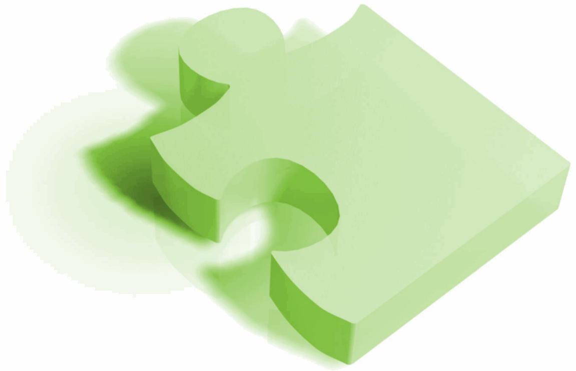
Frontiers in Ab Initio Nuclear Structure Theory

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

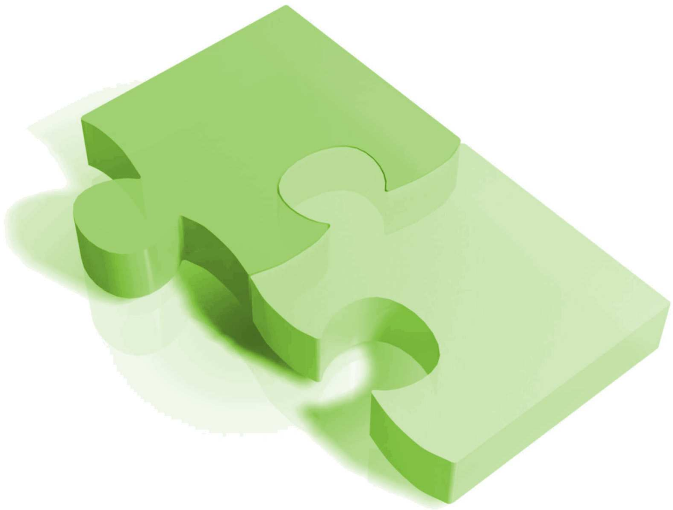
New Era of Nuclear Structure Theory



- **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

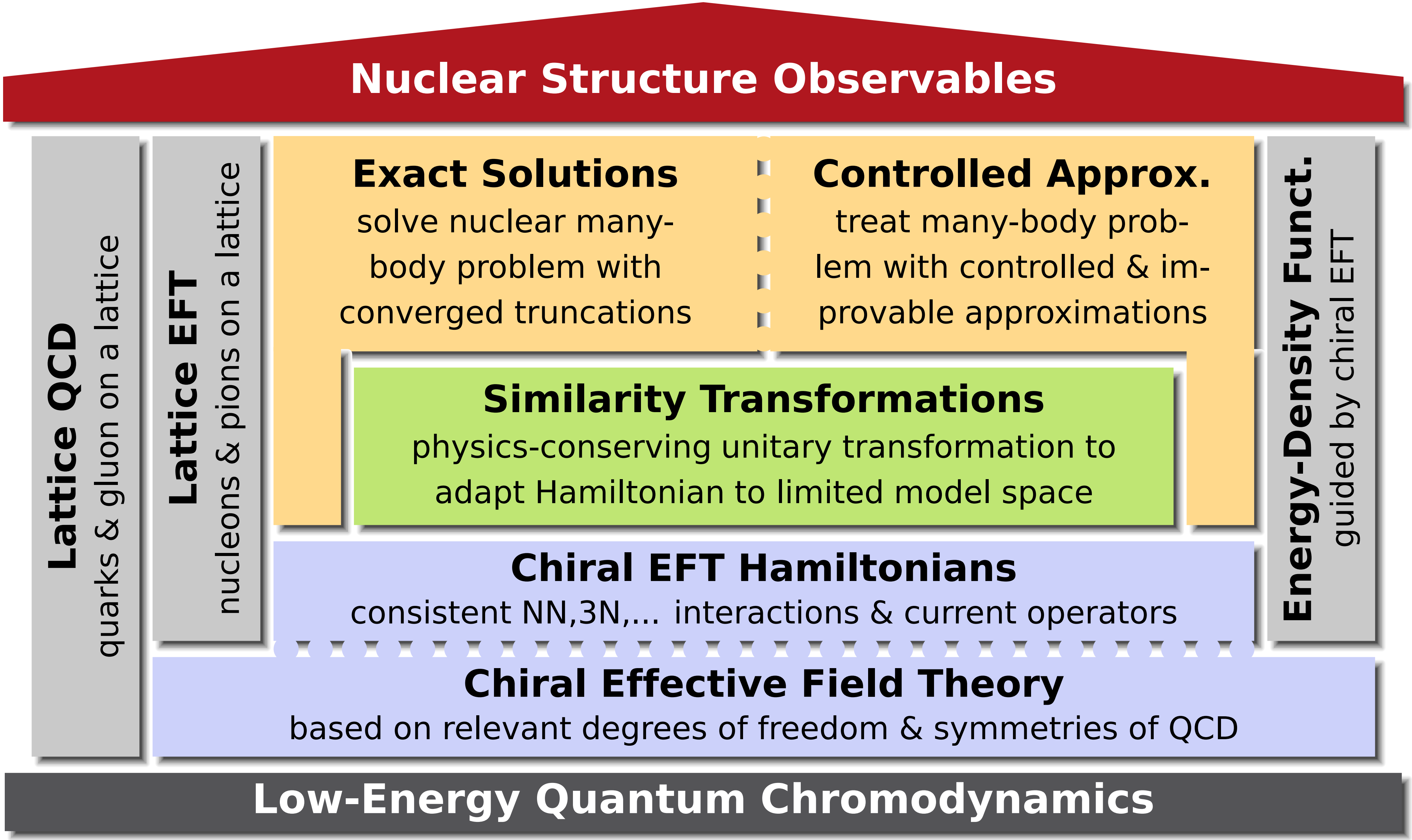
- **computing & algorithms**

  increase of computational resources & improved algorithms

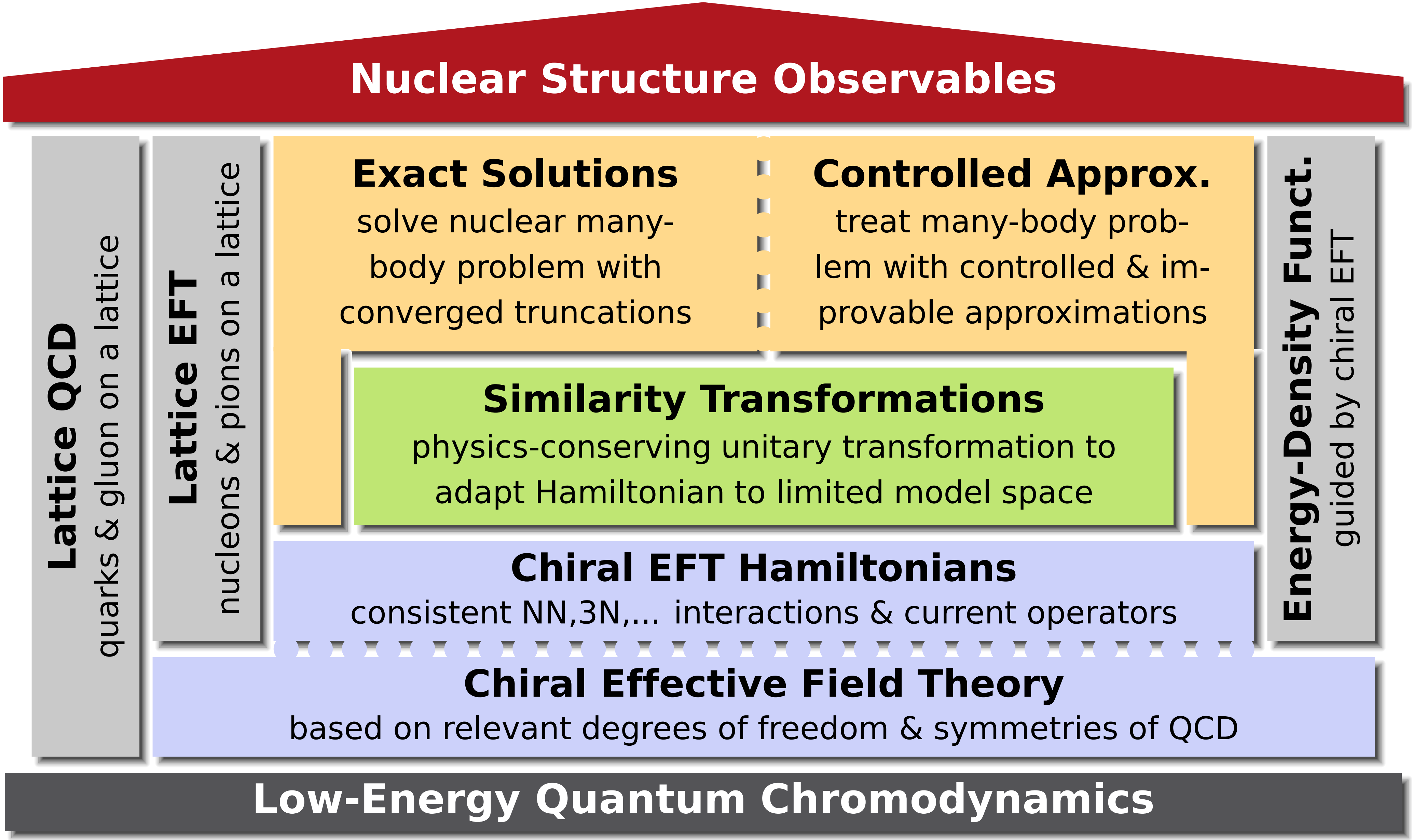
New Era of Nuclear Structure Theory

- **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

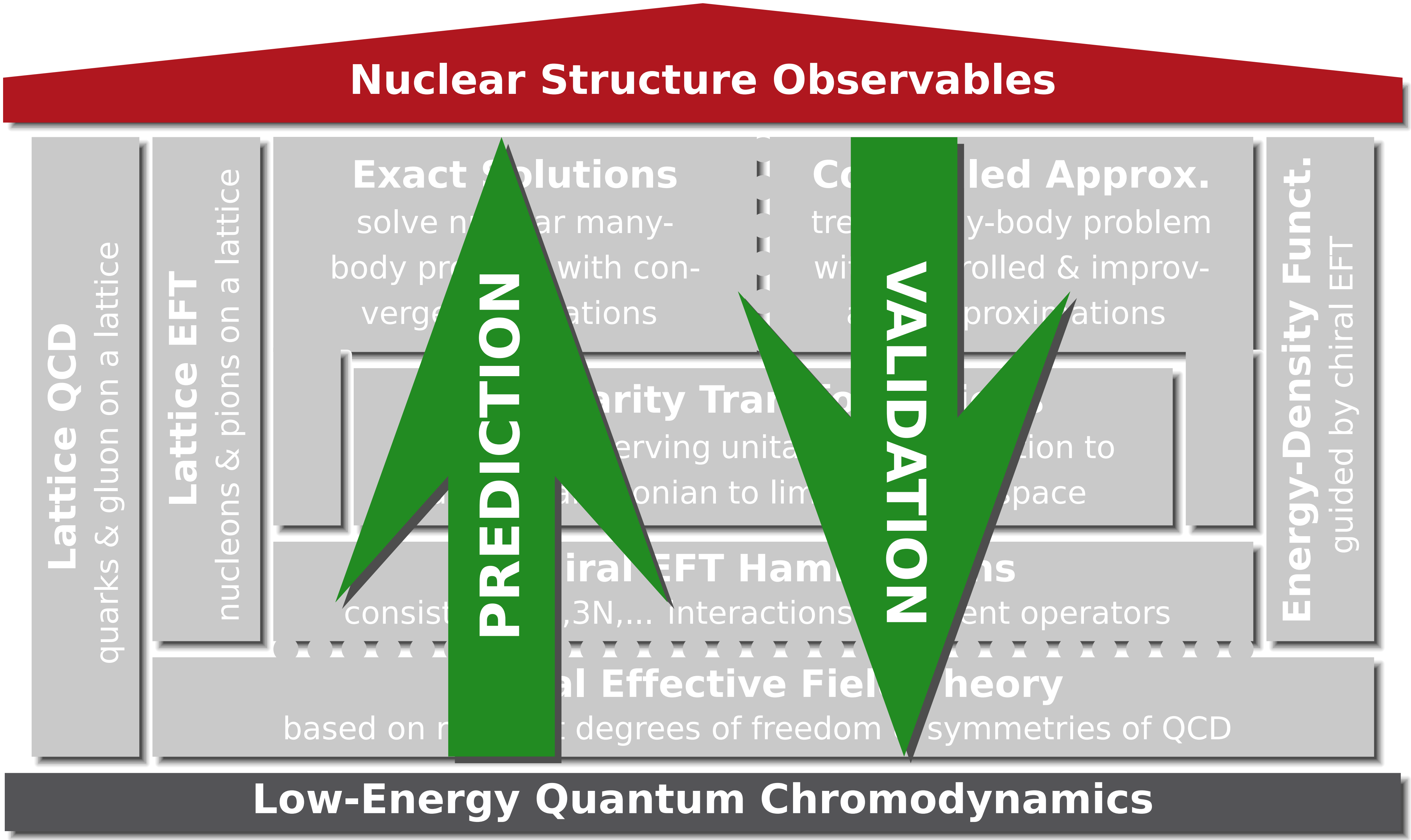
Ab Initio Nuclear Structure



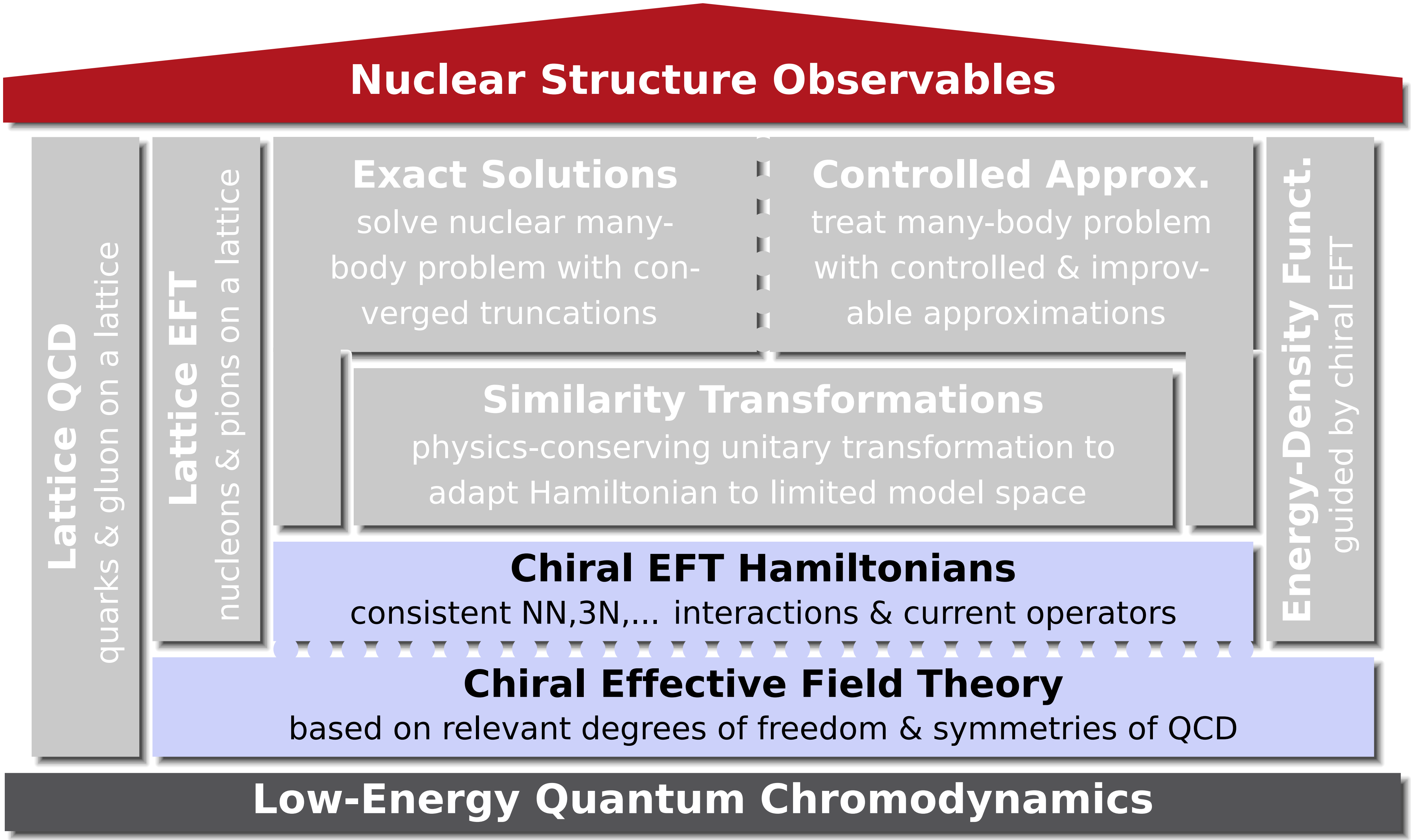
Ab Initio Nuclear Structure



Ab Initio Nuclear Structure



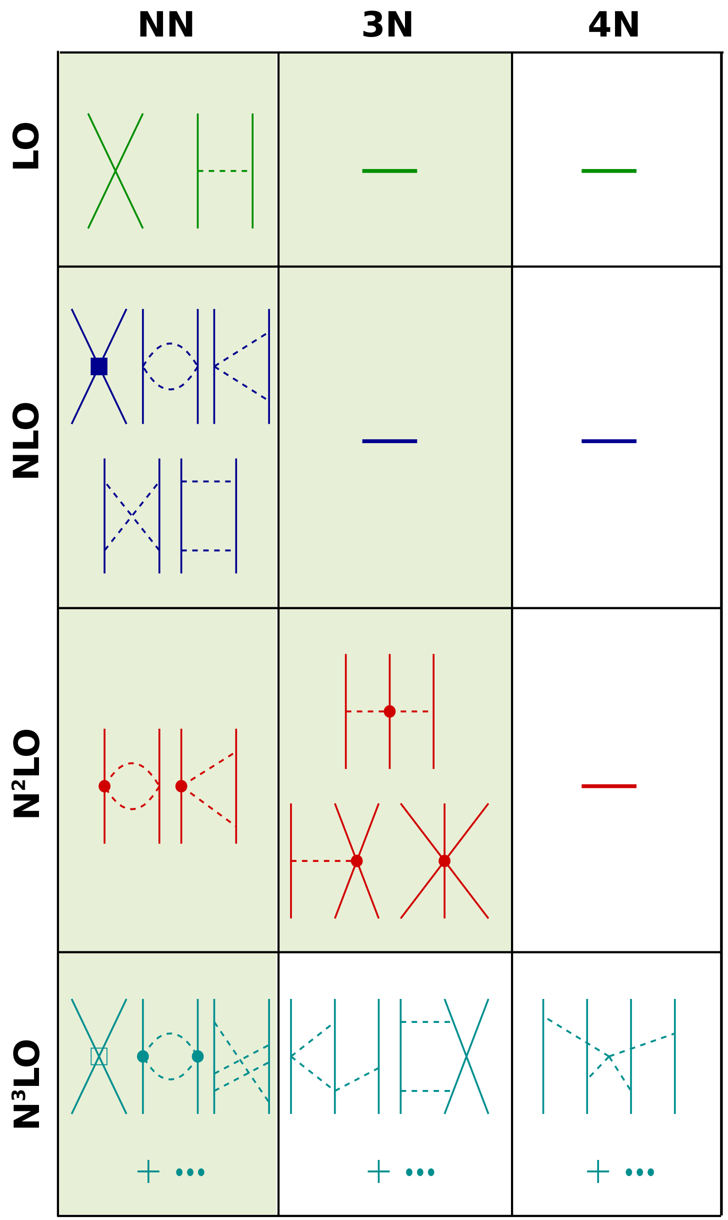
Ab Initio Nuclear Structure



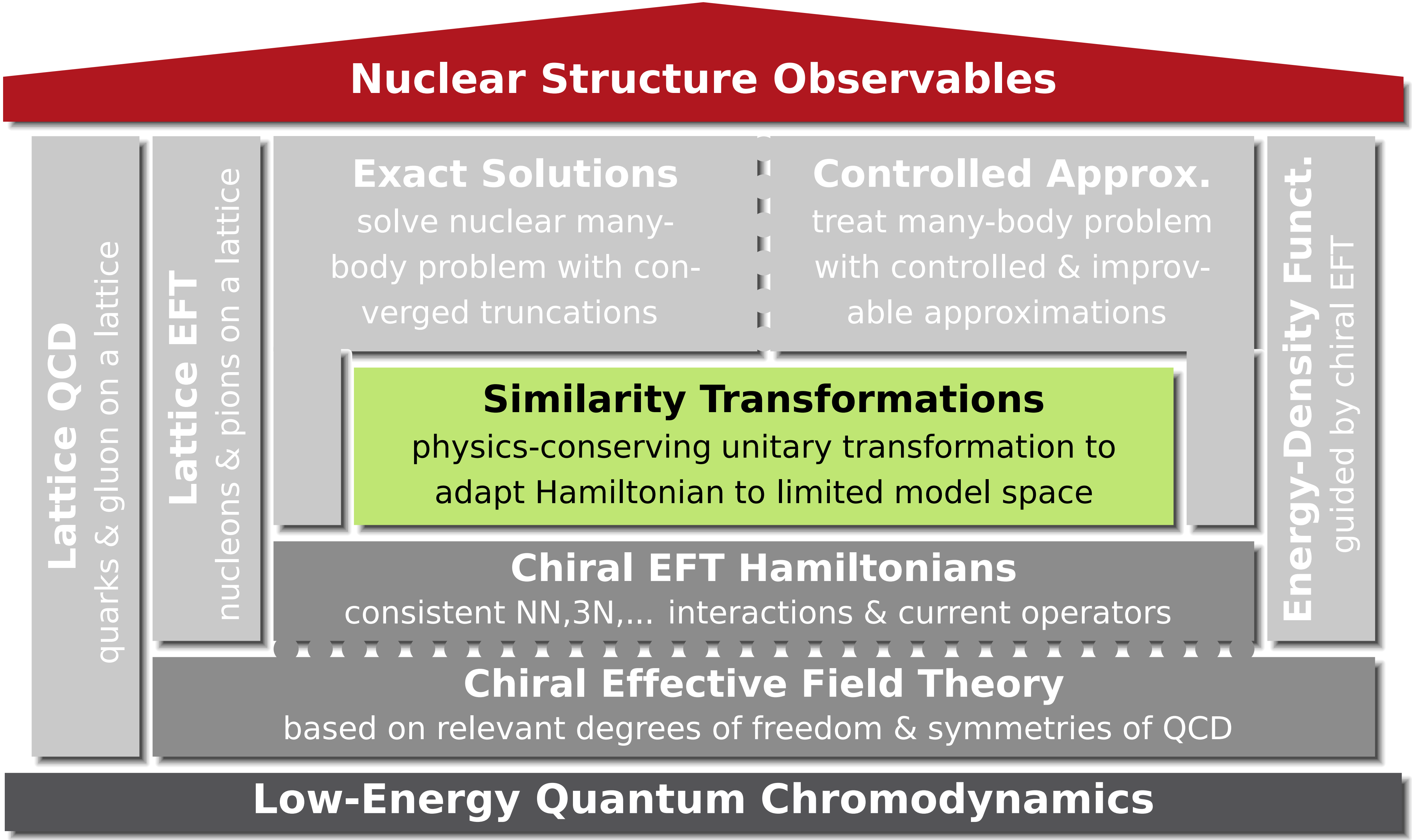
Nuclear Interactions from Chiral EFT

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** fitted to data (NN, πN,...)
- 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
- many ongoing developments



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

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

- **unitary transformation** of Hami

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

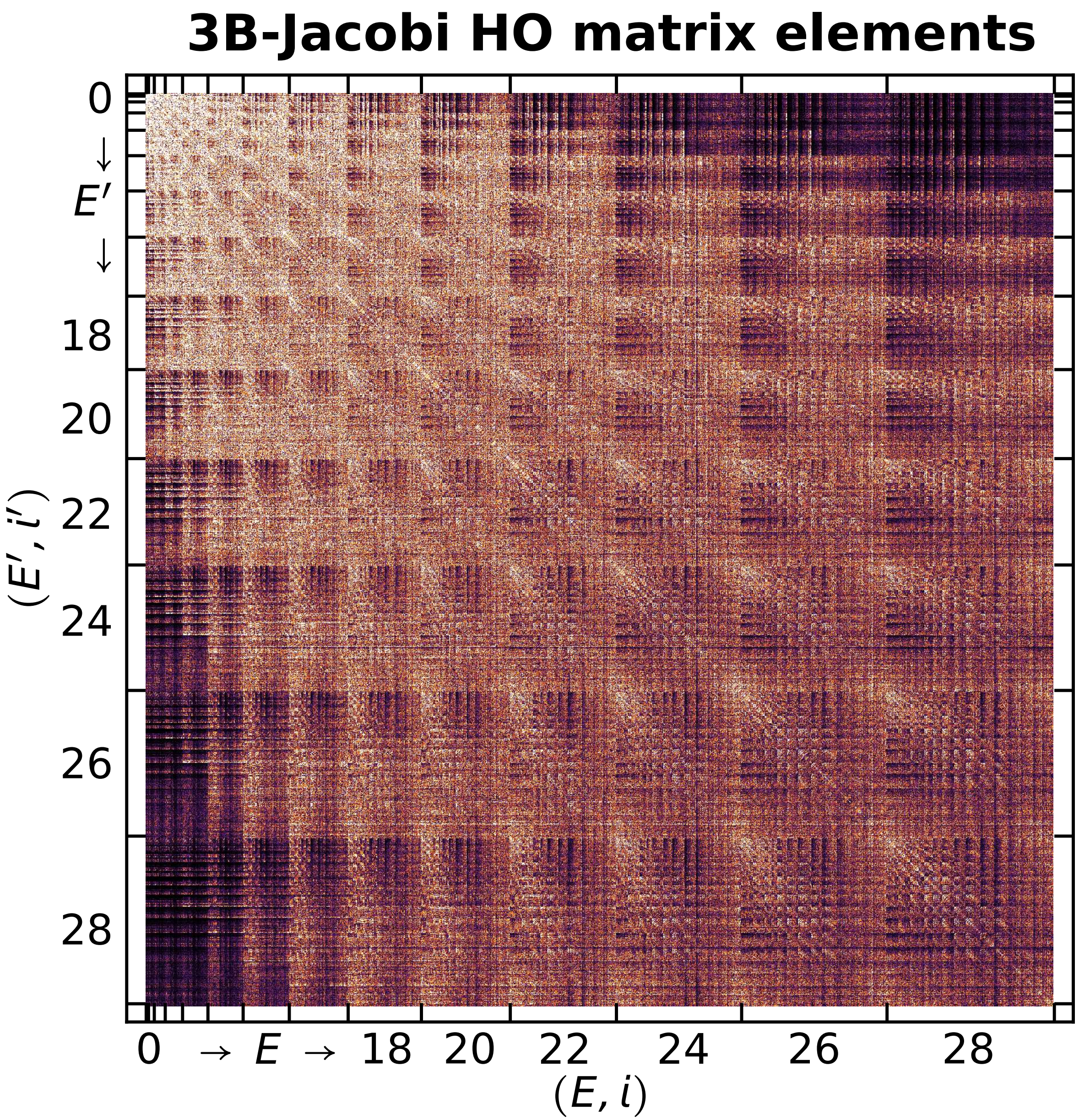
- **evolution equations** for H_α and U

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

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

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

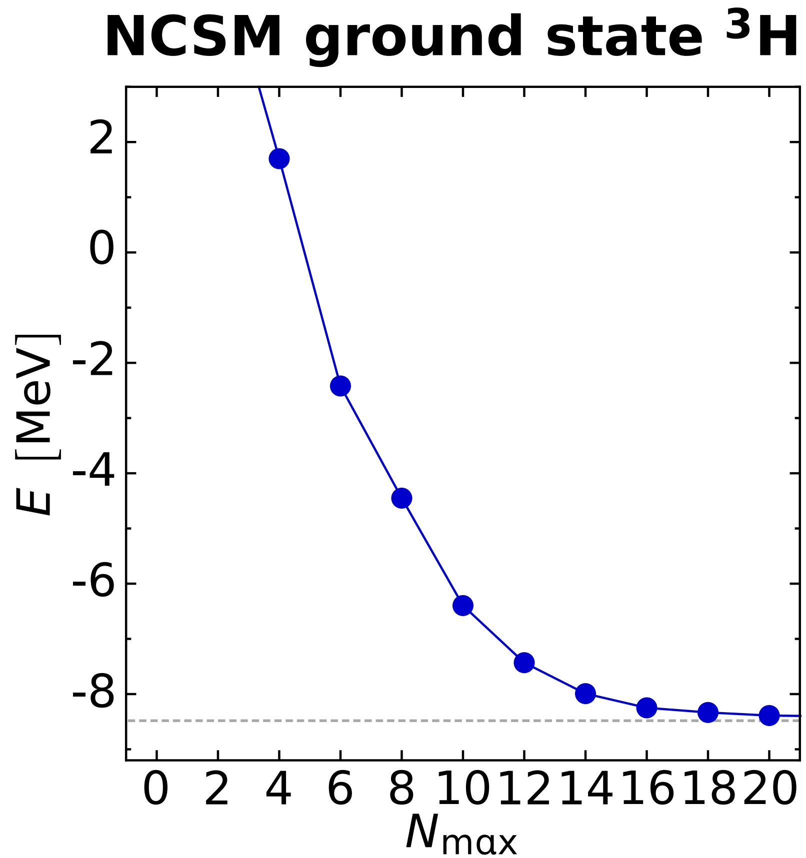
SRG Evolution in Three-Body Space



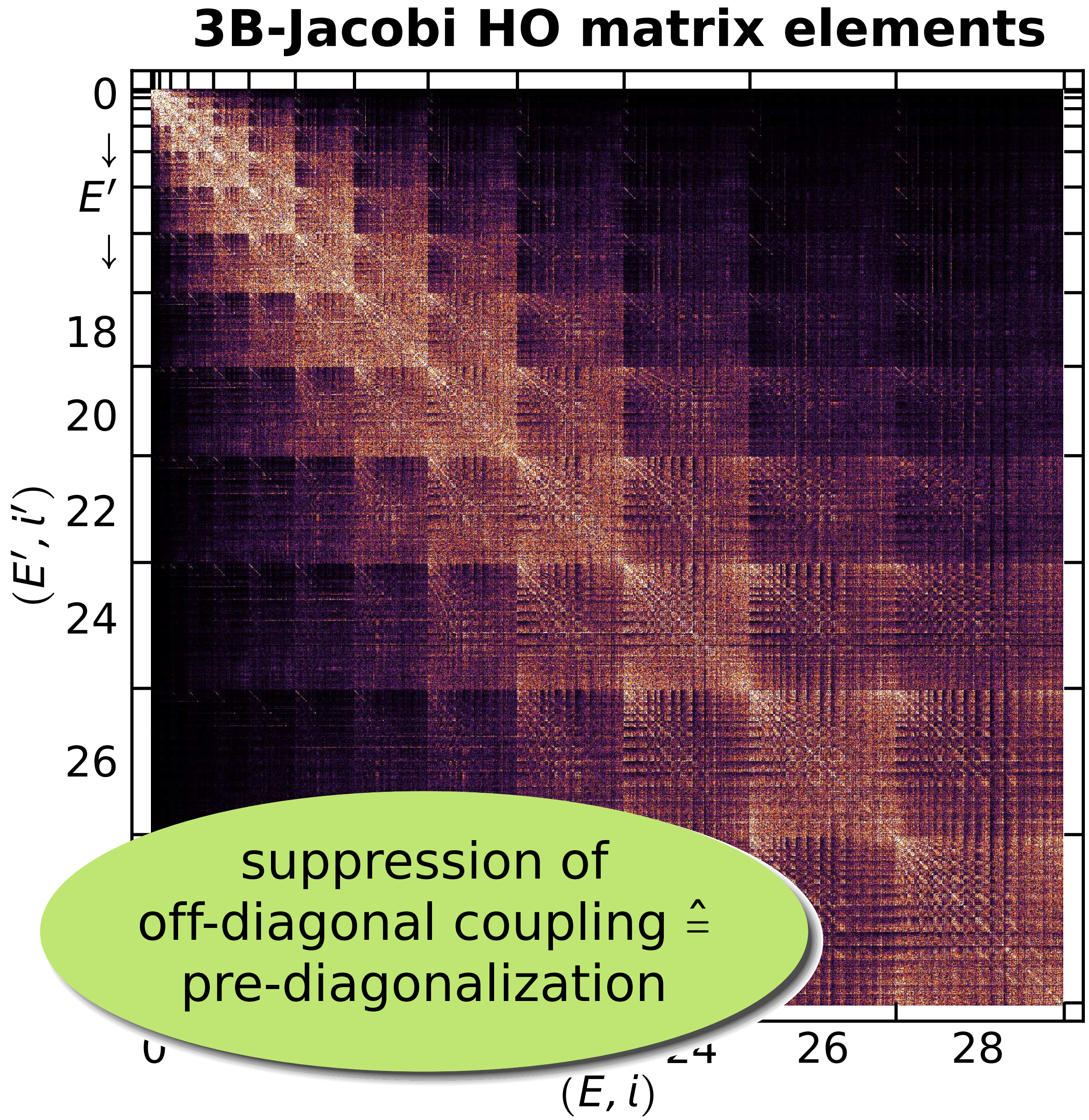
$\alpha = 0.000\,\text{fm}^4$

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

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



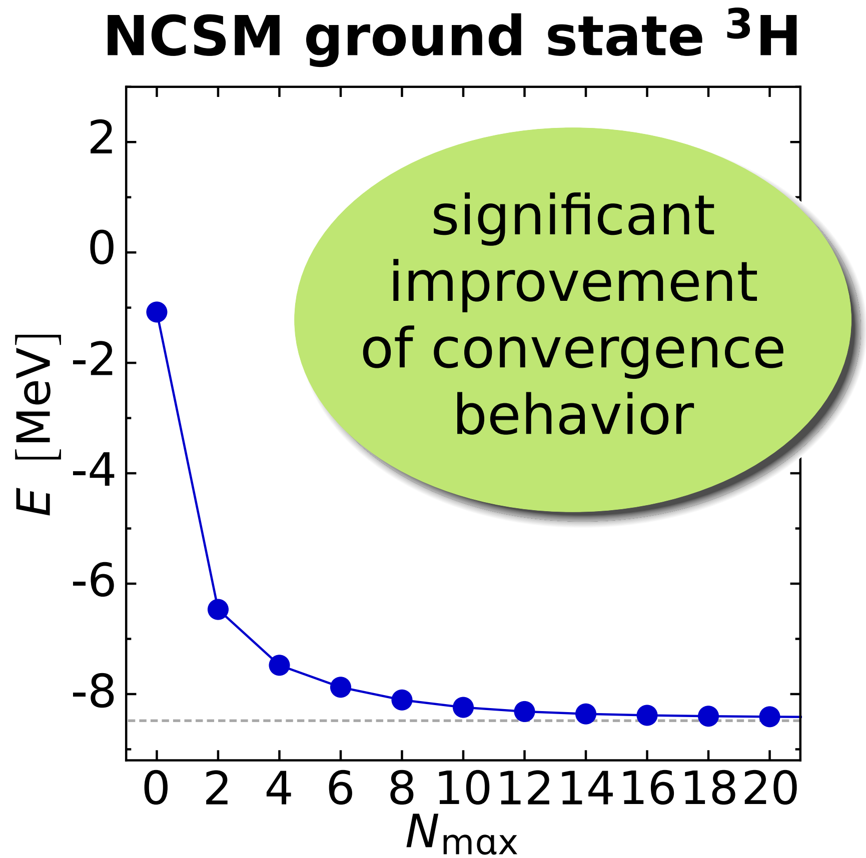
SRG Evolution in Three-Body Space



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

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

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



Hamiltonian in A-Body Space

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

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

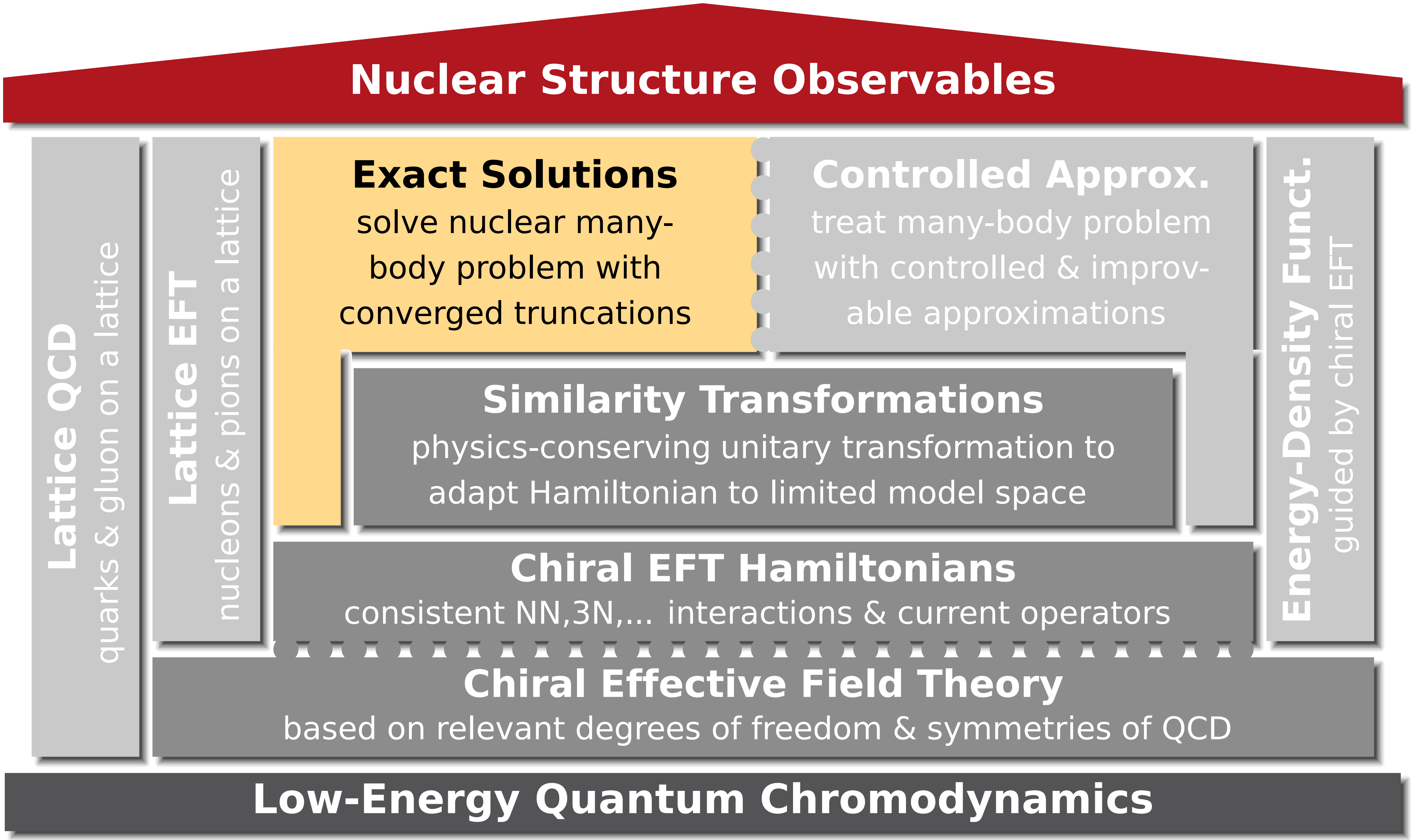
- **truncation of cluster series** formally destroys unitarity and invariance of energy eigenvalues (independence of α)

- 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

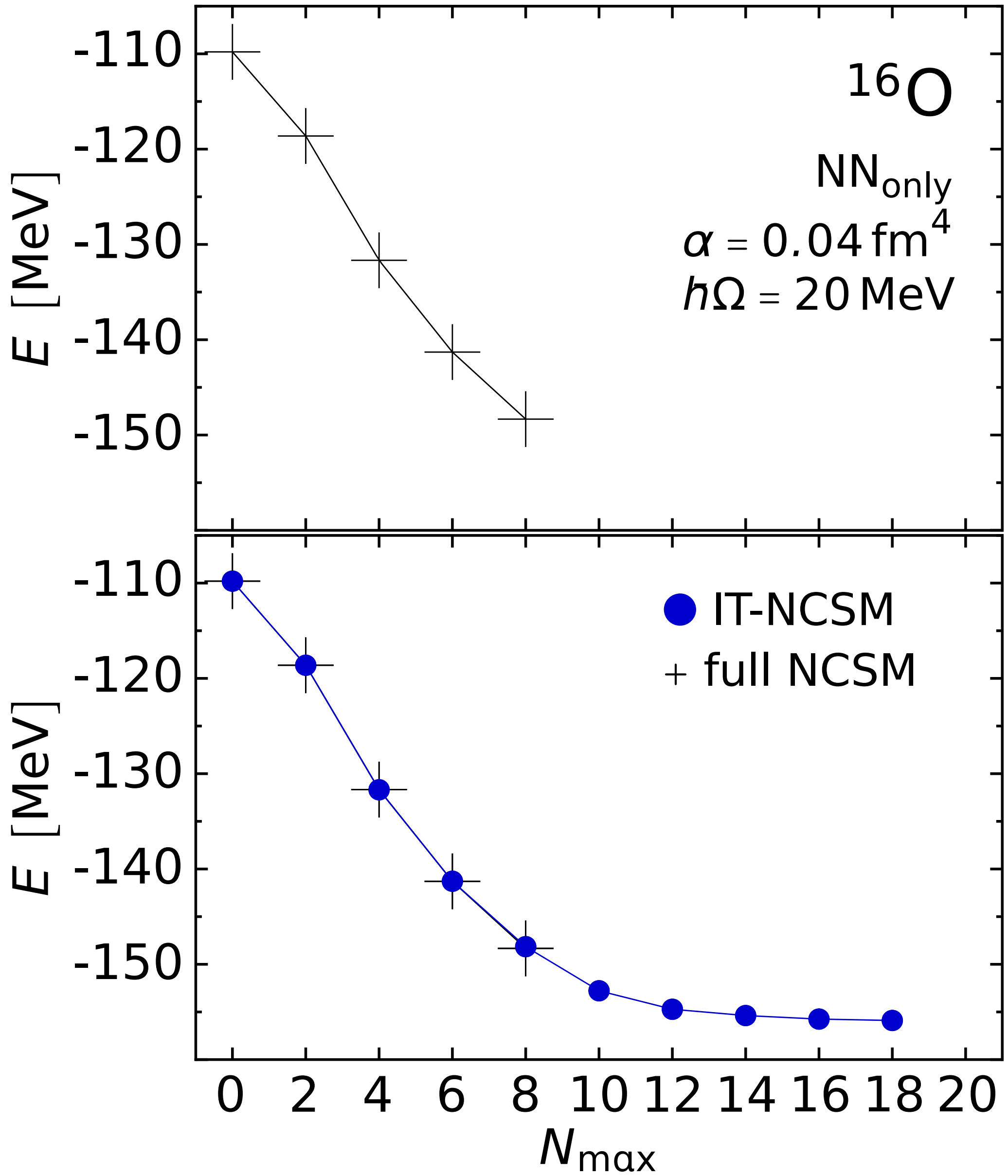
Importance Truncated NCSM

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})

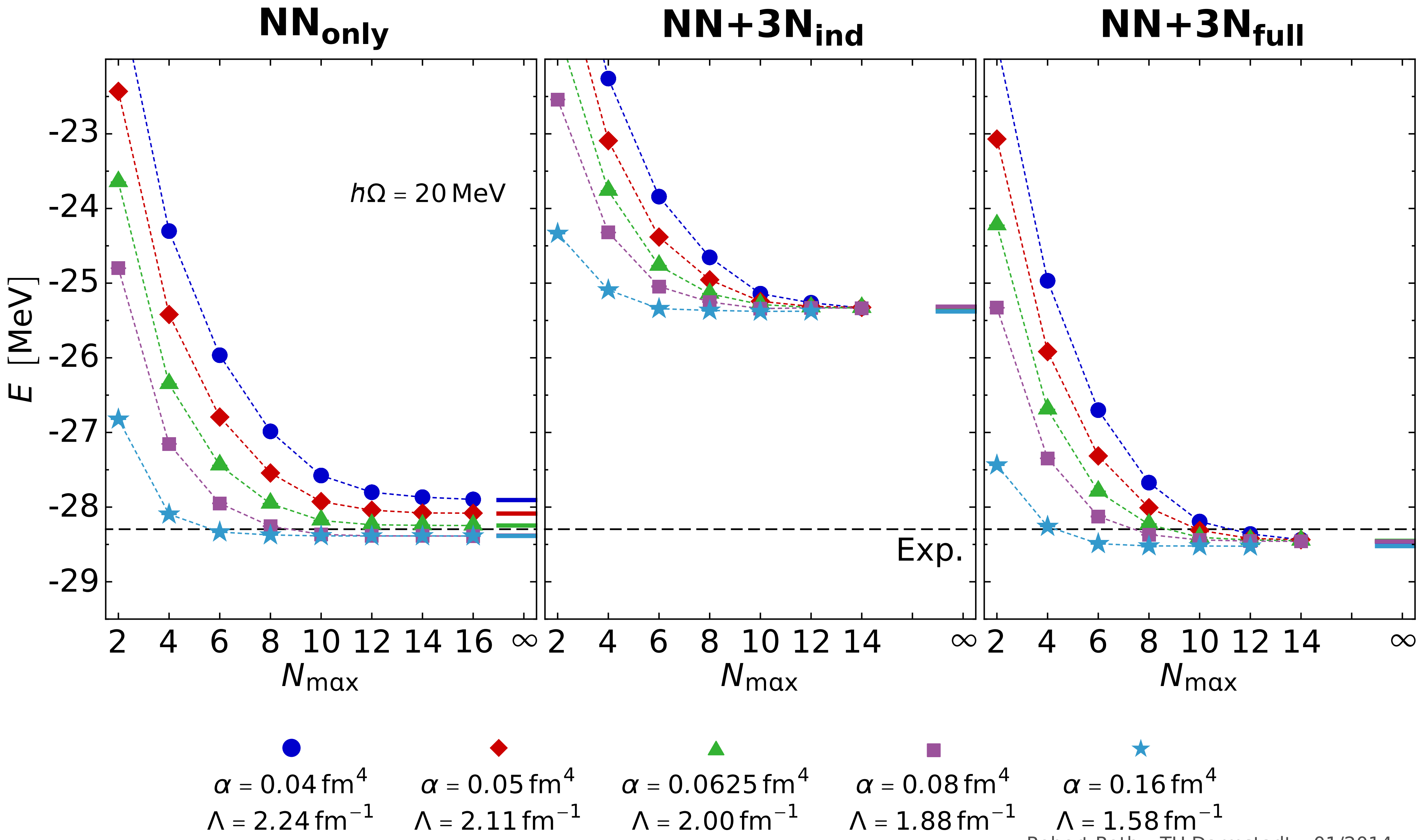
Importance Truncation

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



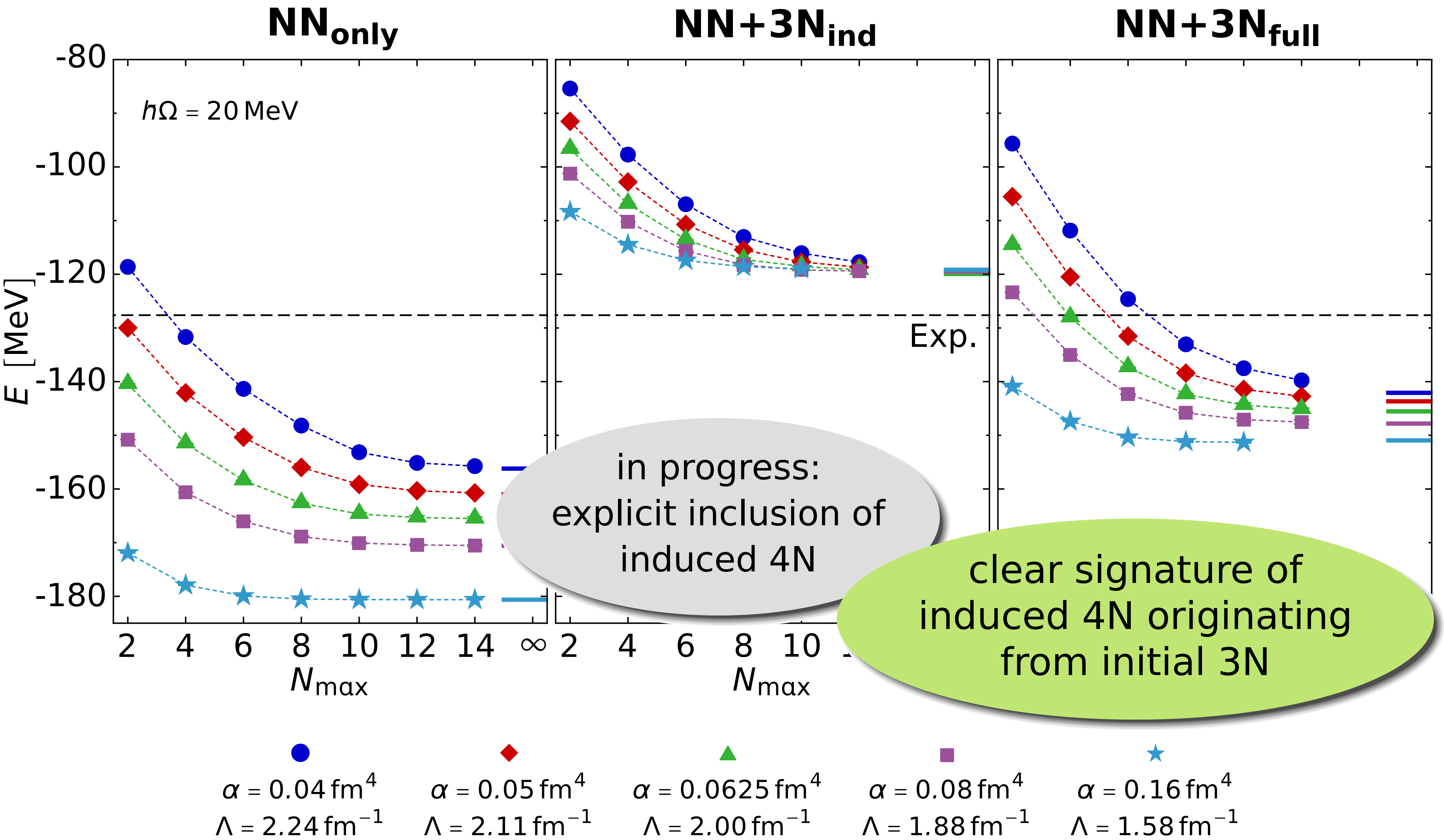
^{4}He: Ground-State Energies

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

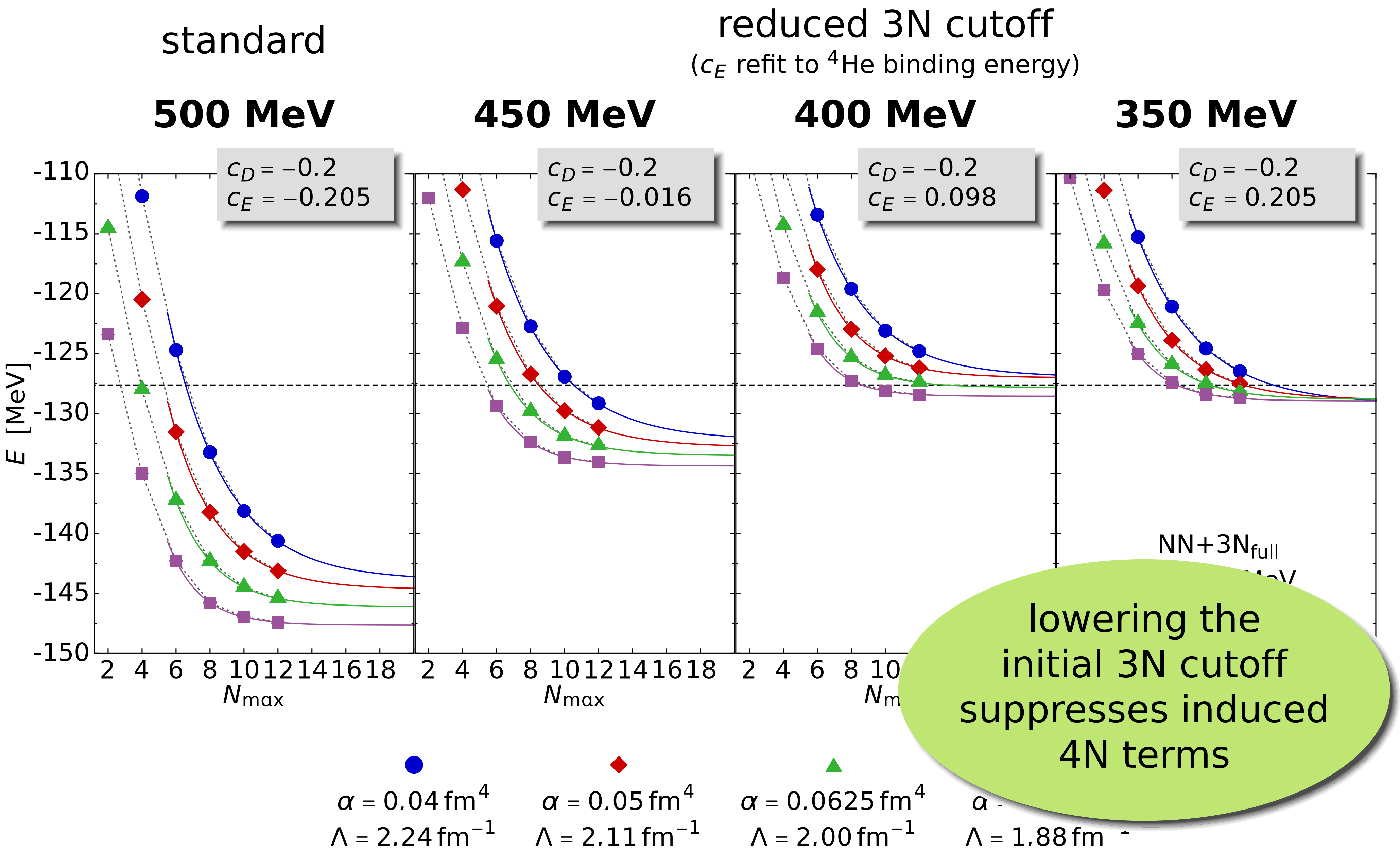


^{16}O: Ground-State Energies

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



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



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)

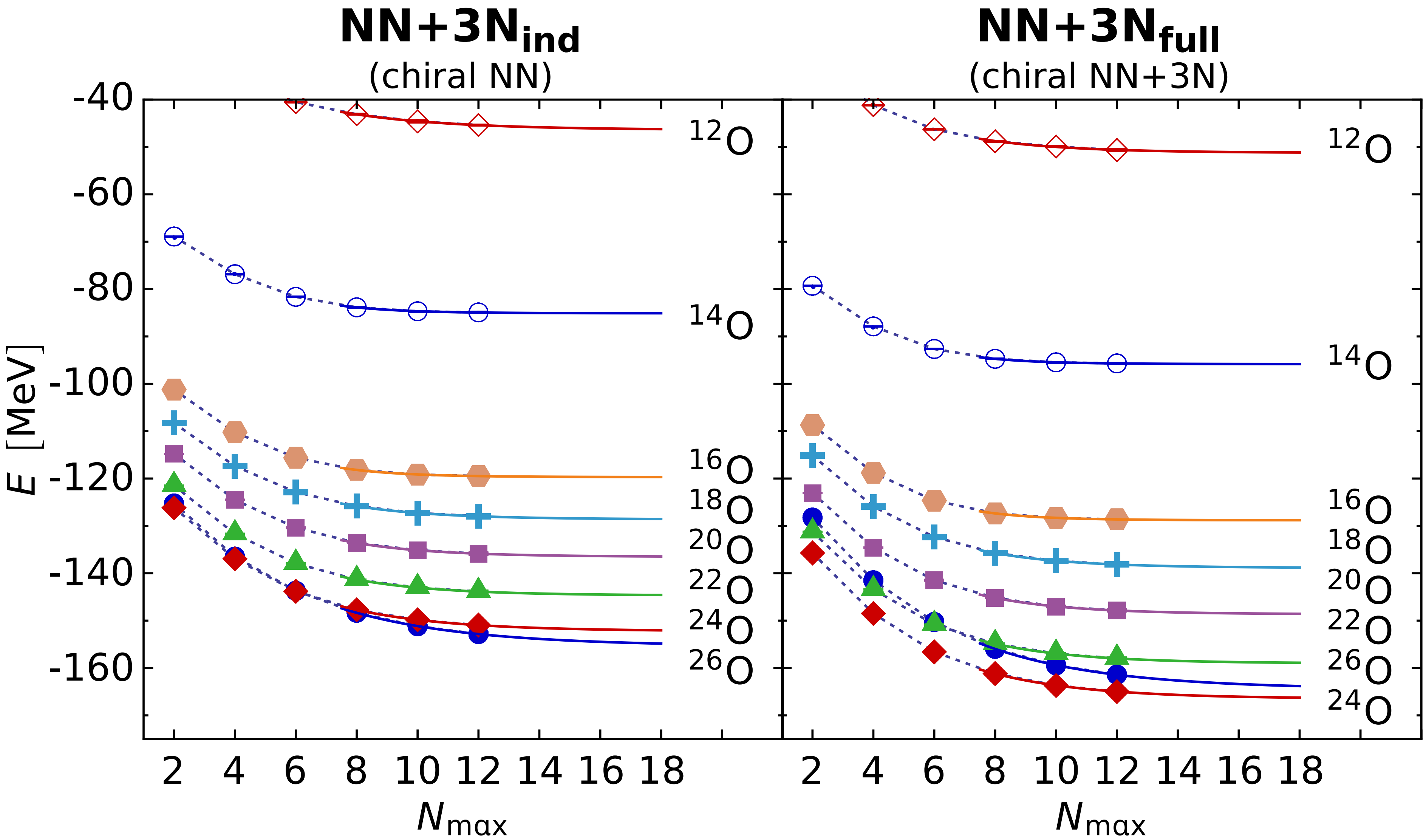
- 2012: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

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

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

Ground States of Oxygen Isotopes

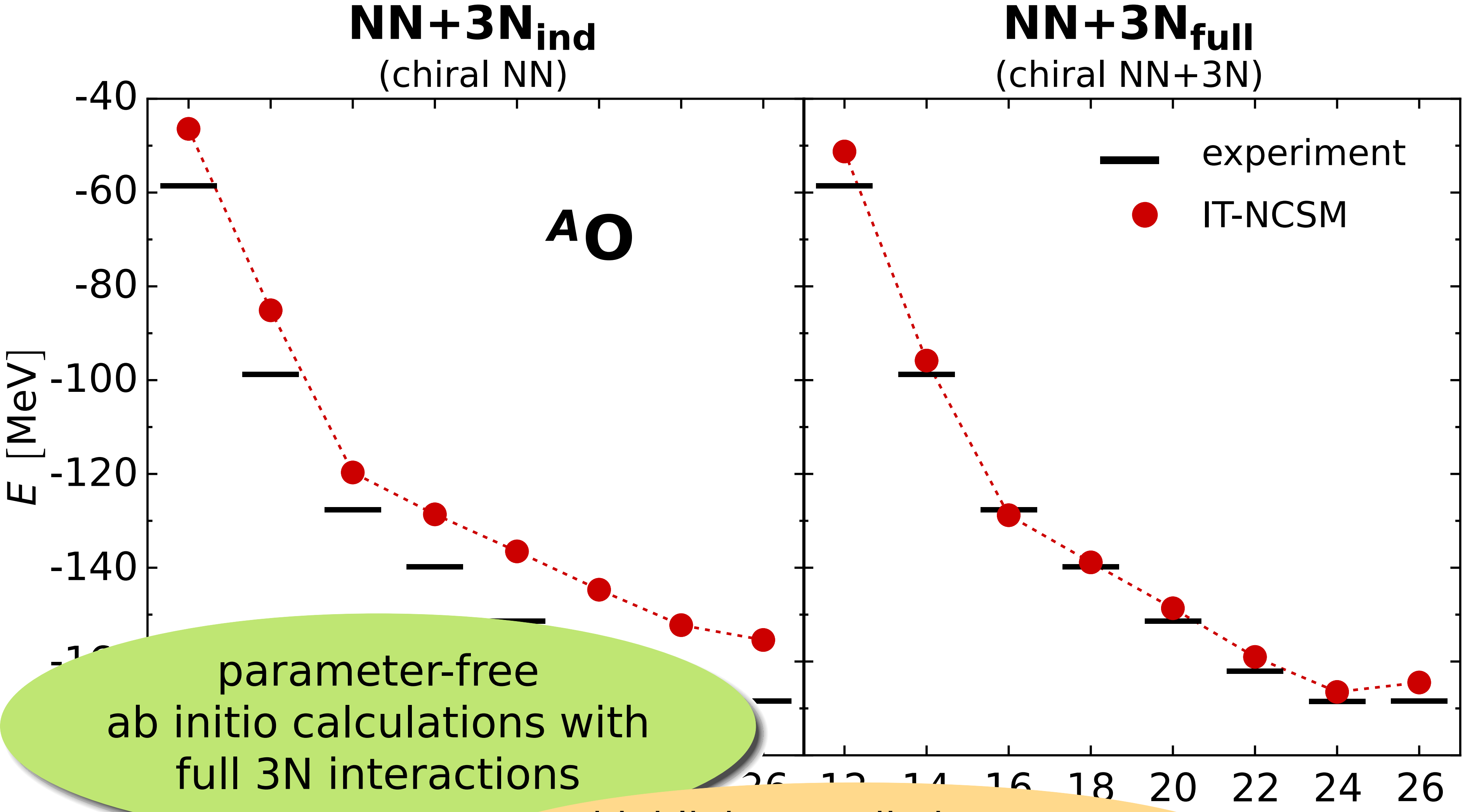
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



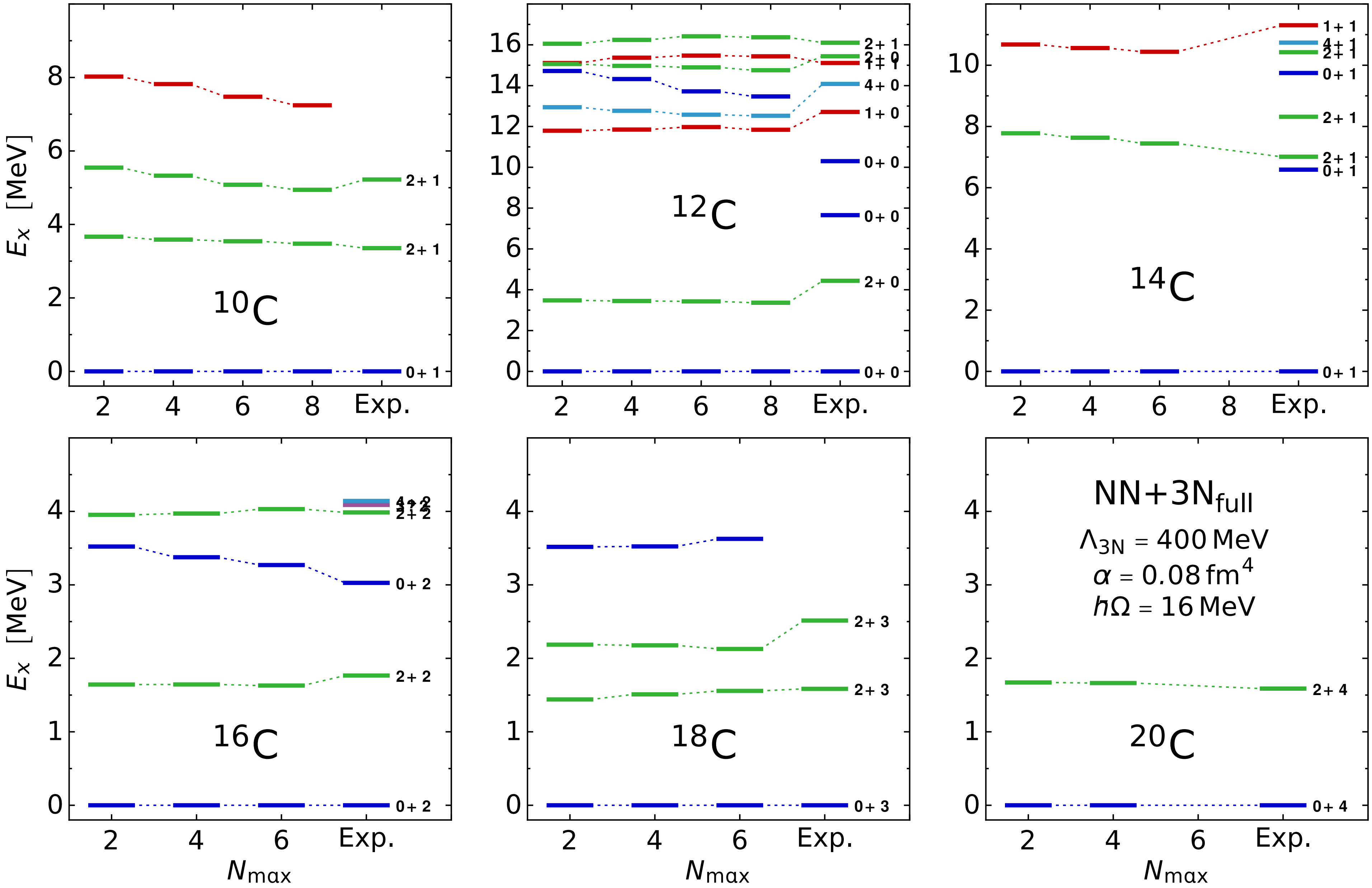
parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

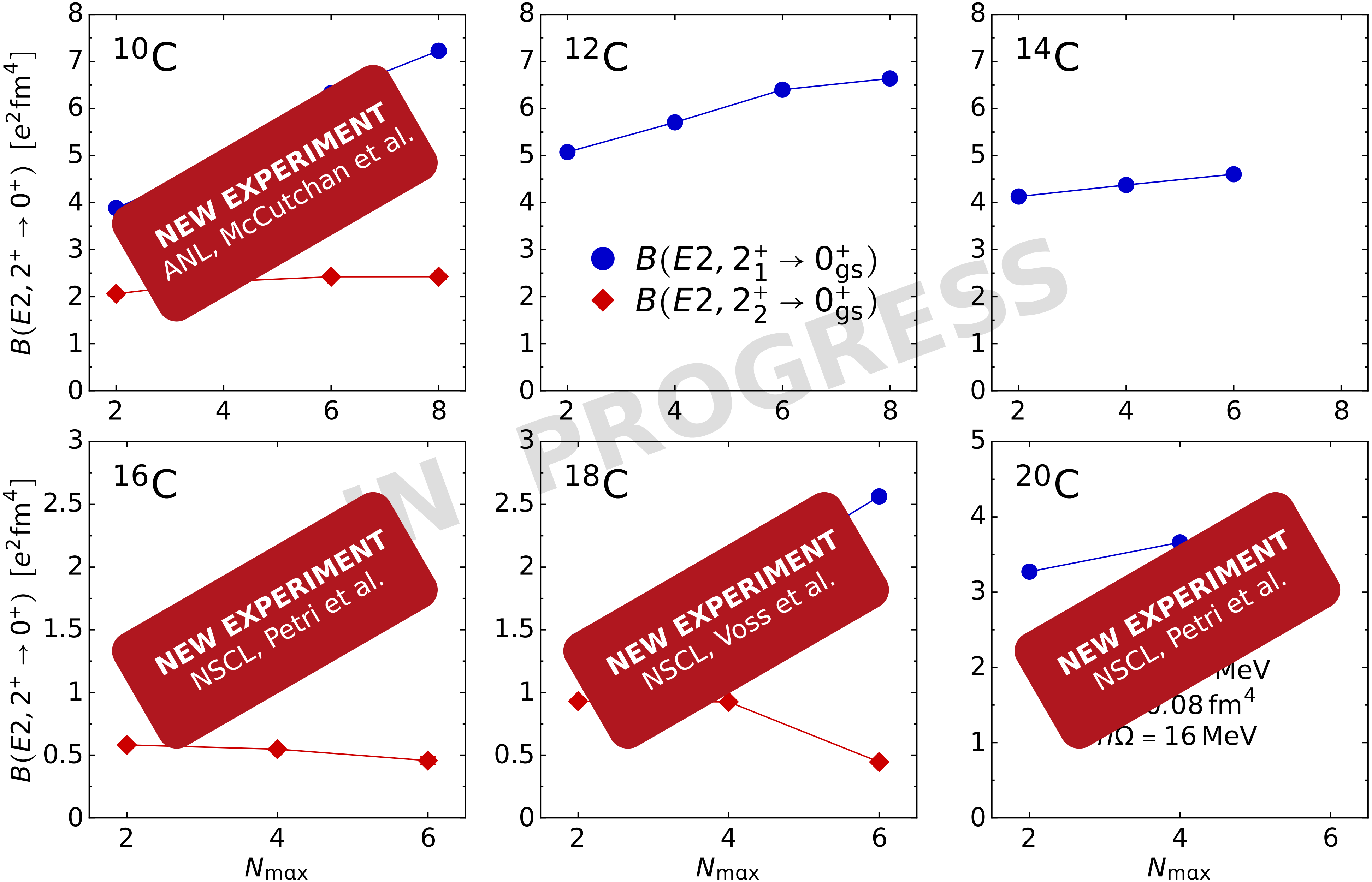
Λ_{3N} = 400 MeV, ... optimal $\hbar\Omega$

Spectroscopy of Carbon Isotopes

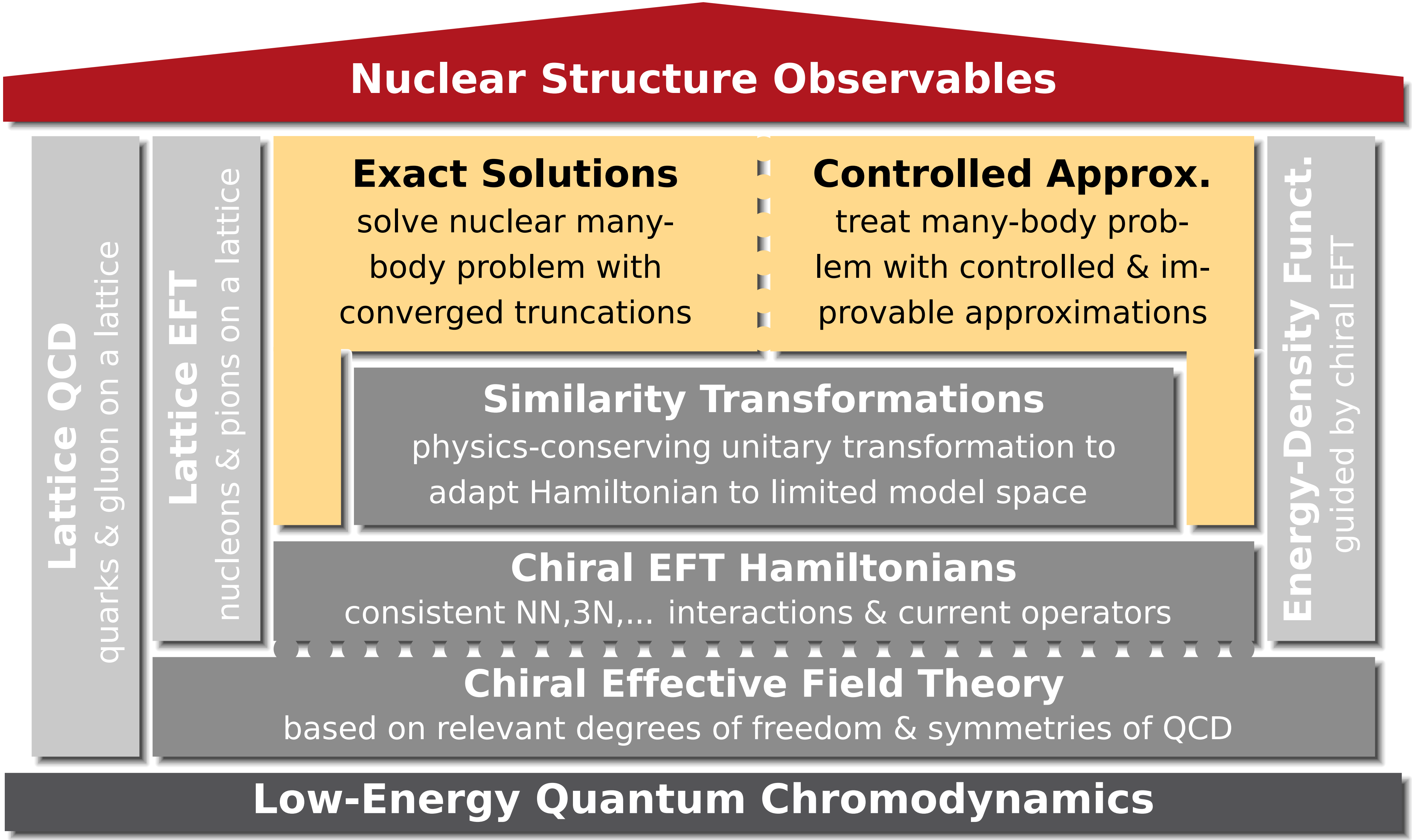
Forssen et al., JPG 40, 055105 (2013); Roth et al., in prep.



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

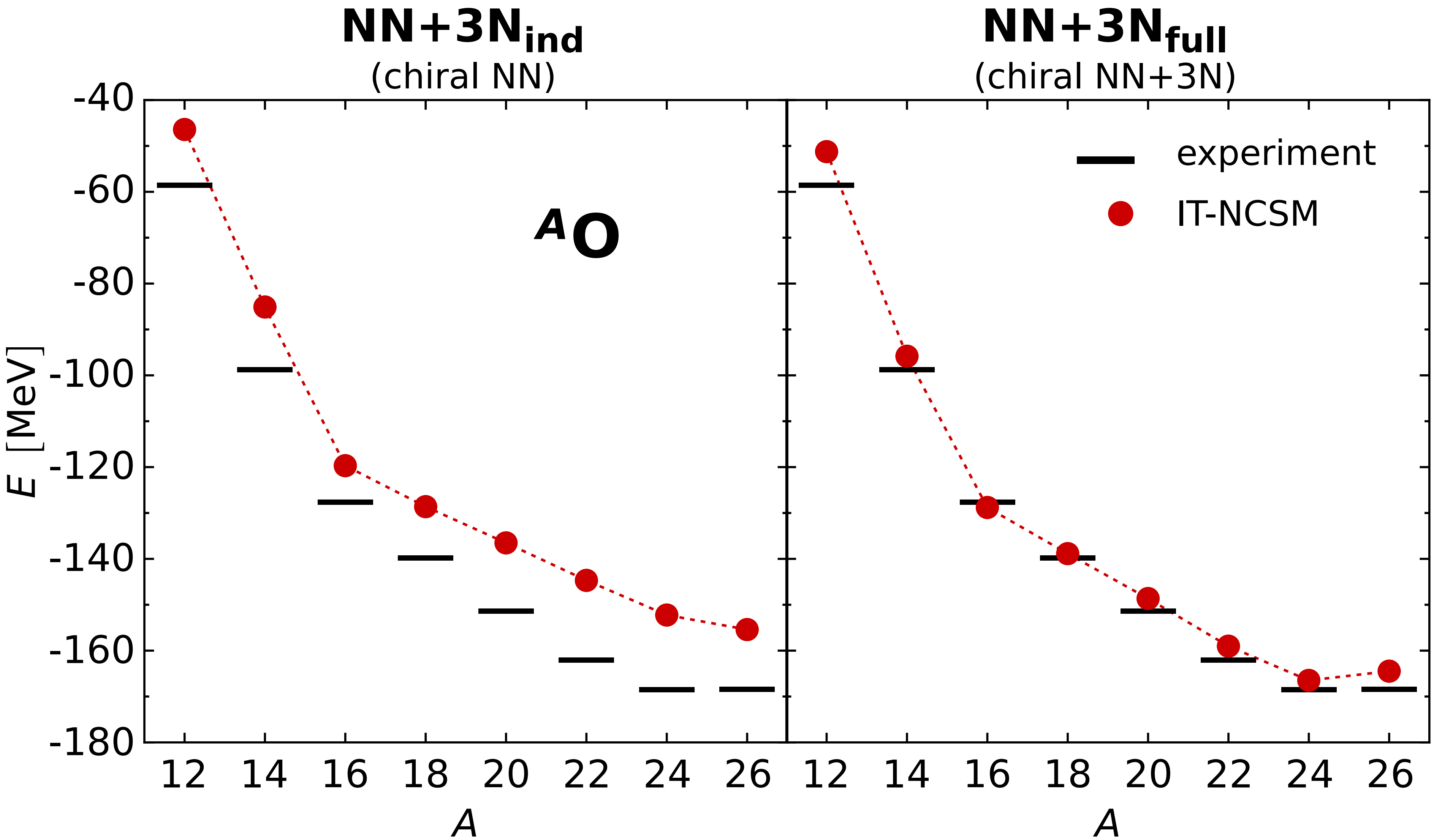
controlling and quantifying the uncertainties due to various truncations is major challenge

Barbieri, Soma, Duguet,...

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

Ground States of Oxygen Isotopes

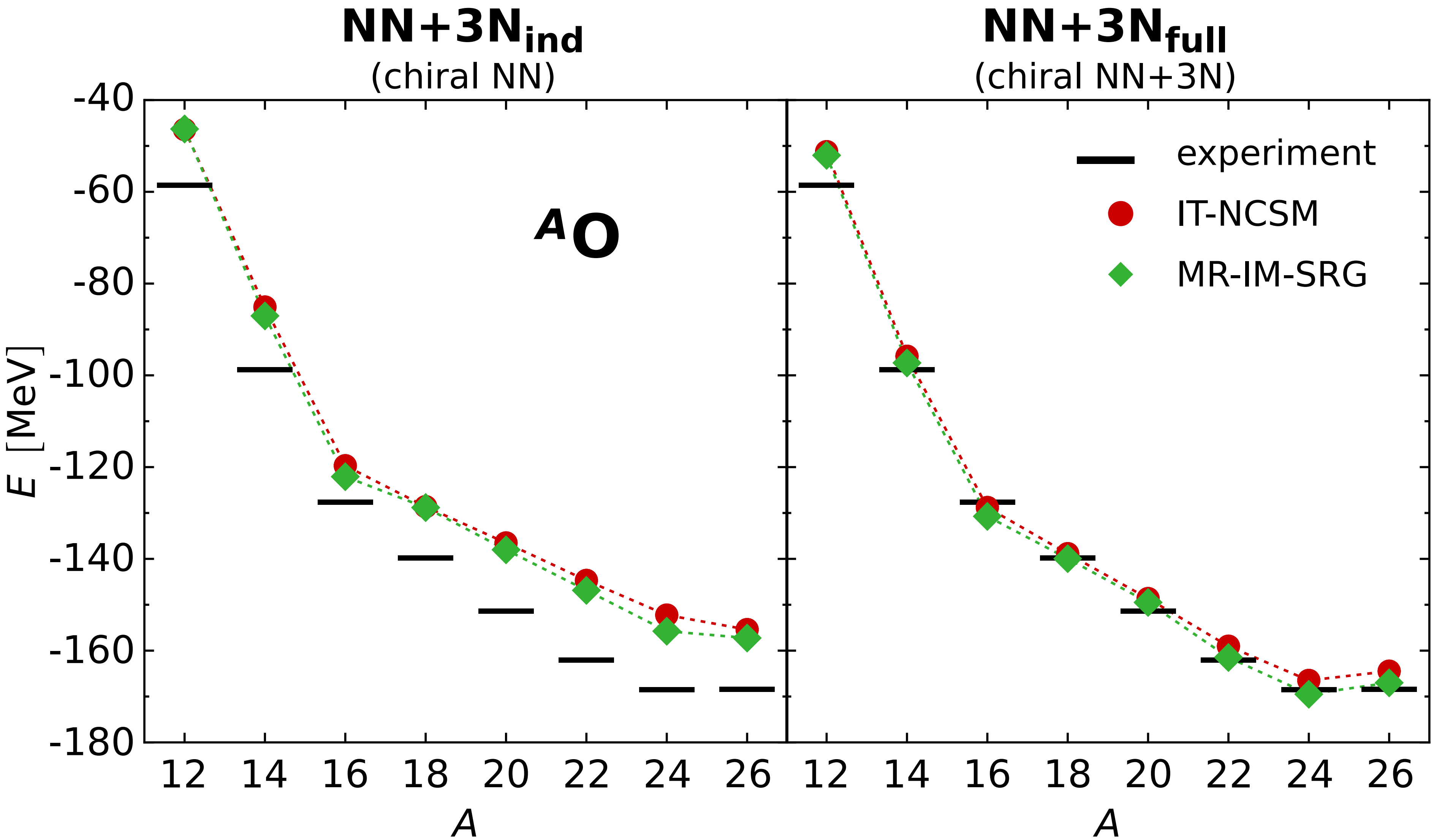
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

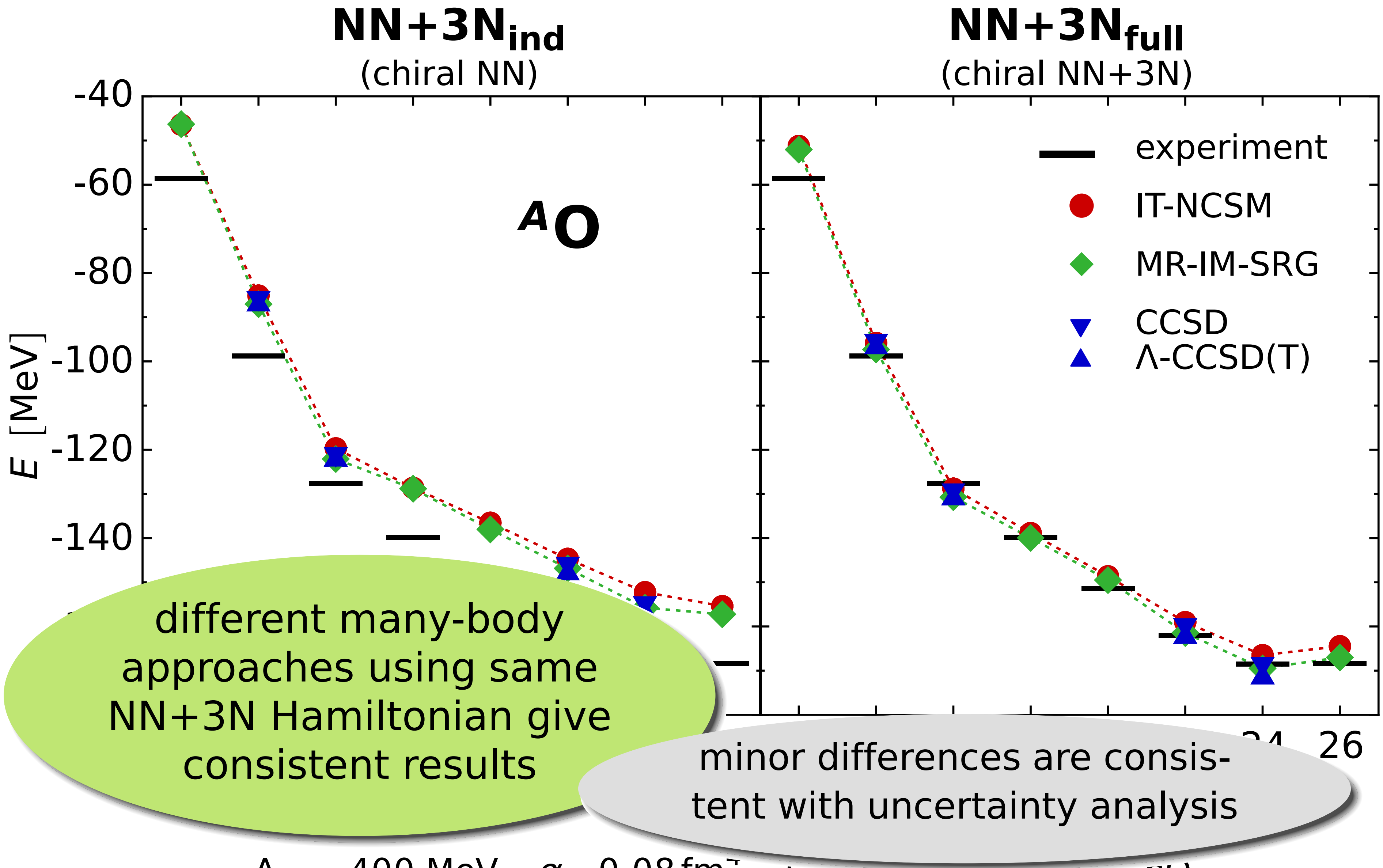
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



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

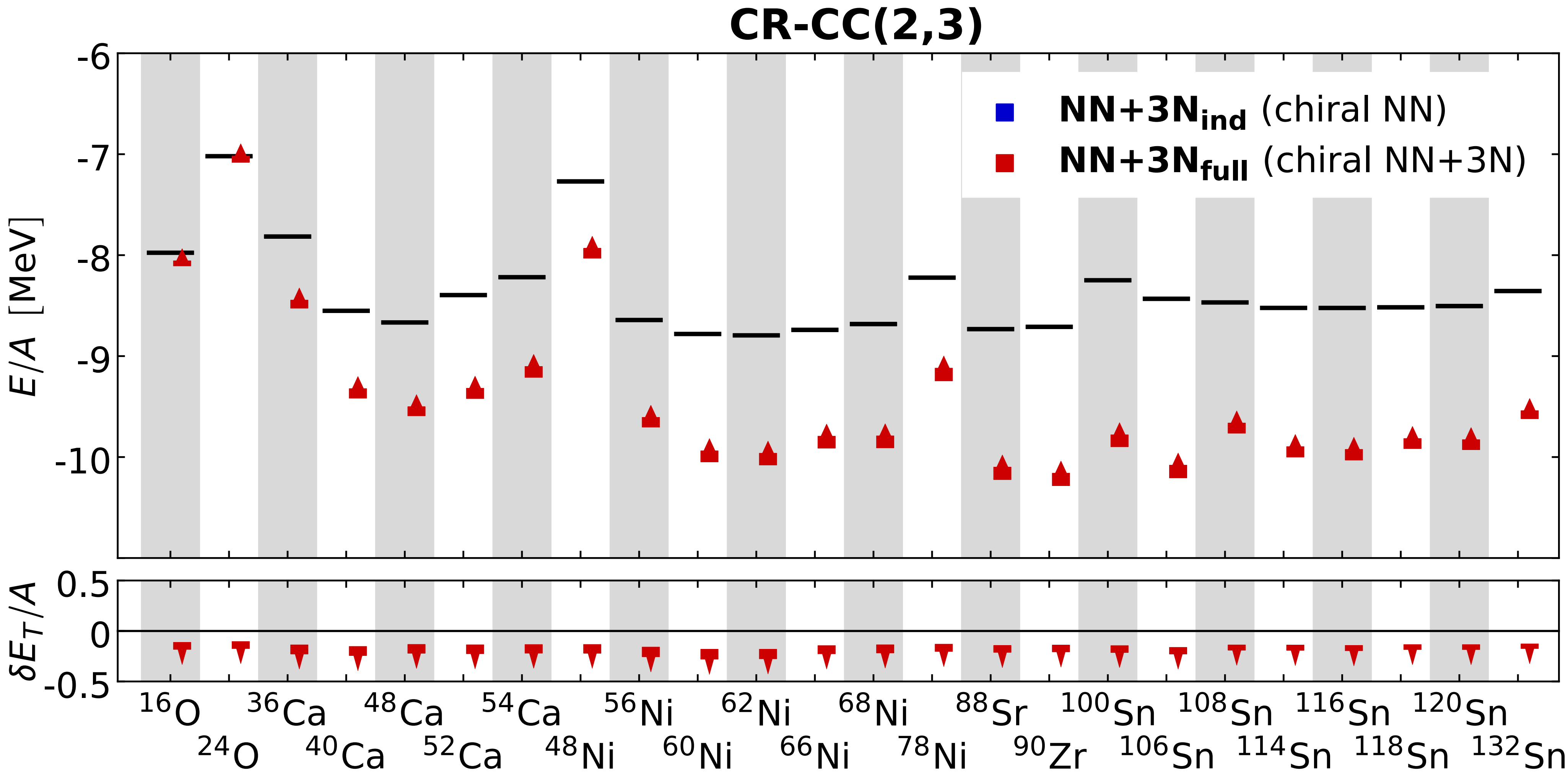
Towards Heavy Nuclei - Ab Initio ?

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013); PRC 88, 054319 (2013); arXiv:1312.5685 (2013)

- calculations for medium-mass and heavy nuclei are **computationally feasible** with CC or IM-SRG
- however, many of the **technical truncations** that are good in light nuclei **fail for heavier systems**
- we **analysed and improved** all of these truncations...
- **2% residual uncertainty** of the many-body approach for $A \lesssim 130$

Towards Heavy Nuclei - Ab Initio !

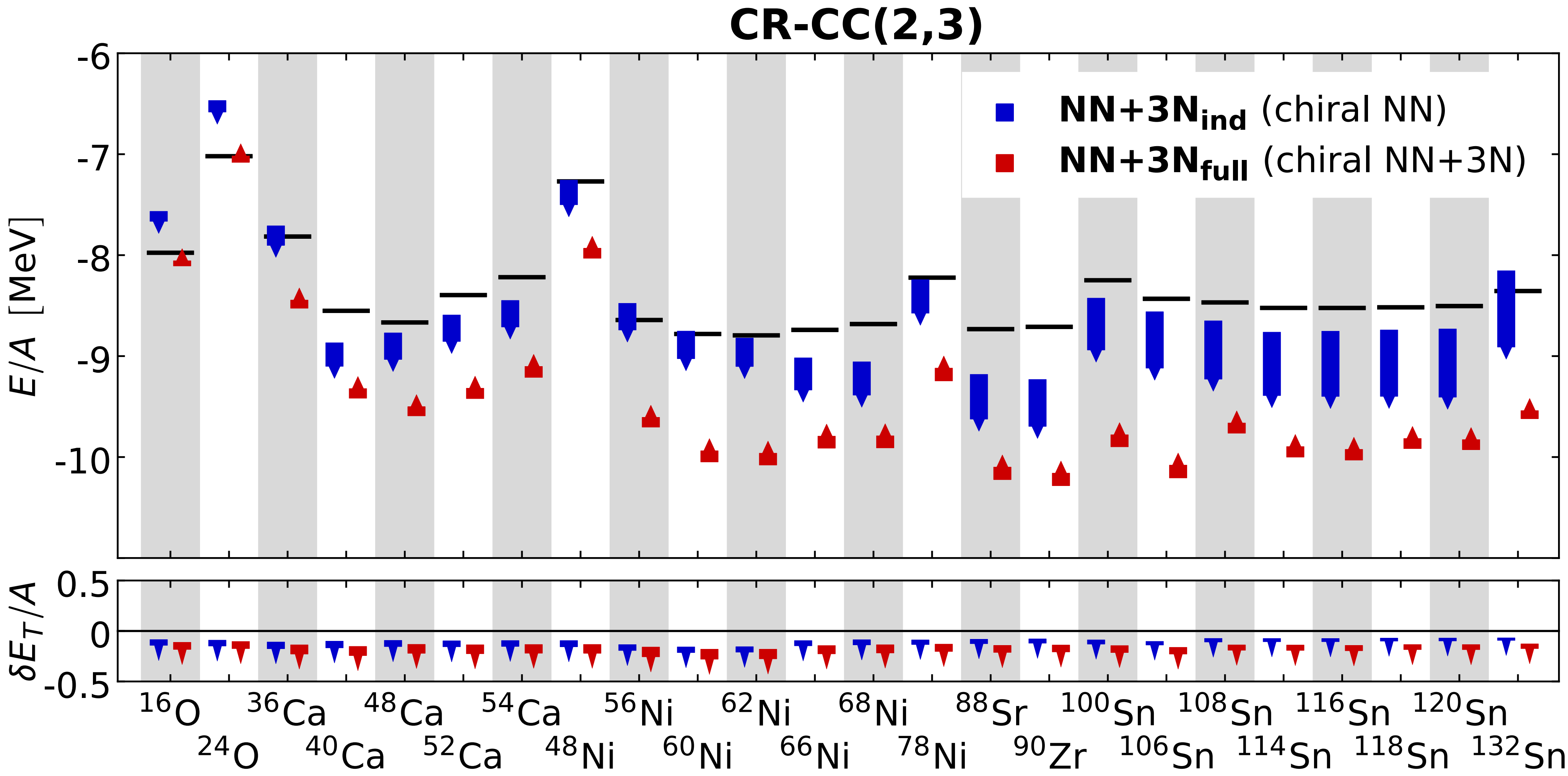
Binder et al., arXiv:1312.5685 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\text{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

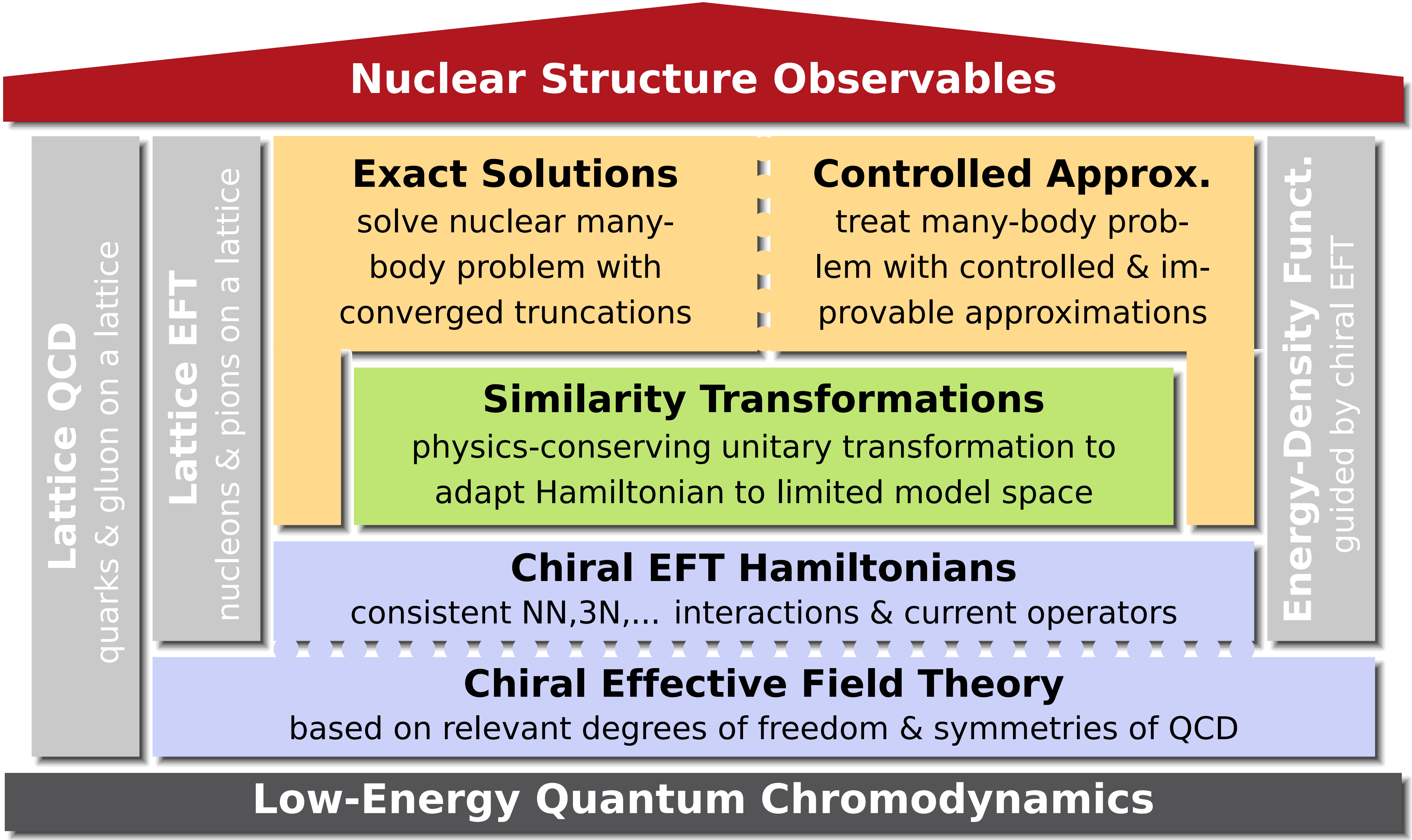
Towards Heavy Nuclei - Ab Initio !

Binder et al., arXiv:1312.5685 (2013)

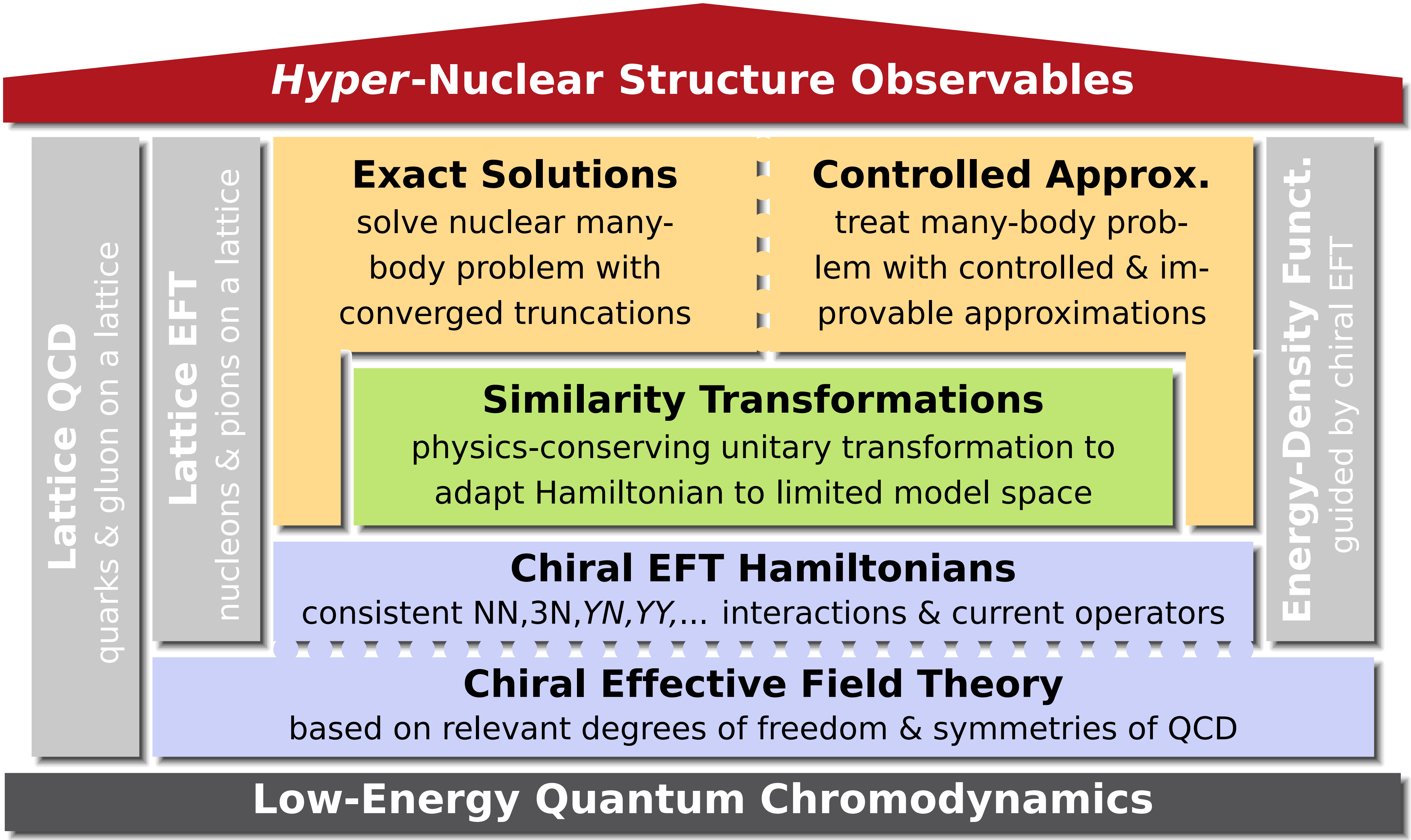


$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\text{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

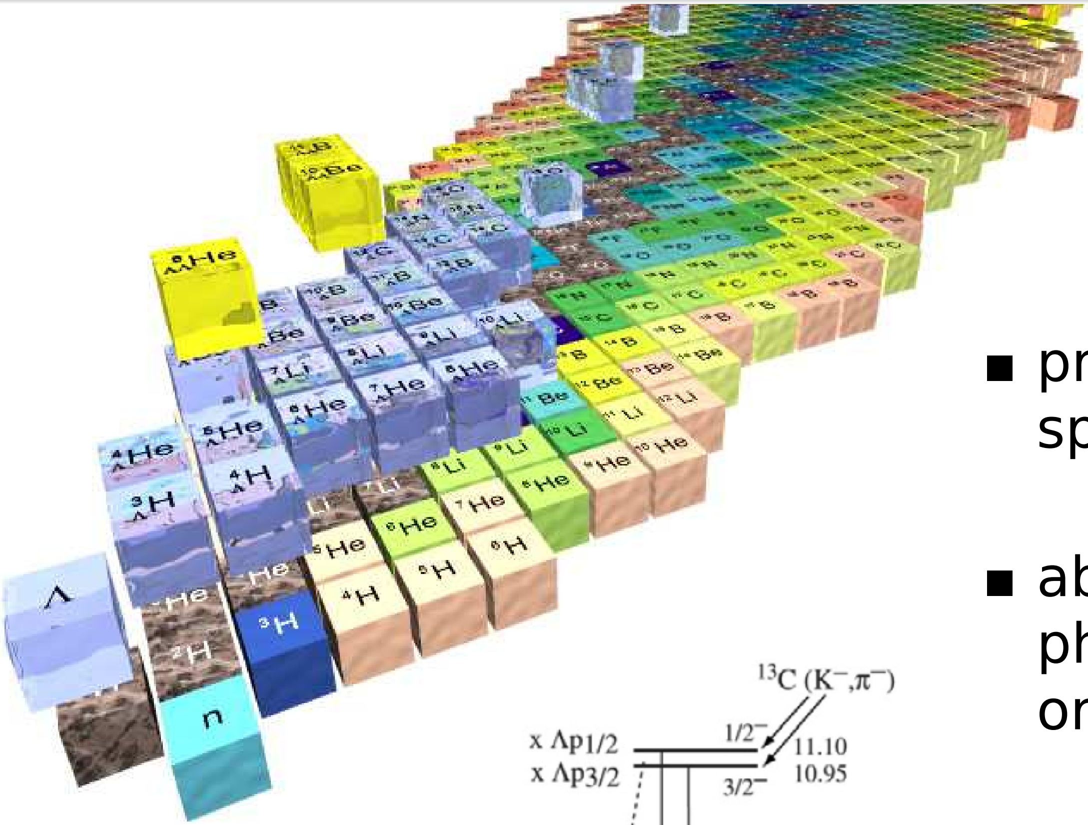
Ab Initio Nuclear Structure

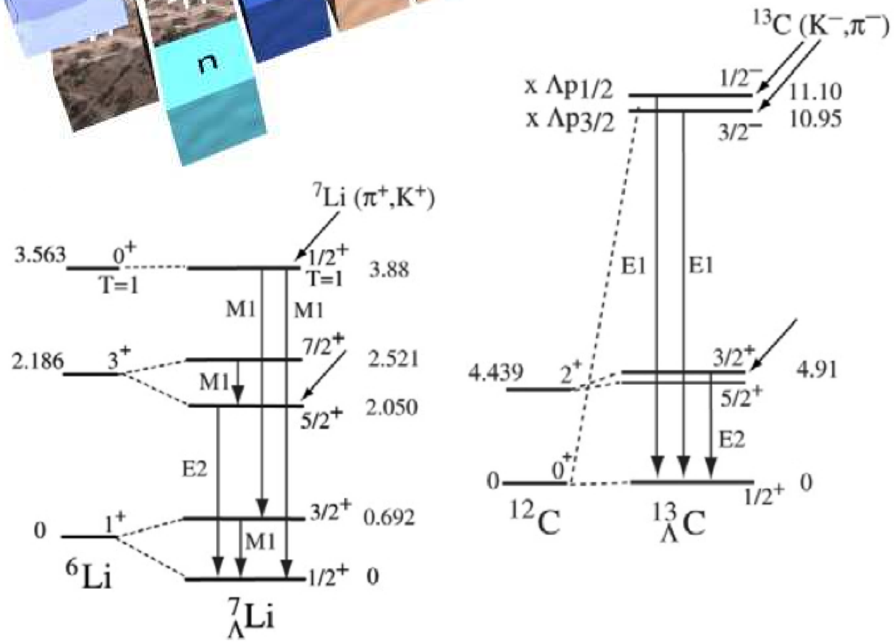


Ab Initio *Hyper*-Nuclear Structure



Ab Initio *Hyper*-Nuclear Structure



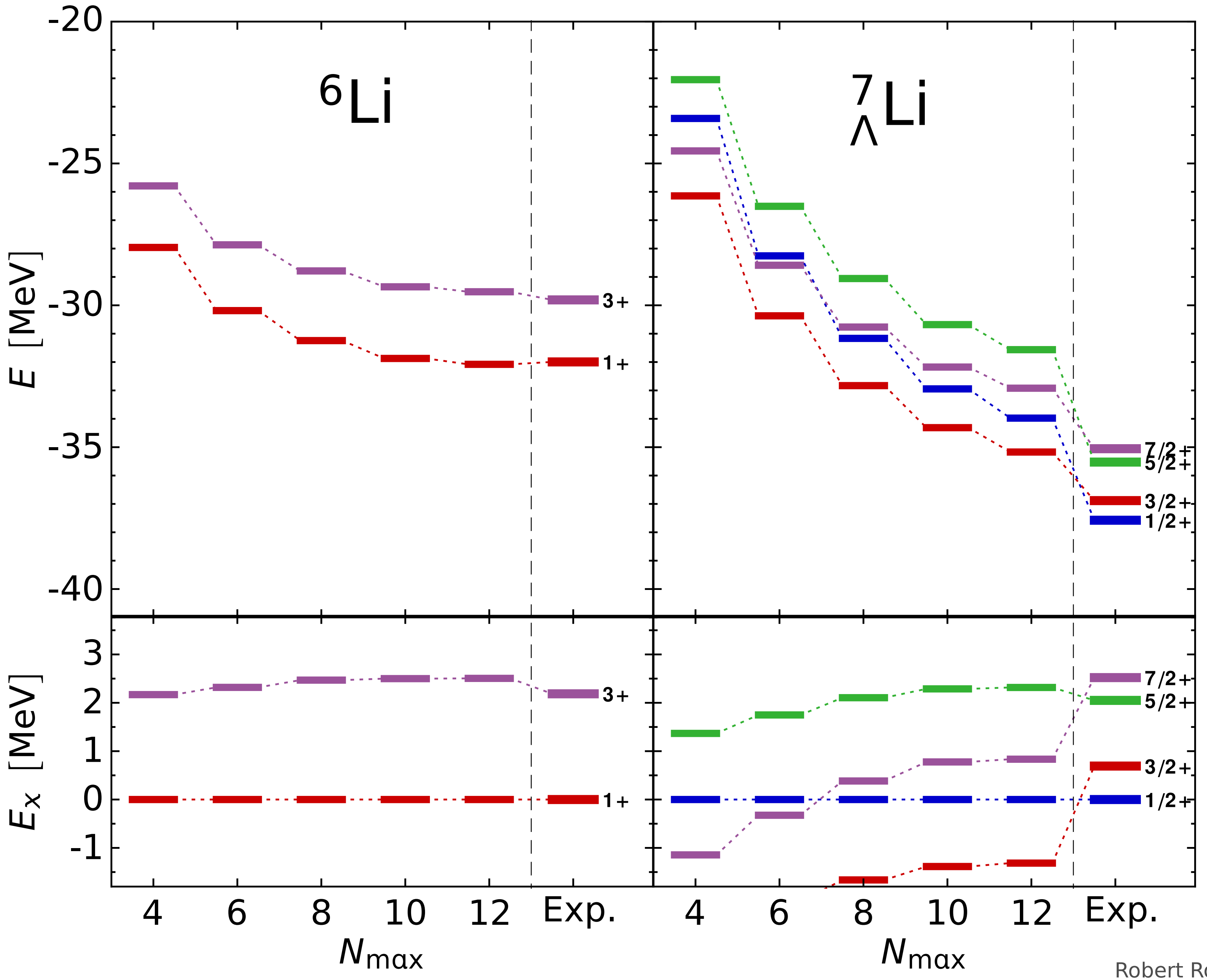


- precise data on ground states & spectroscopy of hyper-nuclei
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations
- chiral YN & YY interactions at (N)LO are available
- constrain YN & YY interaction by ab initio hyper-nuclear structure calculations

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



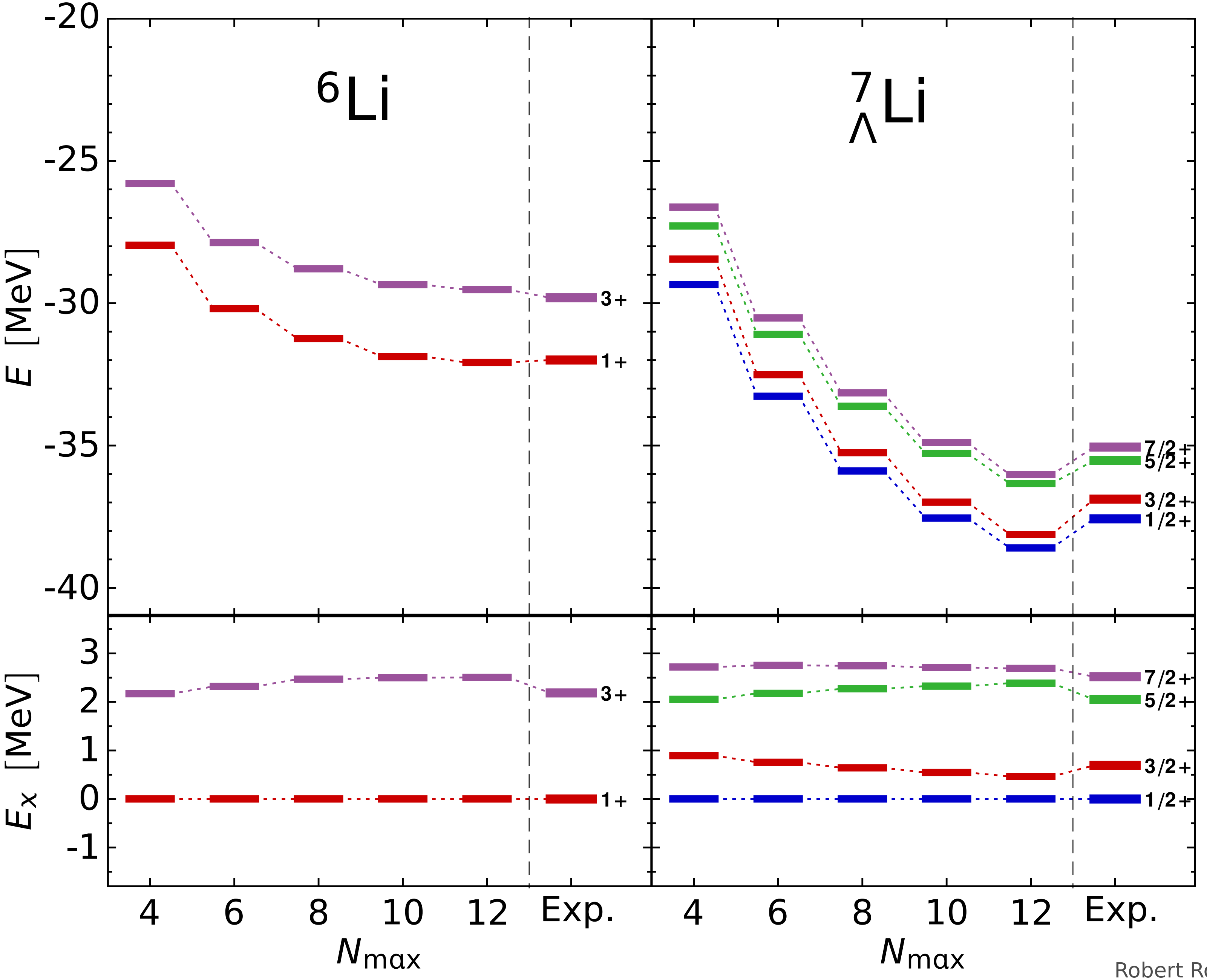
NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

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

Jülich'04
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega$ = 20 MeV

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



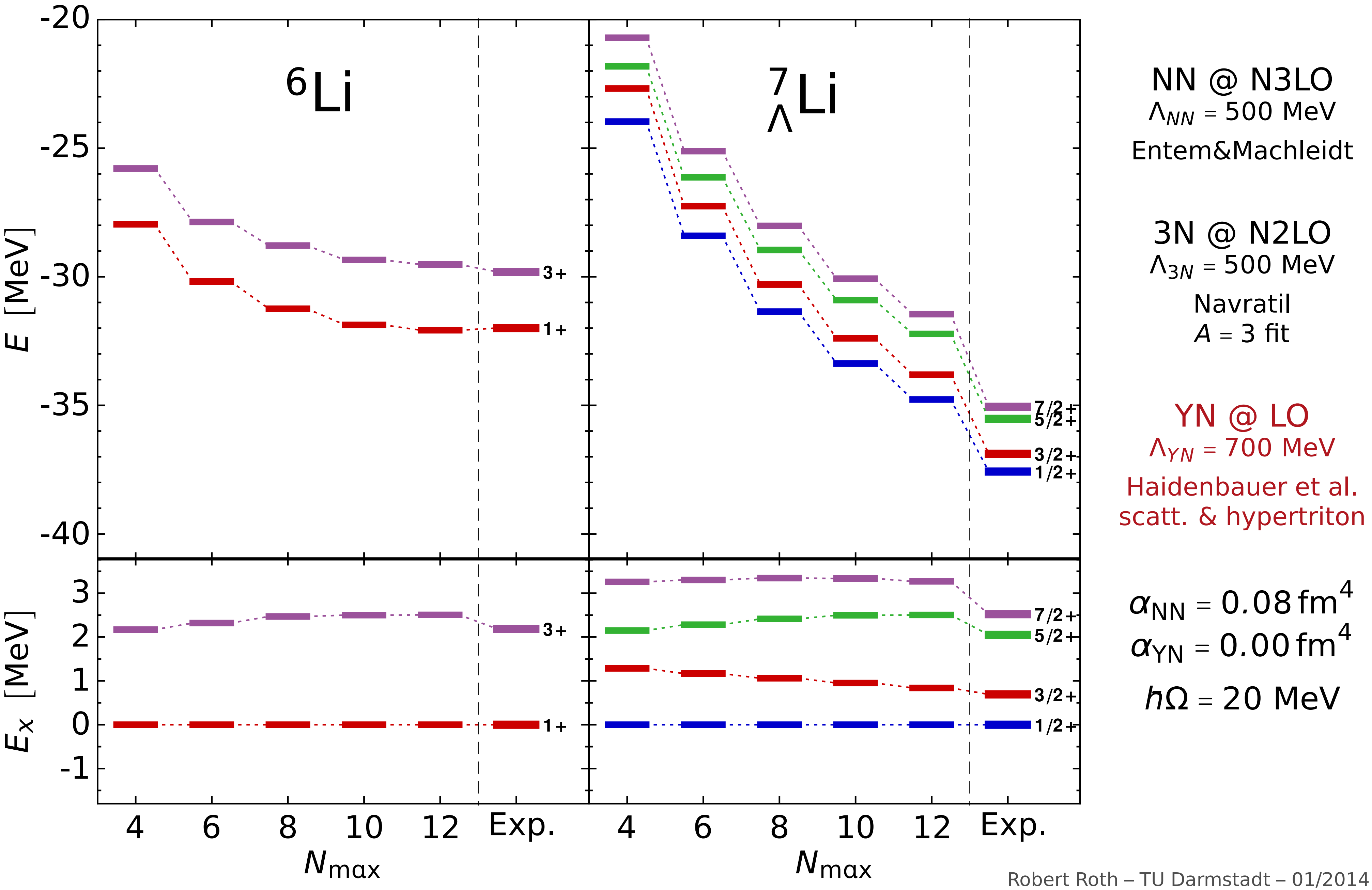
NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

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

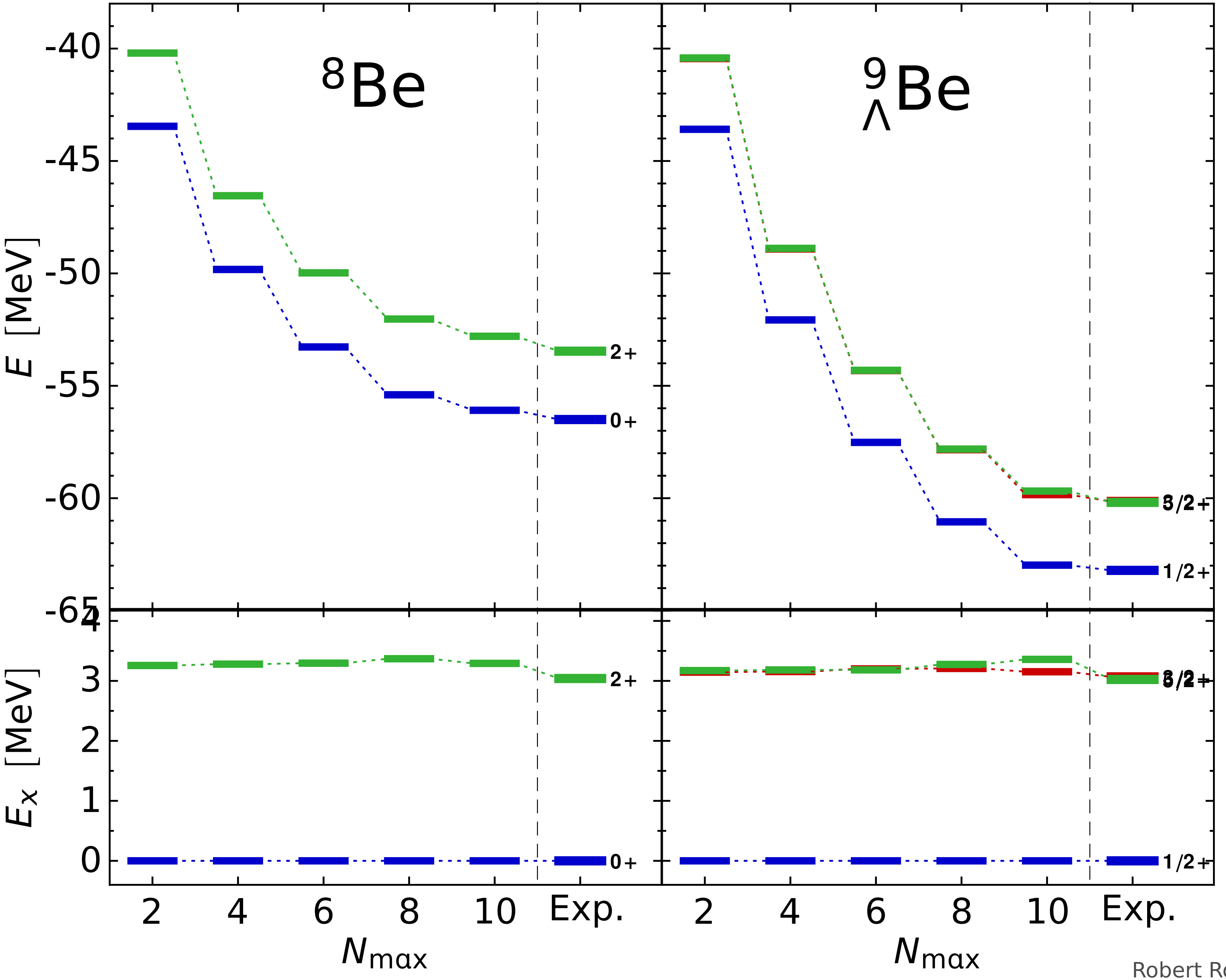
YN @ LO
Λ_{YN} = 600 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

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



Application: $^{9}_{\Lambda}\mathrm{Be}$



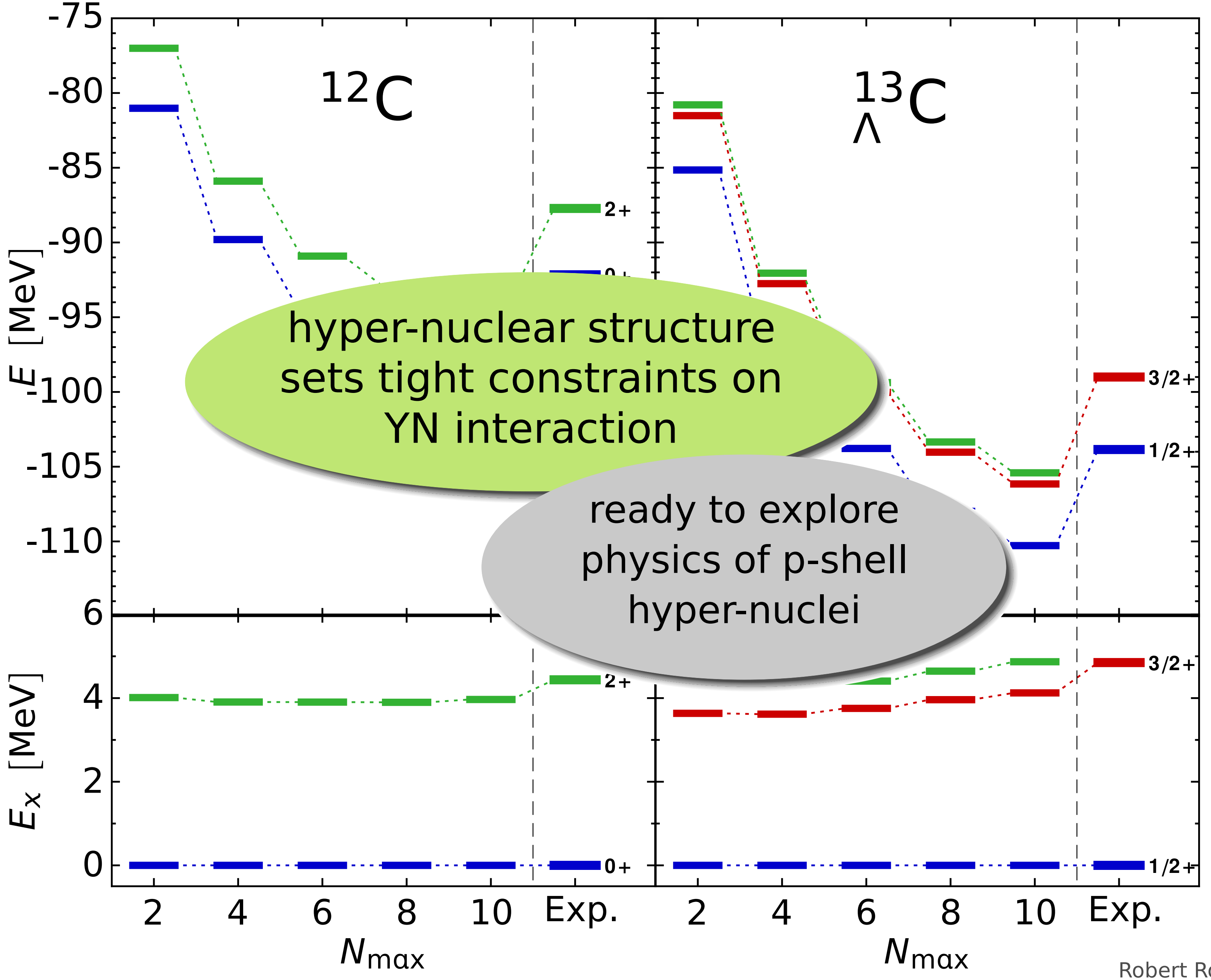
NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

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

YN @ LO
Λ_{YN} = 600 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{\mathrm{NN}} = 0.08\,\mathrm{fm}^4$
$\alpha_{\mathrm{YN}} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega$ = 20 MeV

Application: $^{13}_{\Lambda}$C



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

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

YN @ LO
Λ_{YN} = 600 MeV
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08\,\text{fm}^4$
$\alpha_{YN} = 0.00\,\text{fm}^4$
$\hbar\Omega = 20$ MeV

Frontiers

- **ab initio theory is entering new territory...**
  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT
  - **precision frontier**
    precision spectroscopy of light nuclei, including current contribution
  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum frontier**
    include continuum effects and scattering observables consistently
  - **strangeness frontier**
    ab initio predictions for hyper-nuclear structure & spectroscopy

...providing a coherent theoretical framework for nuclear structure & reaction calculations

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, J. Braun, **A. Calci**, S. Fischer, E. Gebrerufael, H. Spiess, **J. Langhammer**, 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
    IBS/RISP, Korea
  - 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