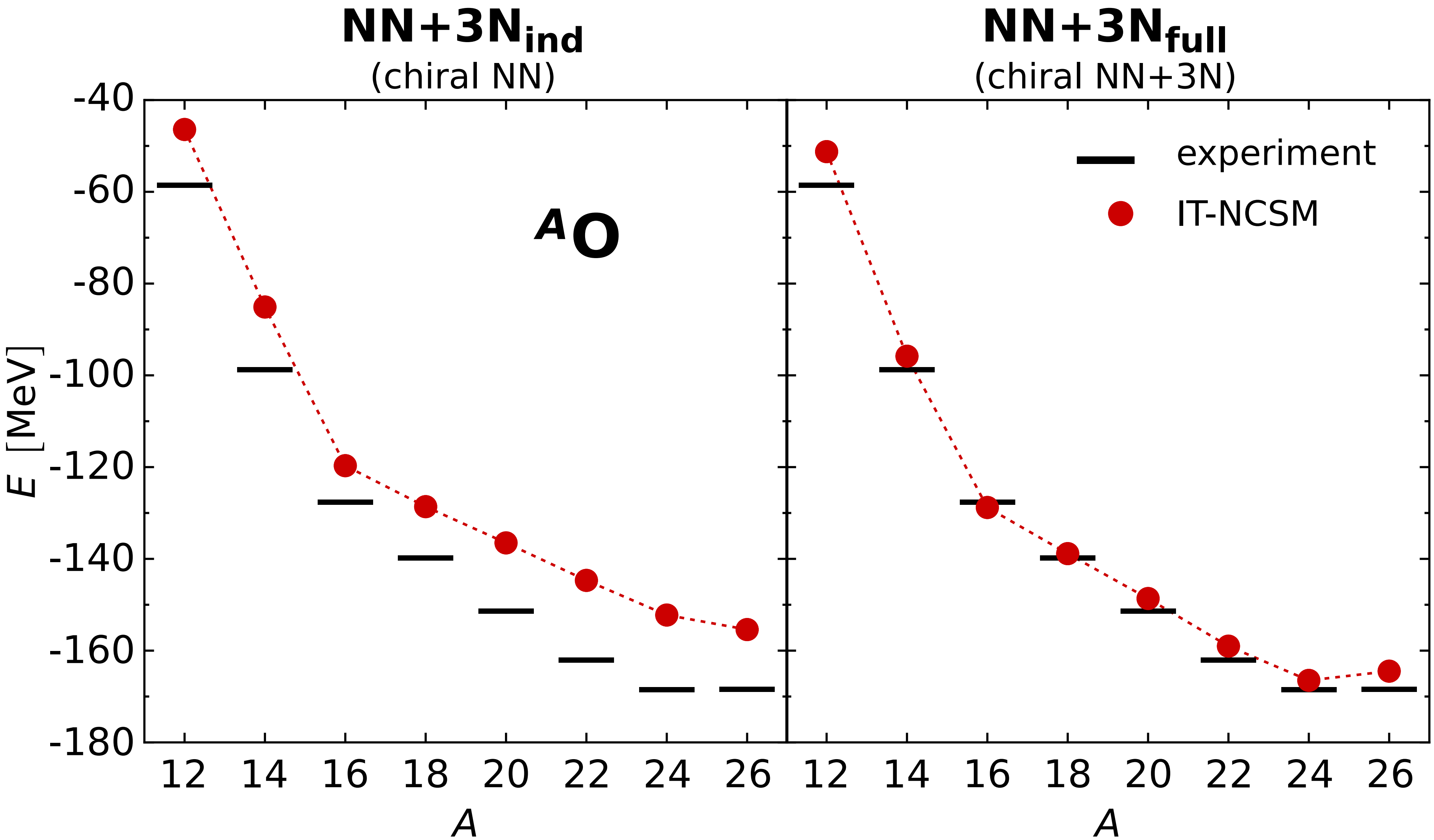
Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)




normal-ordering approximation reproduces explicit-3N results to better than 1%

# Ground States of Oxygen Isotopes

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

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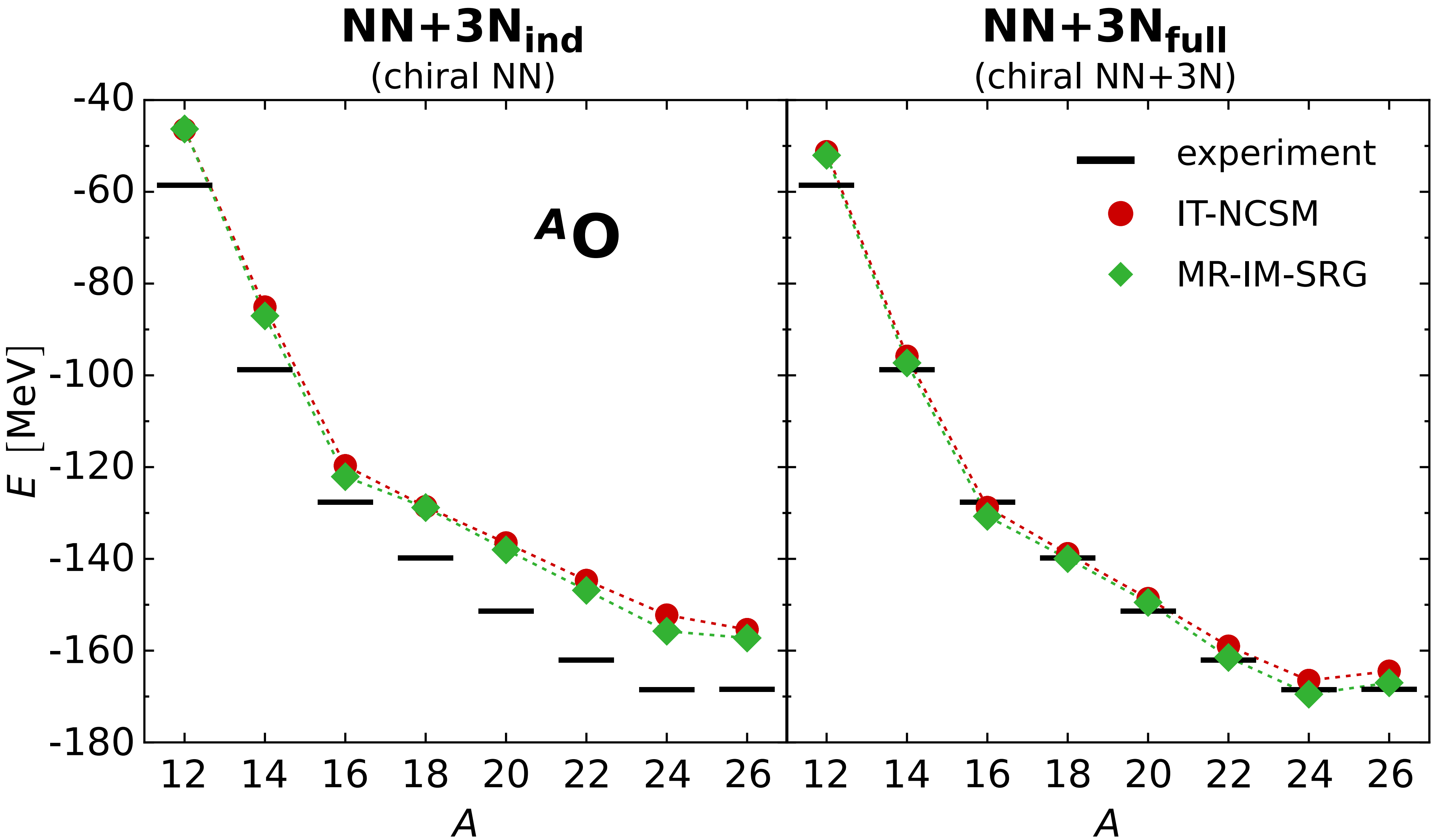


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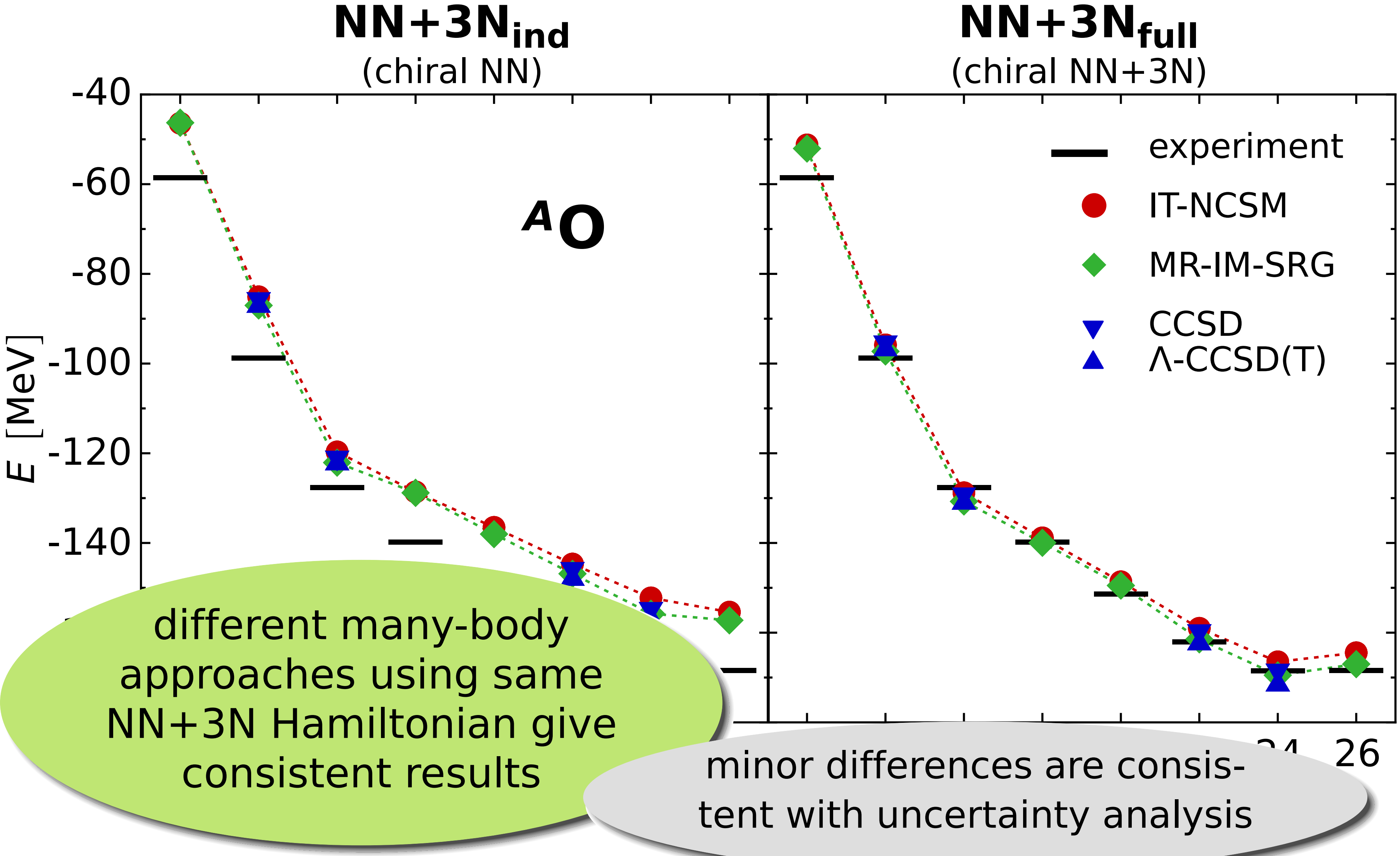


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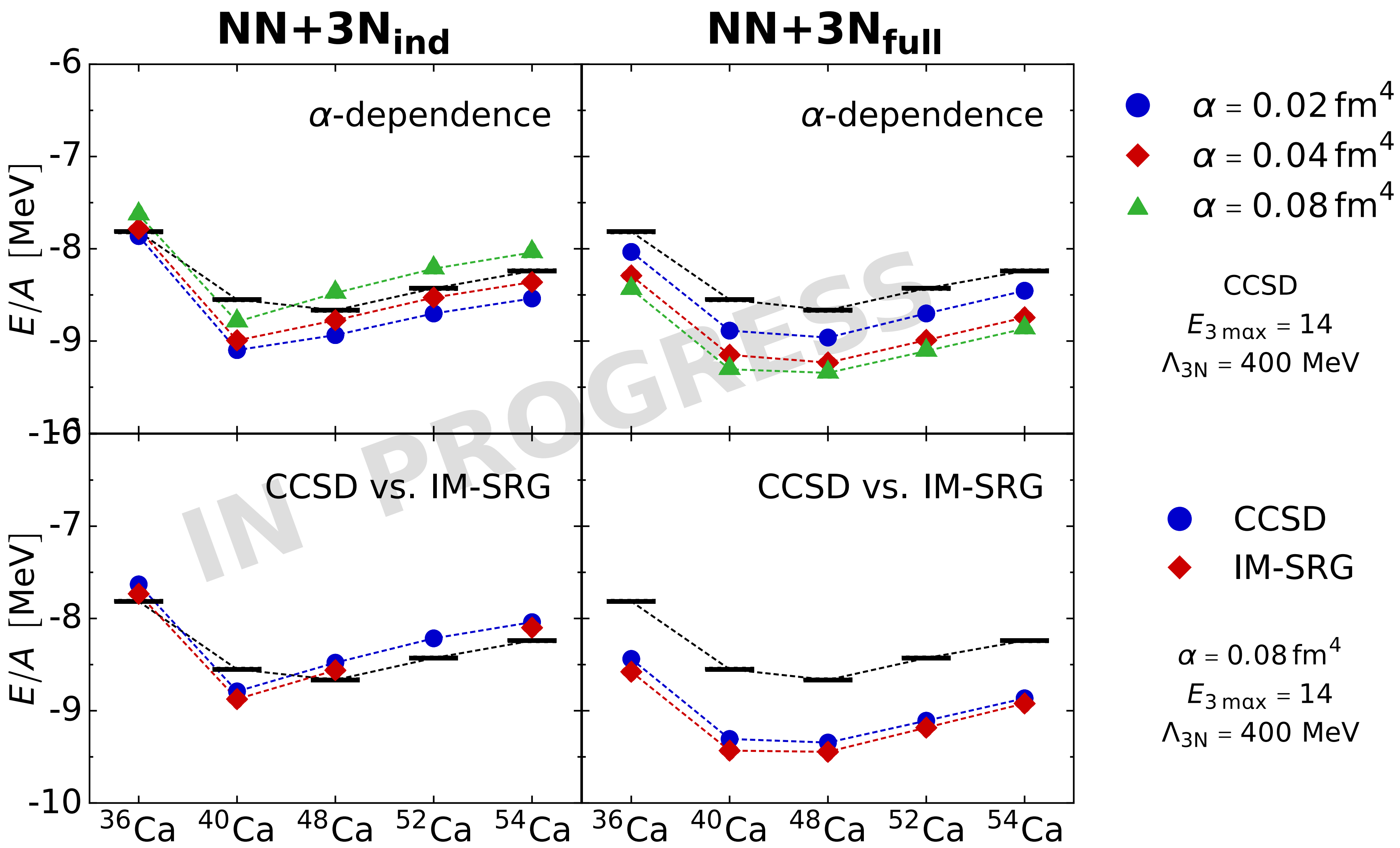
# Next Step: Calcium & Nickel Isotopes



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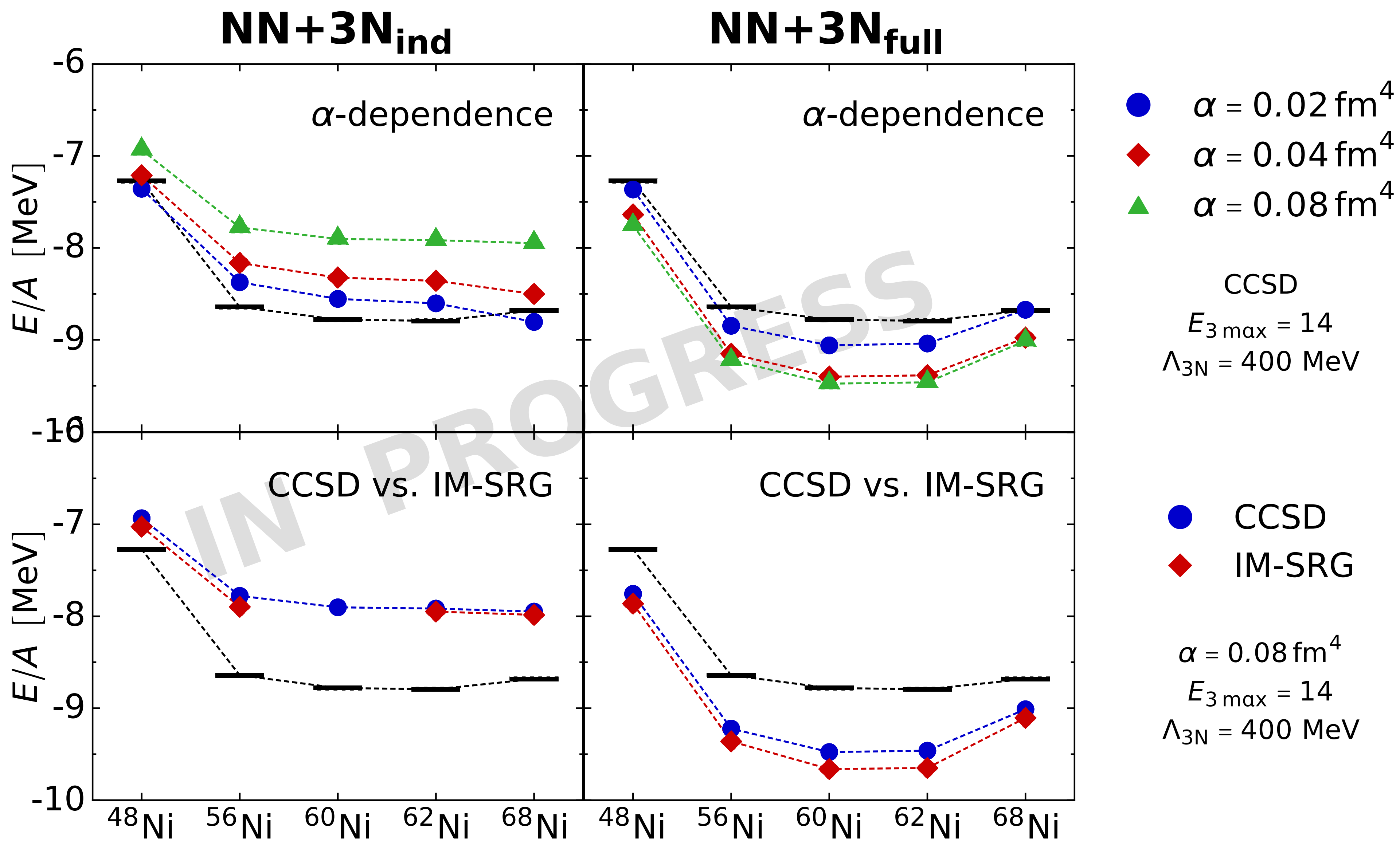

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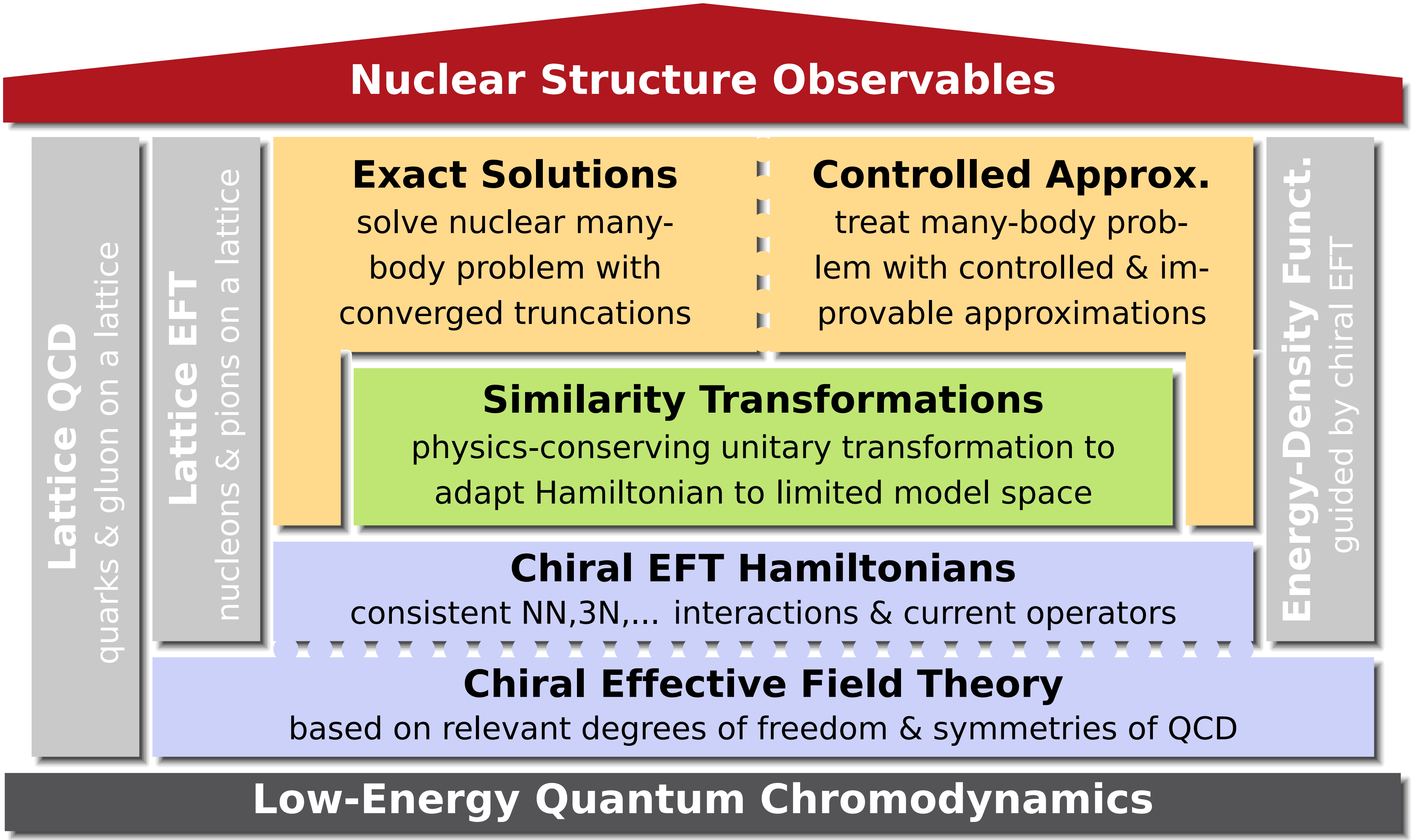
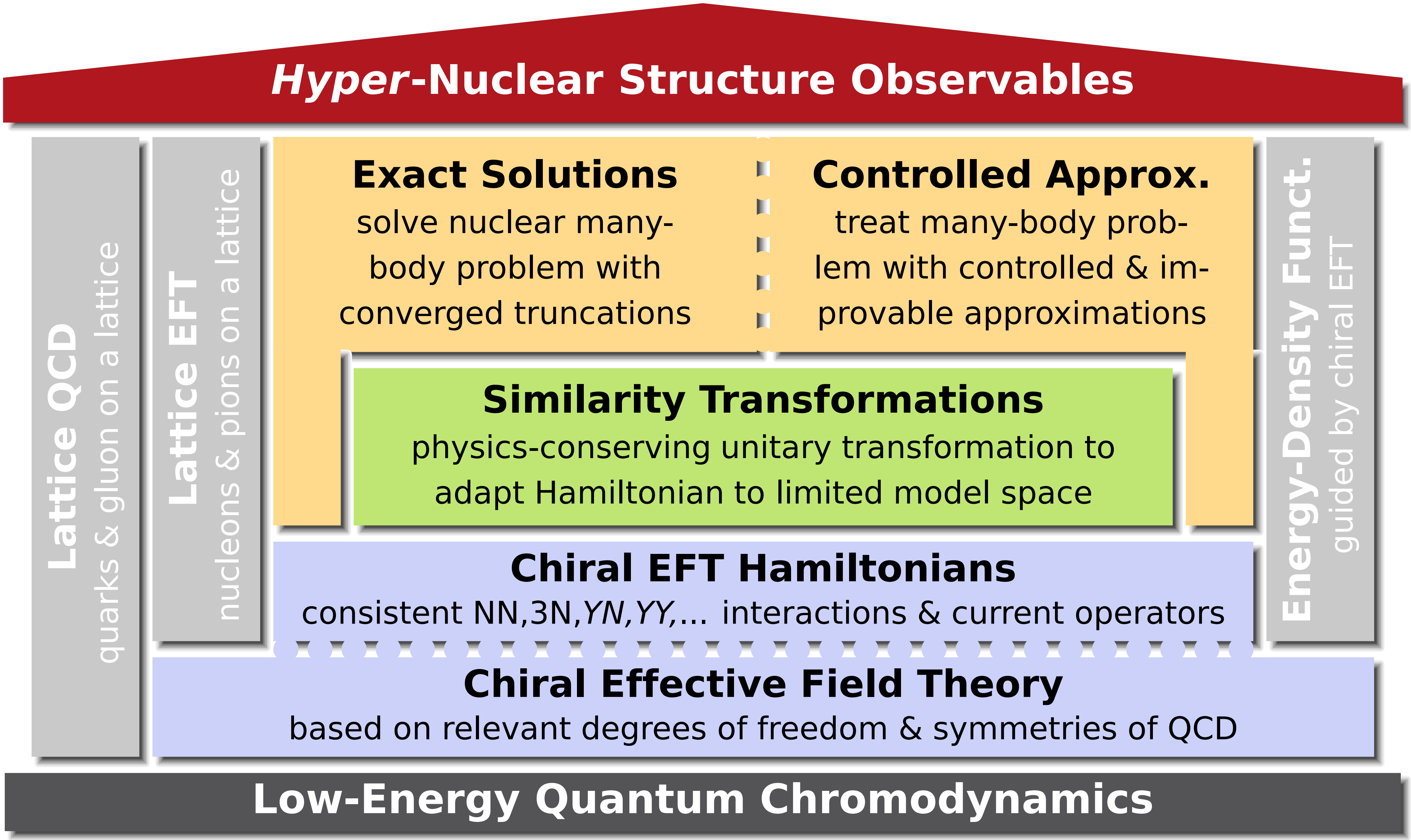
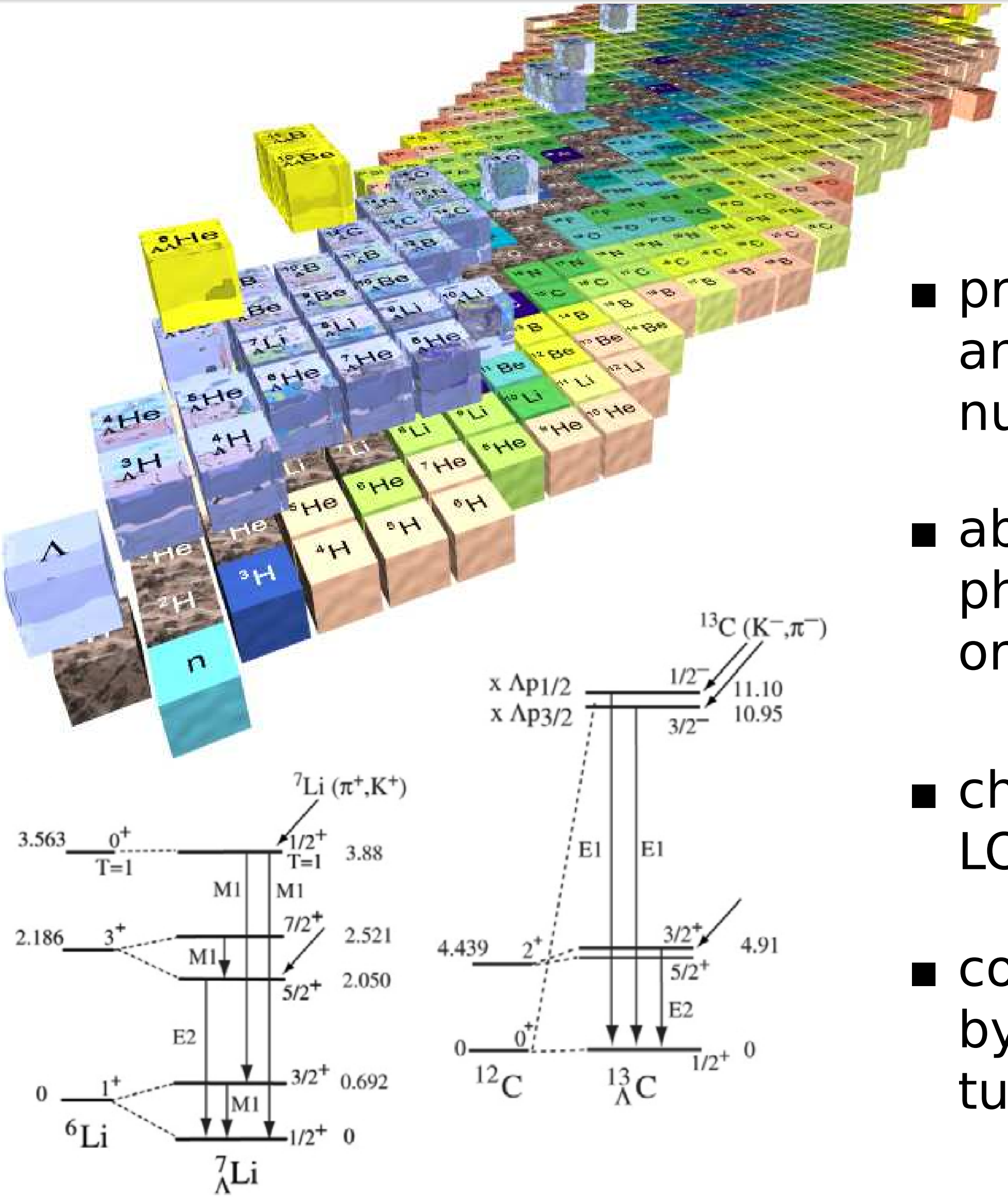


# Ab Initio *Hyper*-Nuclear Structure



# Motivation: Hyper-Nuclear Structure

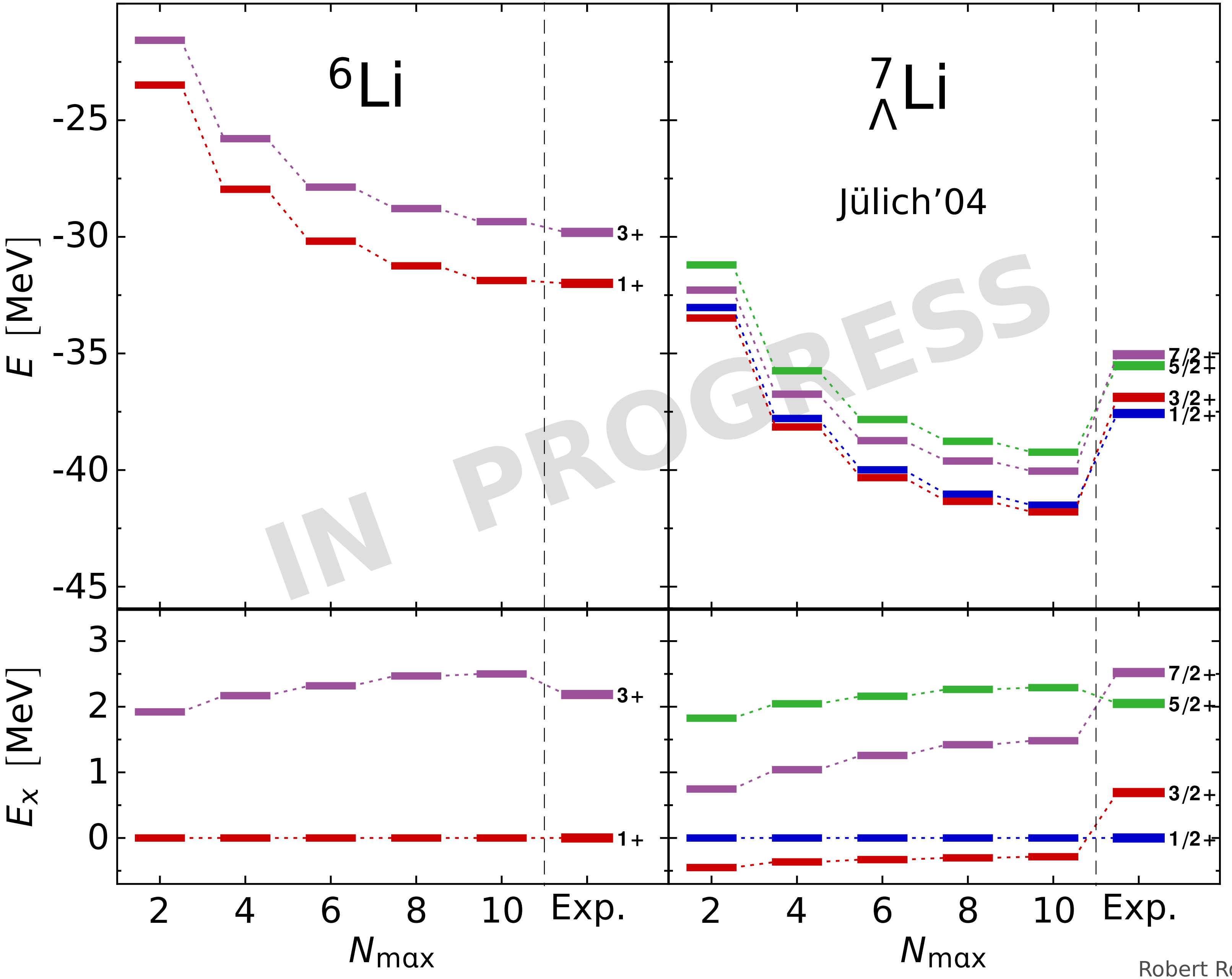



- precision data on ground states and spectroscopy of hyper-nuclei: talk by Nakamura
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations so far

*Haidenbauer et al.*

- chiral YN & YY interactions at LO and NLO are available
- constrain YN & YY interaction by ab initio hyper-nuclear structure calculations

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



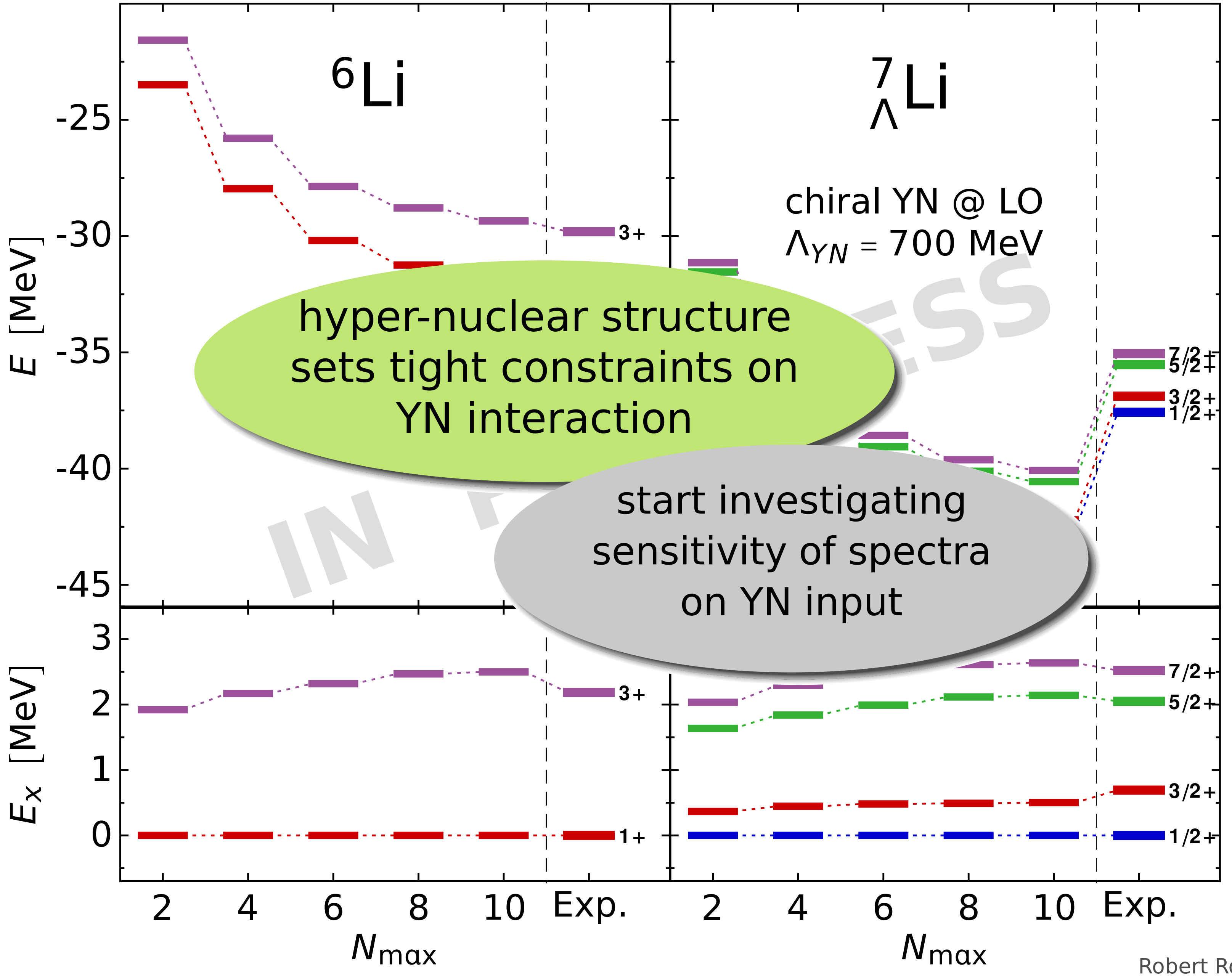

**NN @ N3LO**
Entem&Machleidt
$\Lambda_{NN} = 500$ MeV

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




hyper-nuclear structure sets tight constraints on YN interaction

start investigating sensitivity of spectra on YN input

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

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

YN @ LO
Haidenbauer et al.
$\Lambda_{YN}$ = 700 MeV
scatt. & hypertriton

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

# 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. Krutsch, **J. Langhammer**, S. Reinhardt, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, **R. Wirth**
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    Michigan State University, USA
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    IPN Orsay, F
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    Chalmers University, Sweden
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HIC for FAIR
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Exzellente Forschung für Hessens Zukunft

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COMPUTING TIME