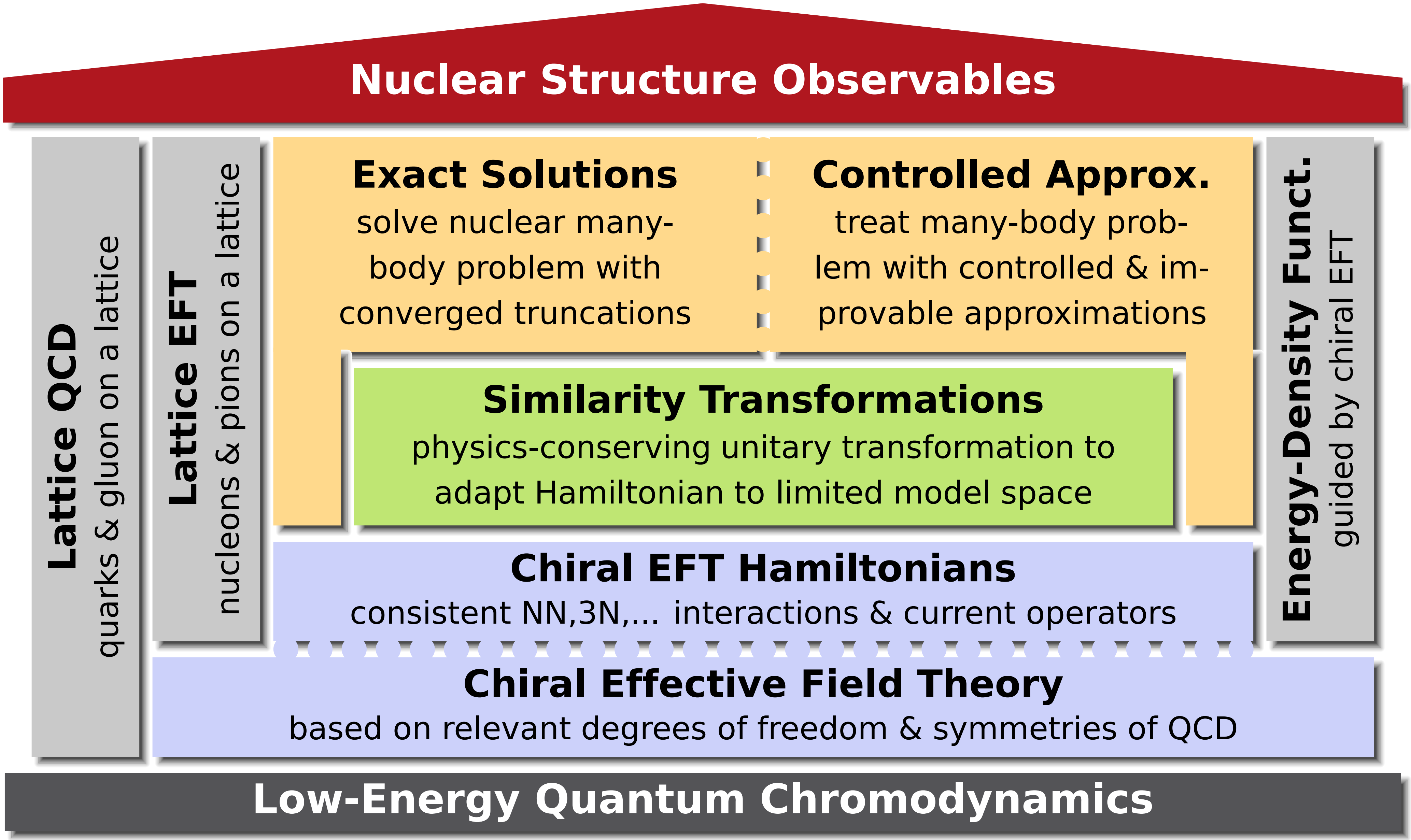
Frontiers in Ab Initio Nuclear Structure Theory

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Nuclear Structure



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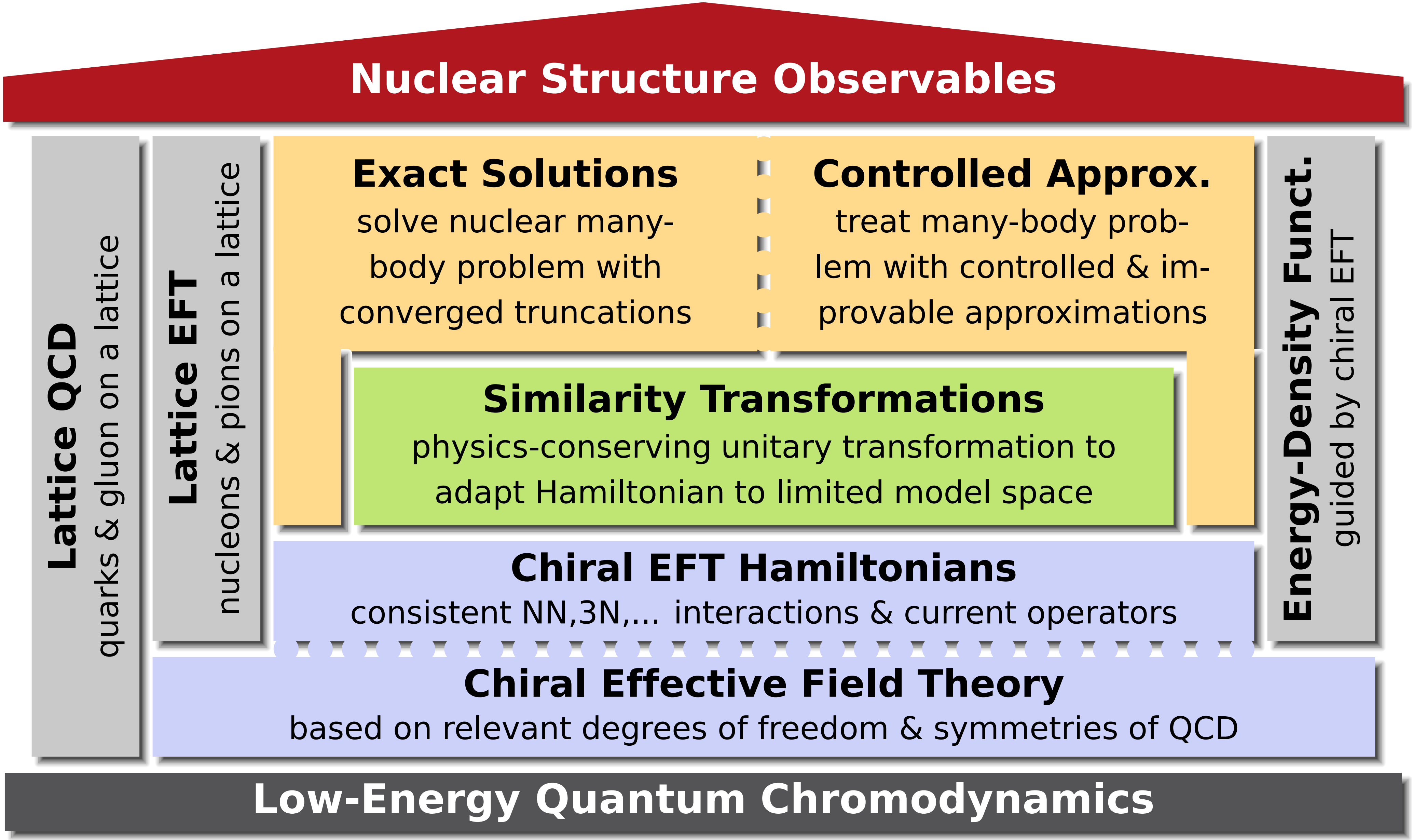

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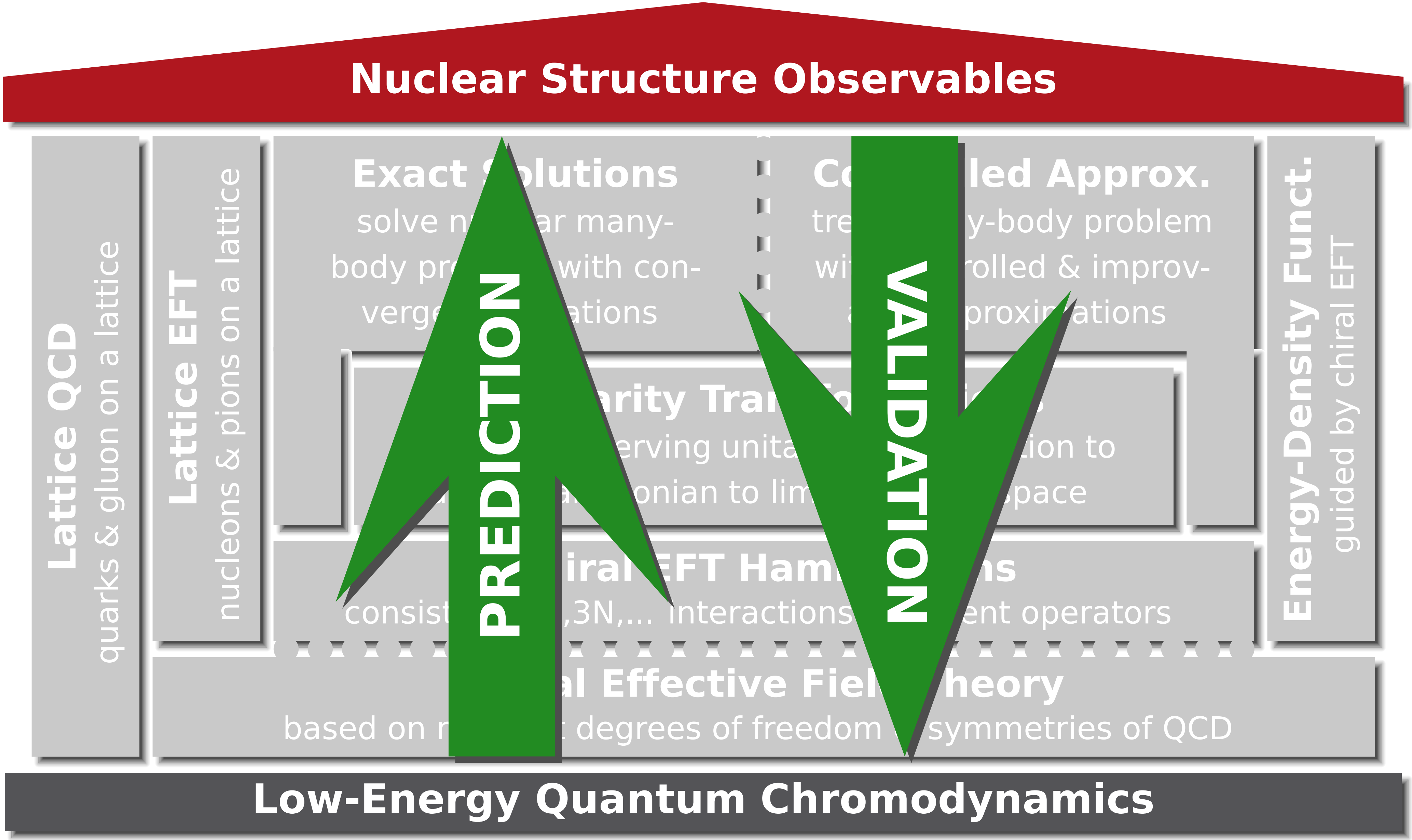

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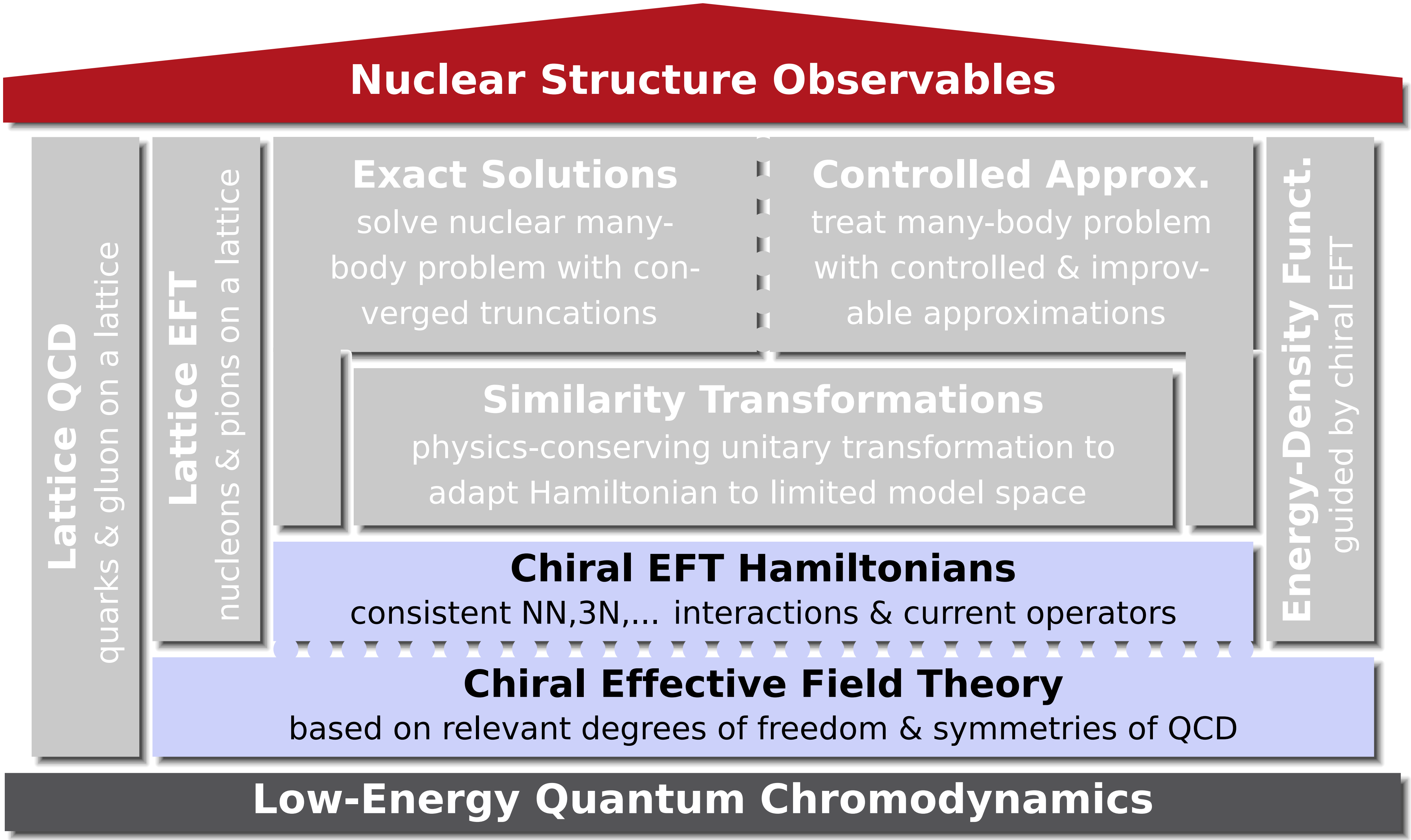
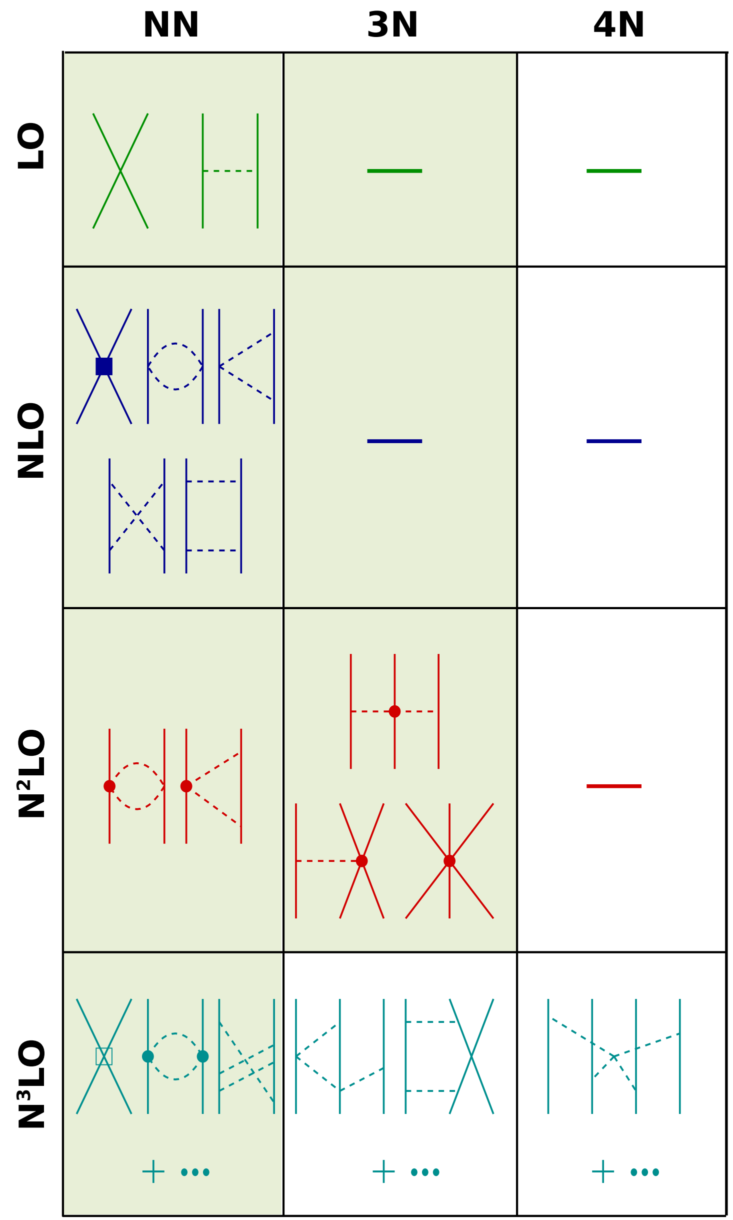


Nuclear Interactions from Chiral EFT

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

- **chiral EFT background**: talks by Ekström, van Kolck, et al.
- **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 variations)
  - consistent Hamiltonians at N2LO (NN: POUNDERs-opt., Epelbaum)
  - consistent Hamiltonians at N3LO (LENPIC Collaboration)



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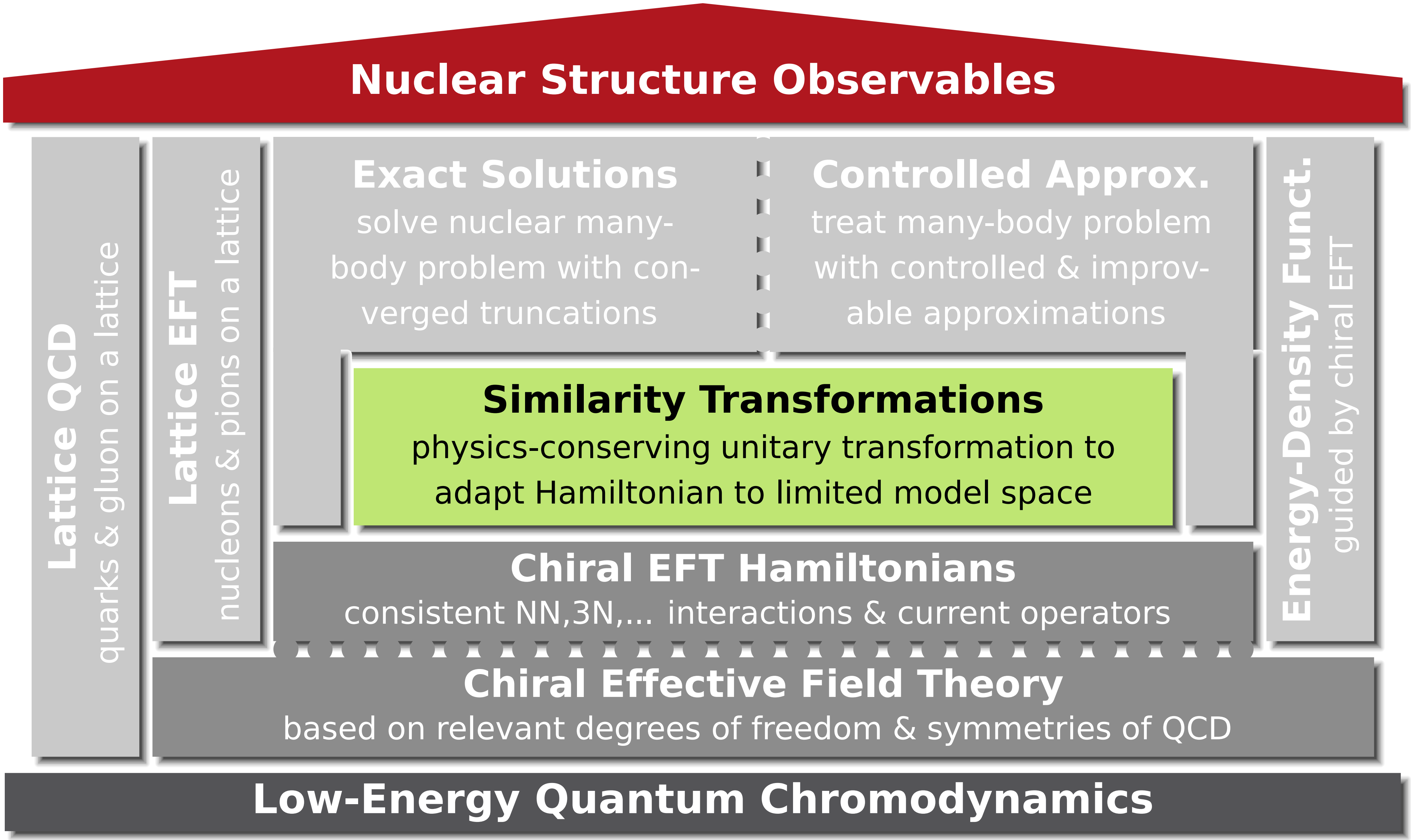


Similarity Renormalization Group

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

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

- **evolution equations** for H_α and U_α depending on generator η_α

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

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

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

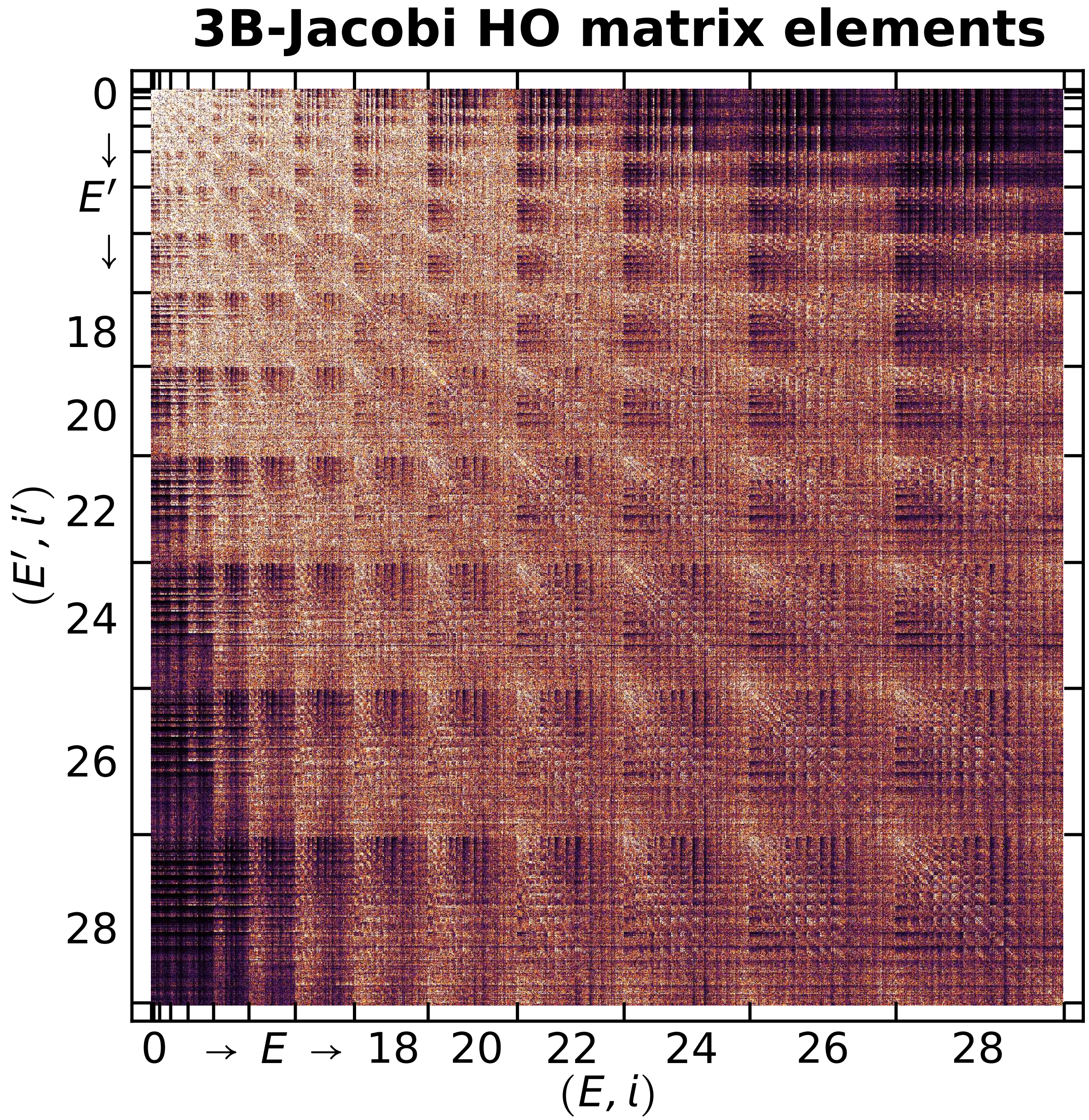
SRG Evolution of Matrix Elements

- convert Fock-space operator equations into **coupled evolution equations for matrix elements** in n-body Hilbert space
- use **antisym. Jacobi harmonic-oscillator states**: $|EiJ^\pi T\rangle$
- system of **coupled evolution equations** for each $J^\pi T$-block

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle EiJ^\pi T|\,\mathrm{H}_\alpha\,|E'i'J^\pi T\rangle = (2\mu)^2 \sum_{E''i''}^{E_\mathrm{SRG}} \sum_{E'''i'''}^{E_\mathrm{SRG}} \Big[$$
$$\langle Ei\ldots|\,\mathrm{T}_\mathrm{int}\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{H}_\alpha\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{H}_\alpha\,|E'i'\ldots\rangle$$
$$-2\langle Ei\ldots|\,\mathrm{H}_\alpha\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{T}_\mathrm{int}\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{H}_\alpha\,|E'i'\ldots\rangle$$
$$+\langle Ei\ldots|\,\mathrm{H}_\alpha\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{H}_\alpha\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{T}_\mathrm{int}\,|E'i'\ldots\rangle\Big]$$

- use J-dependent basis truncation $E_\mathrm{SRG}(J)$ — convergence needs to be validated for system under consideration
- simple **frequency conversion** to change oscillator frequency $\hbar\Omega$

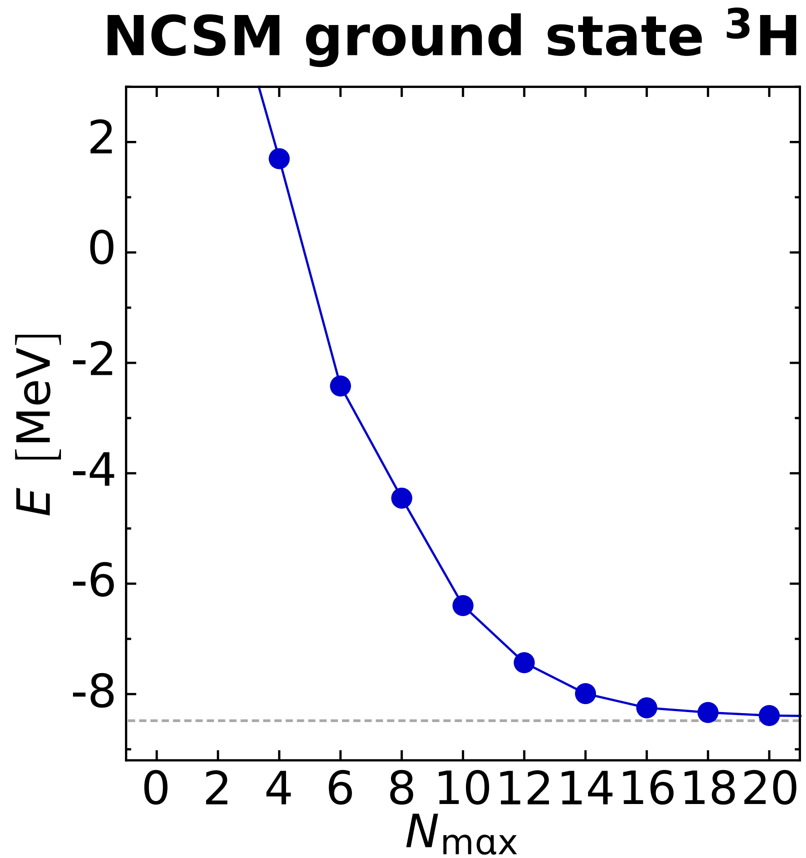
SRG Evolution in Three-Body Space



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

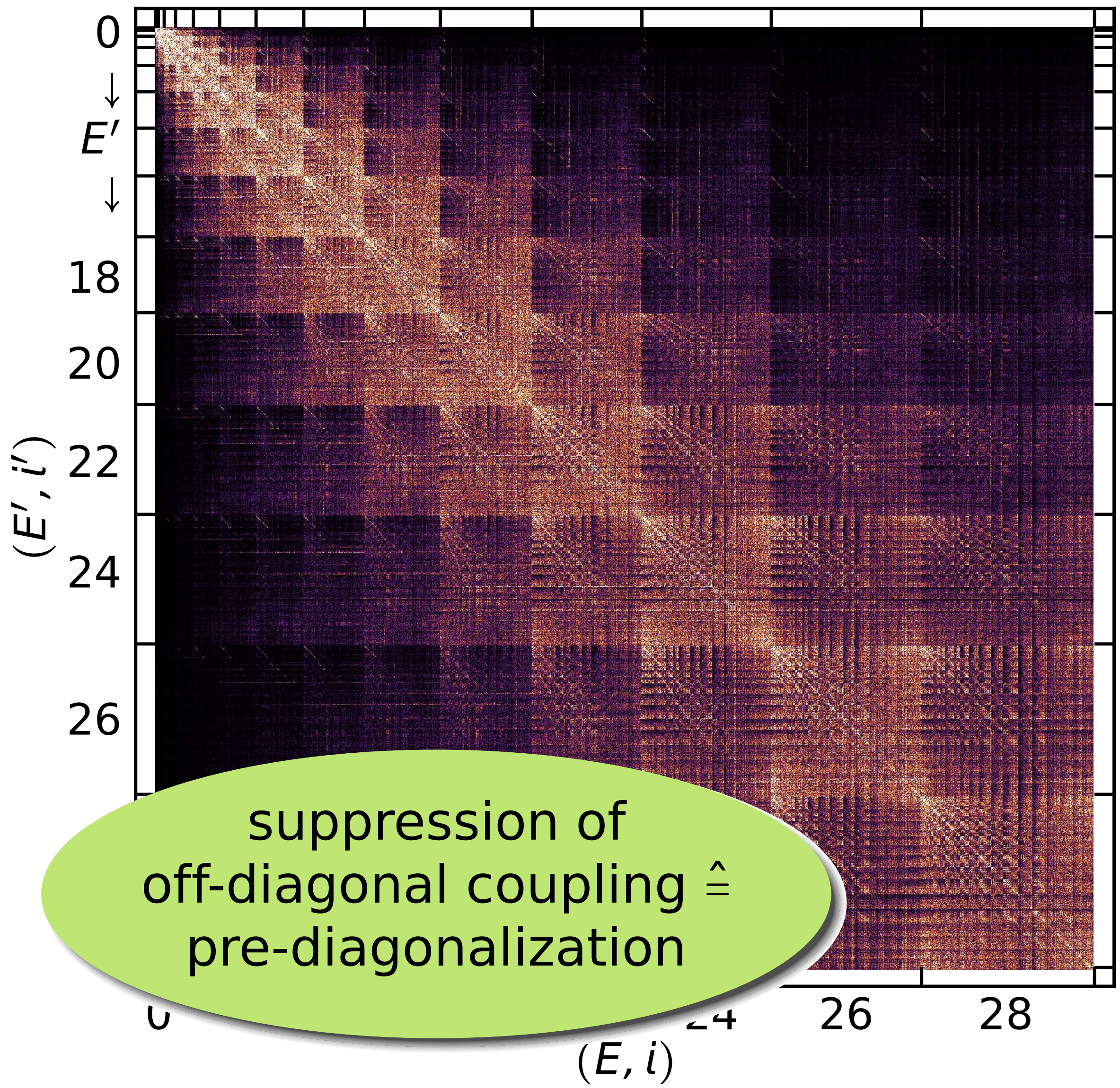
$\Lambda = \infty\,\mathrm{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



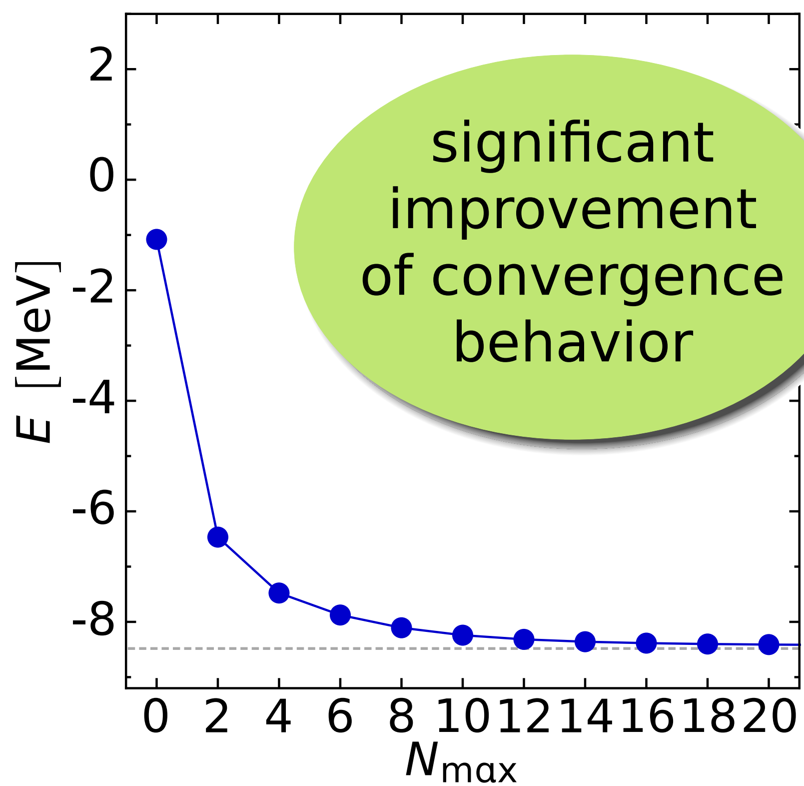
suppression of
off-diagonal coupling ≙
pre-diagonalization

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

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

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

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

Hamiltonian in A-Body Space

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

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

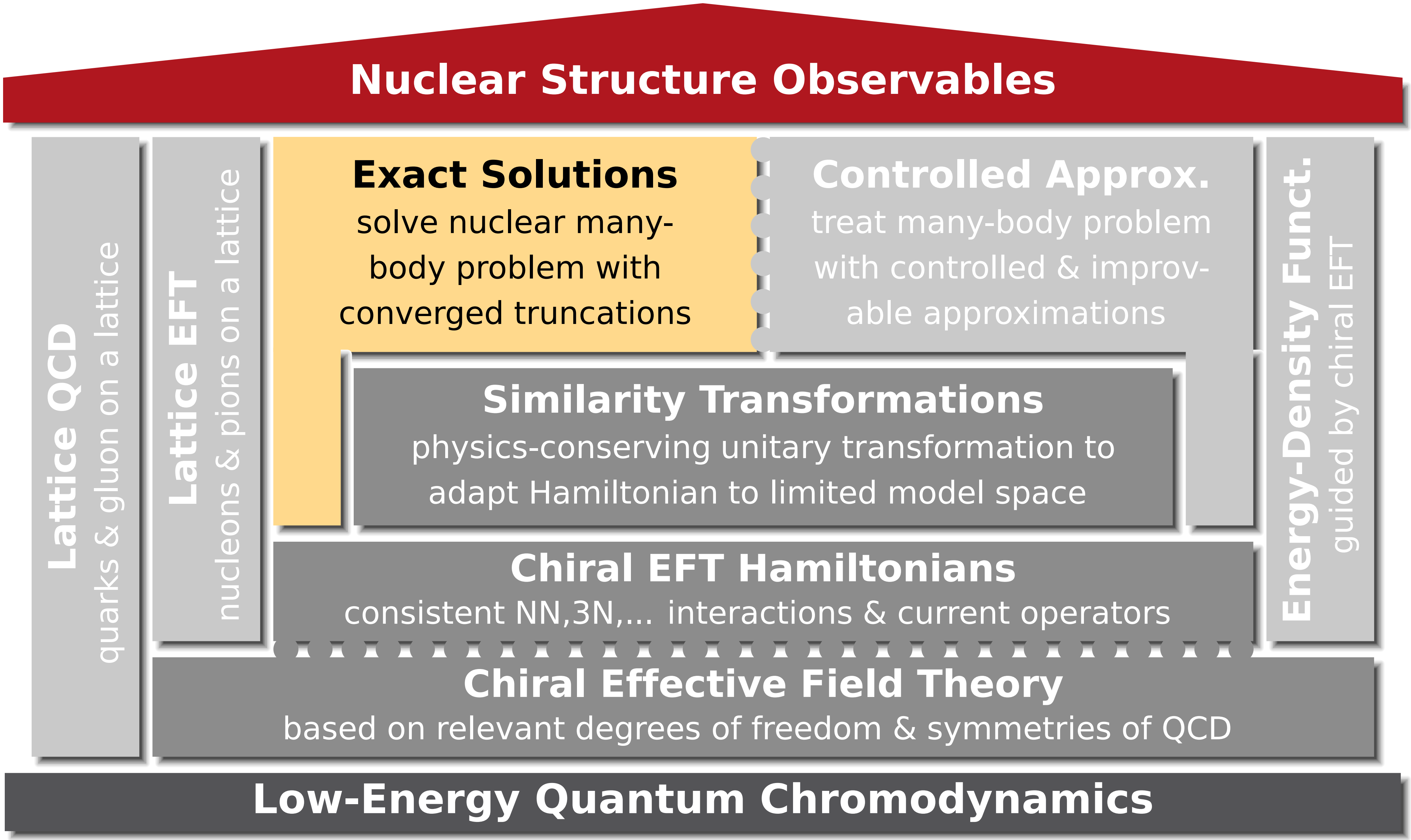
- **truncation of cluster series** formally destroys unitarity and invariance of energy eigenvalues (independence of α)

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

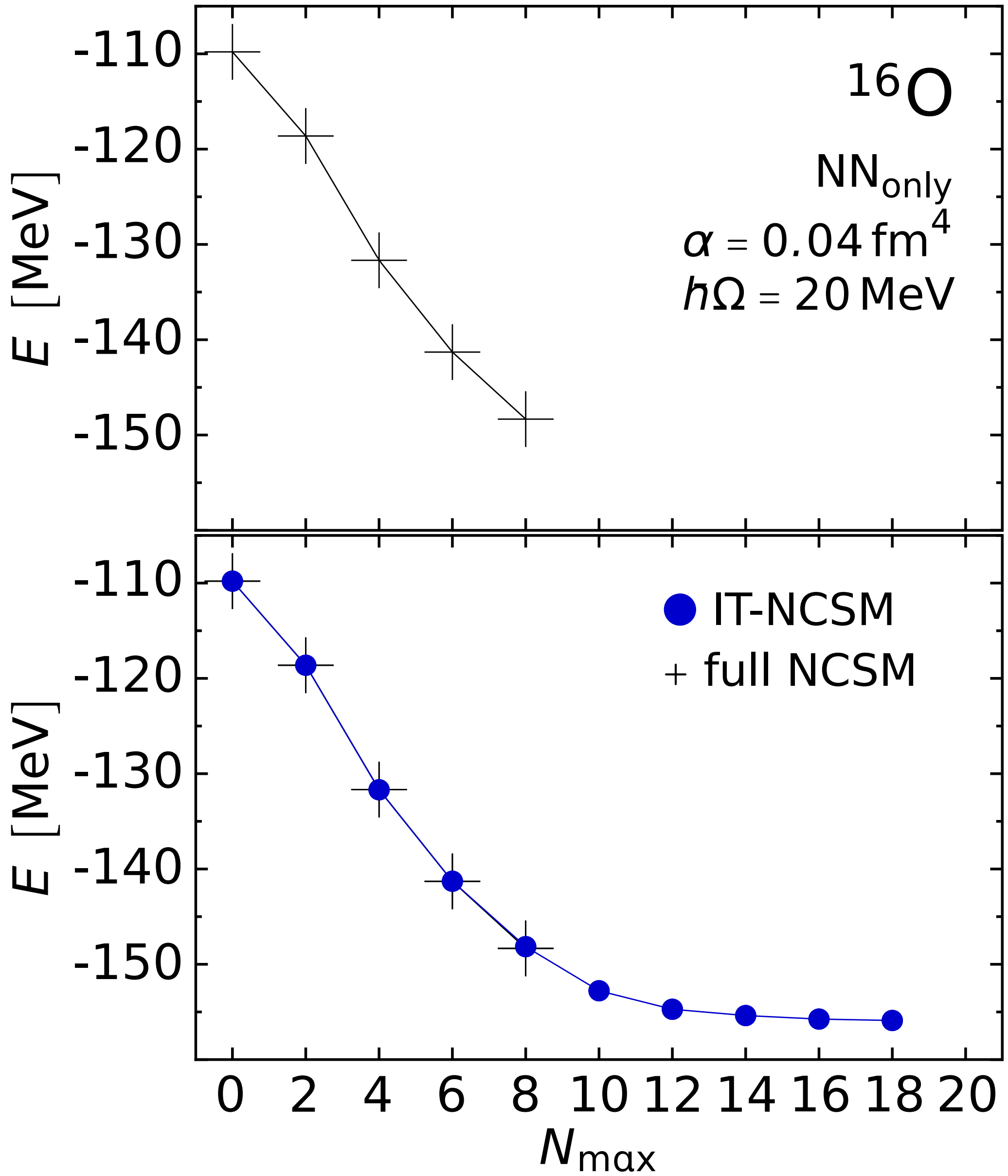
Importance Truncated NCSM

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 $> 10^{10}$)

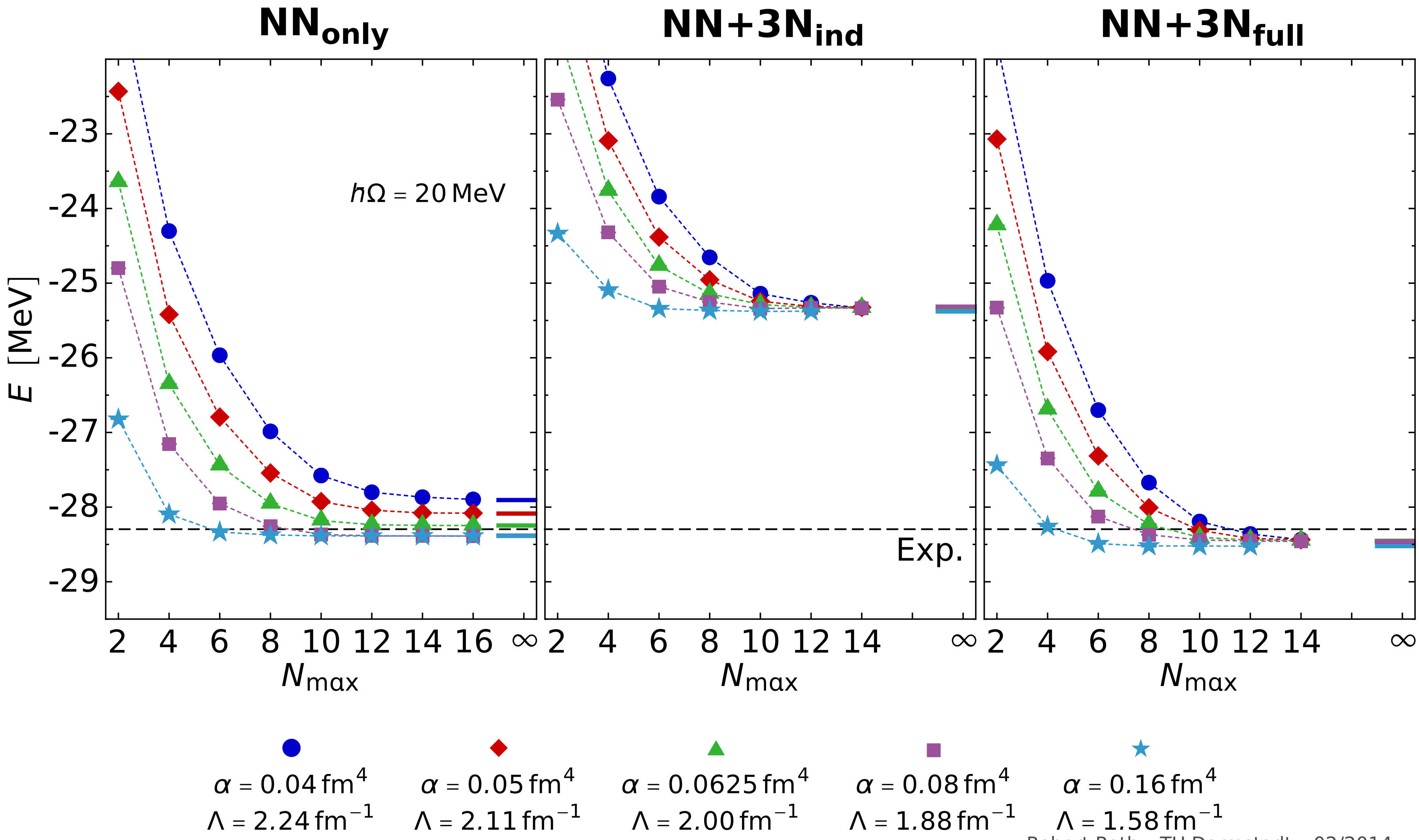
Importance Truncation

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



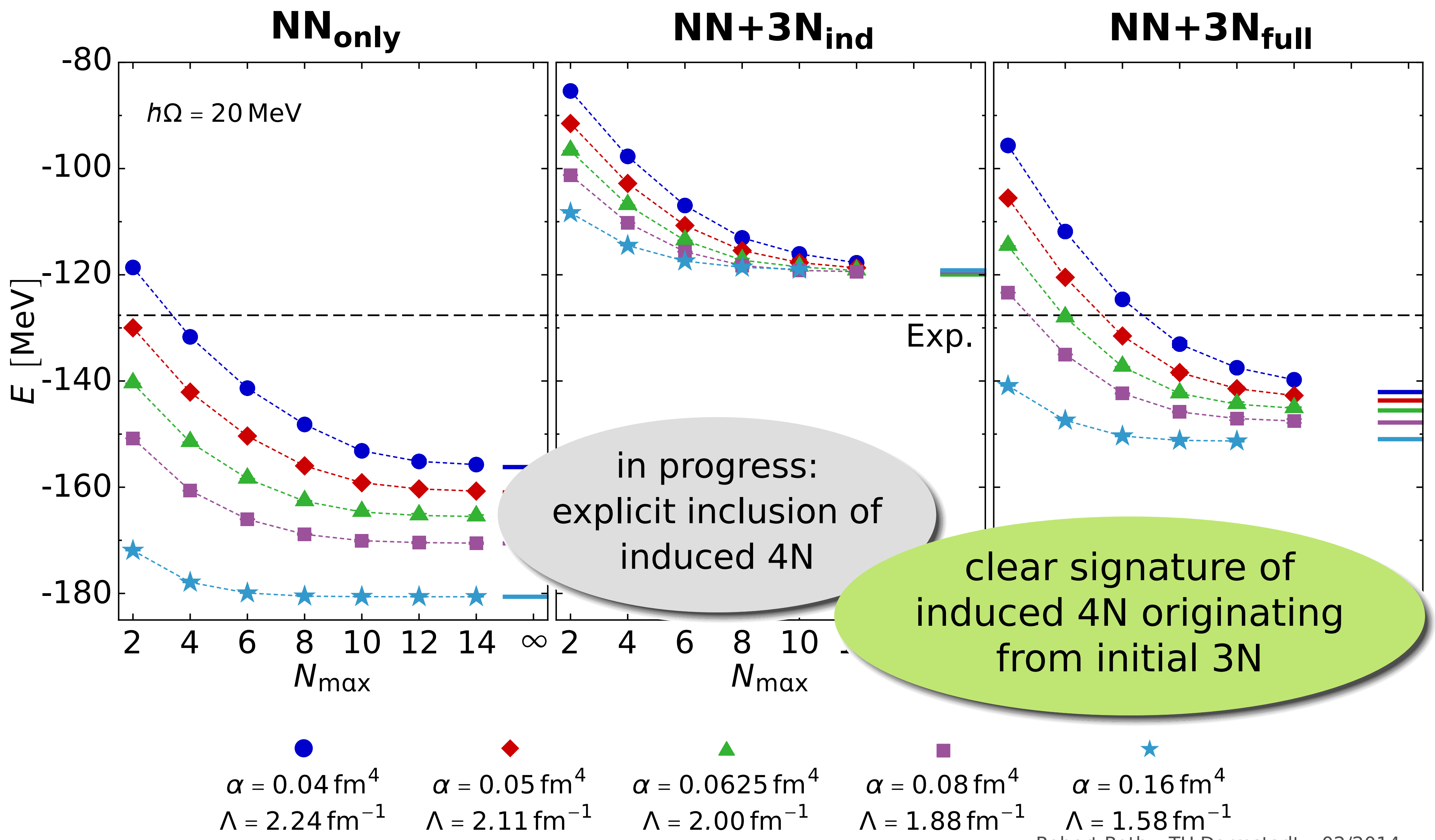
^{4}He: Ground-State Energies

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

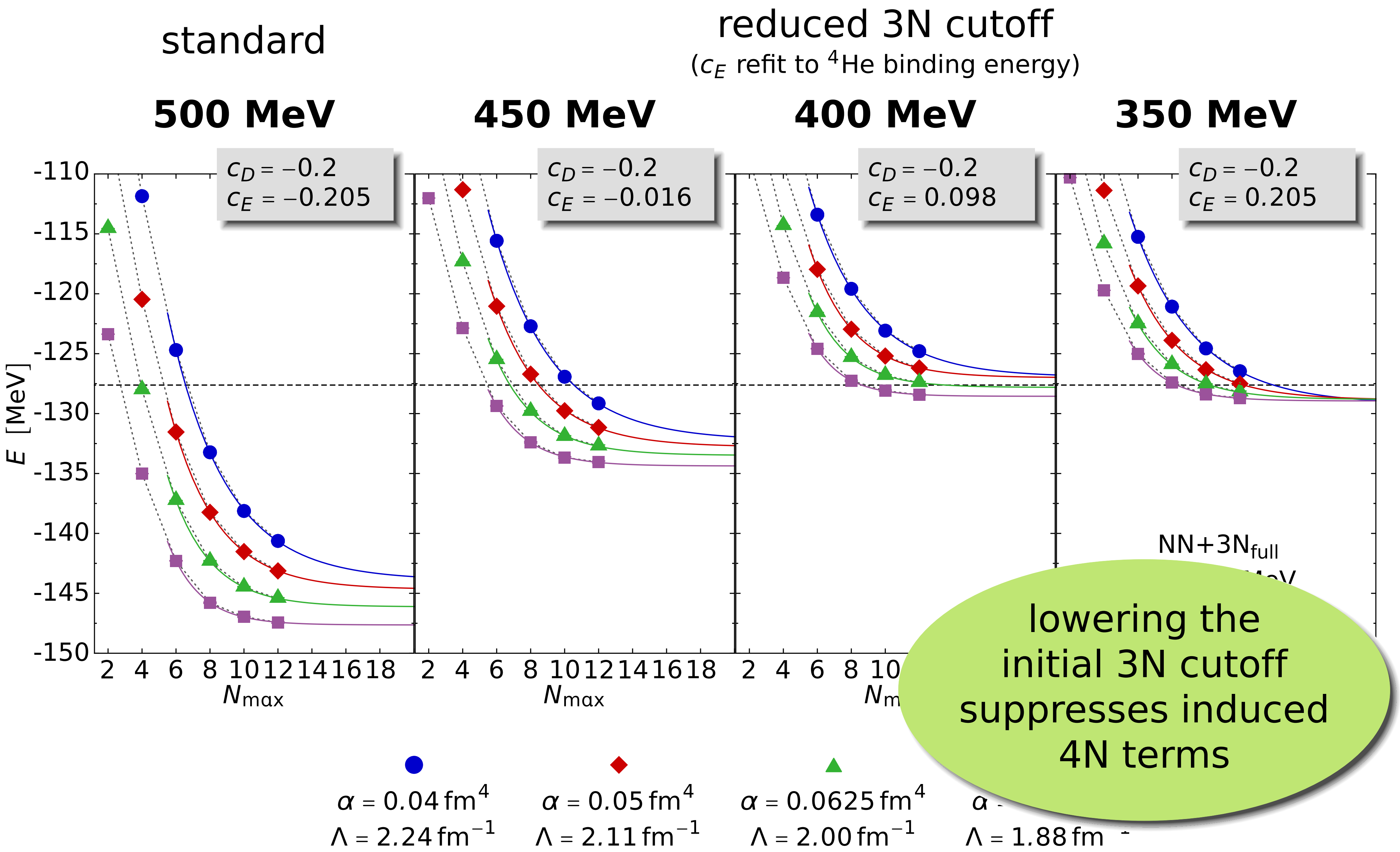


^{16}O: Ground-State Energies

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)

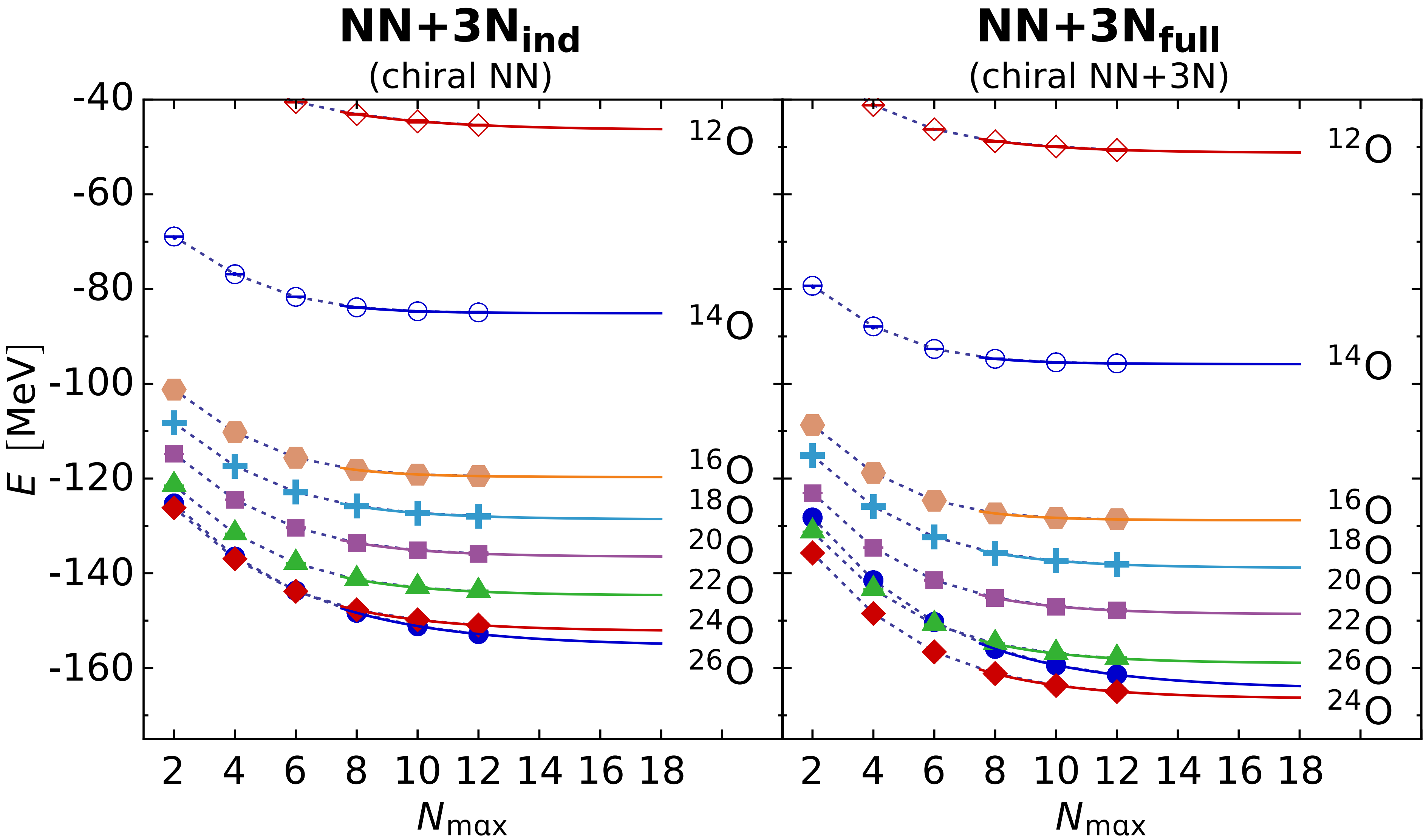
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions...

Cipollone, Barbieri, Duguet, Bogner, Holt, Hergert, Schwenk,...

- more ab initio studies since then...

Ground States of Oxygen Isotopes

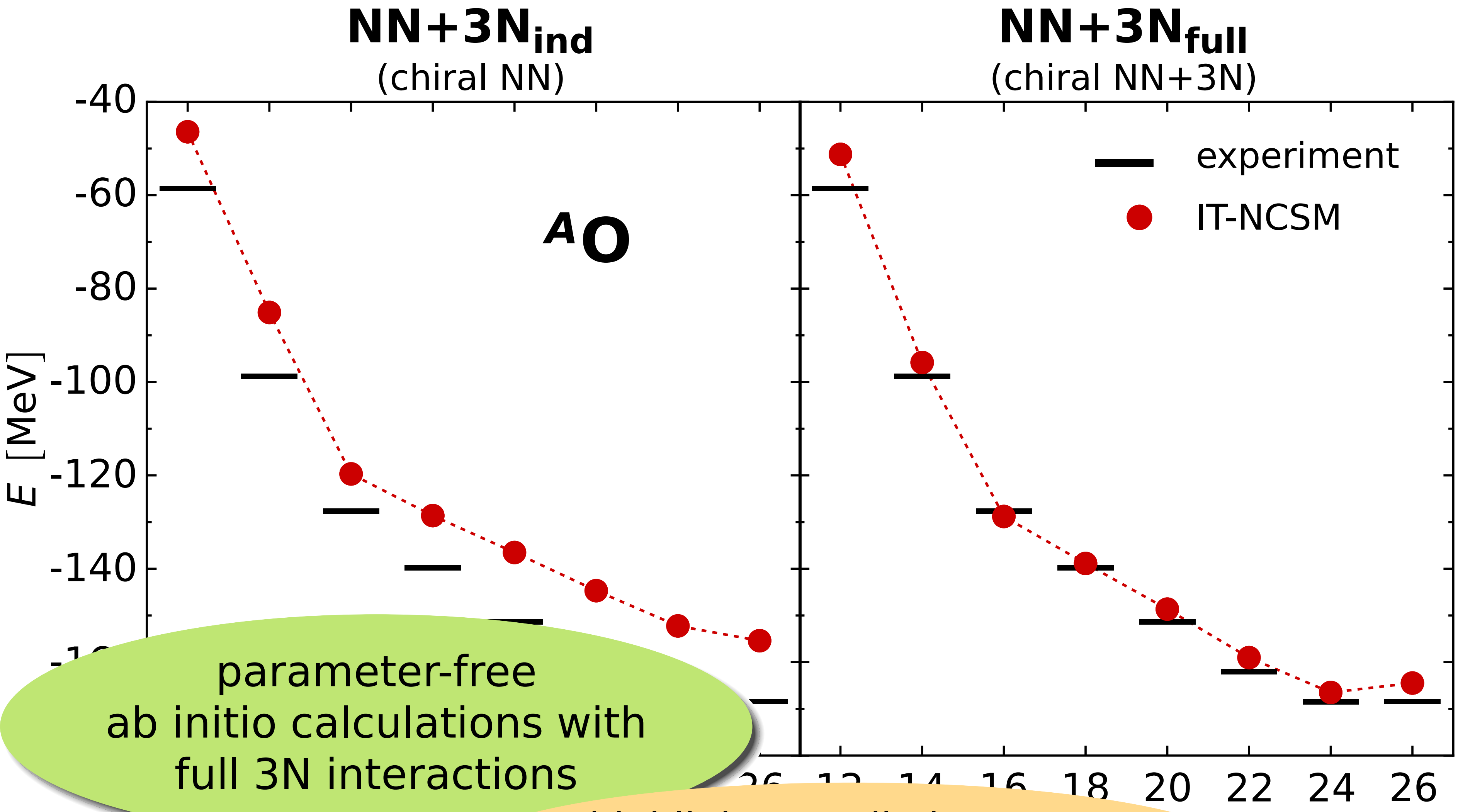
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



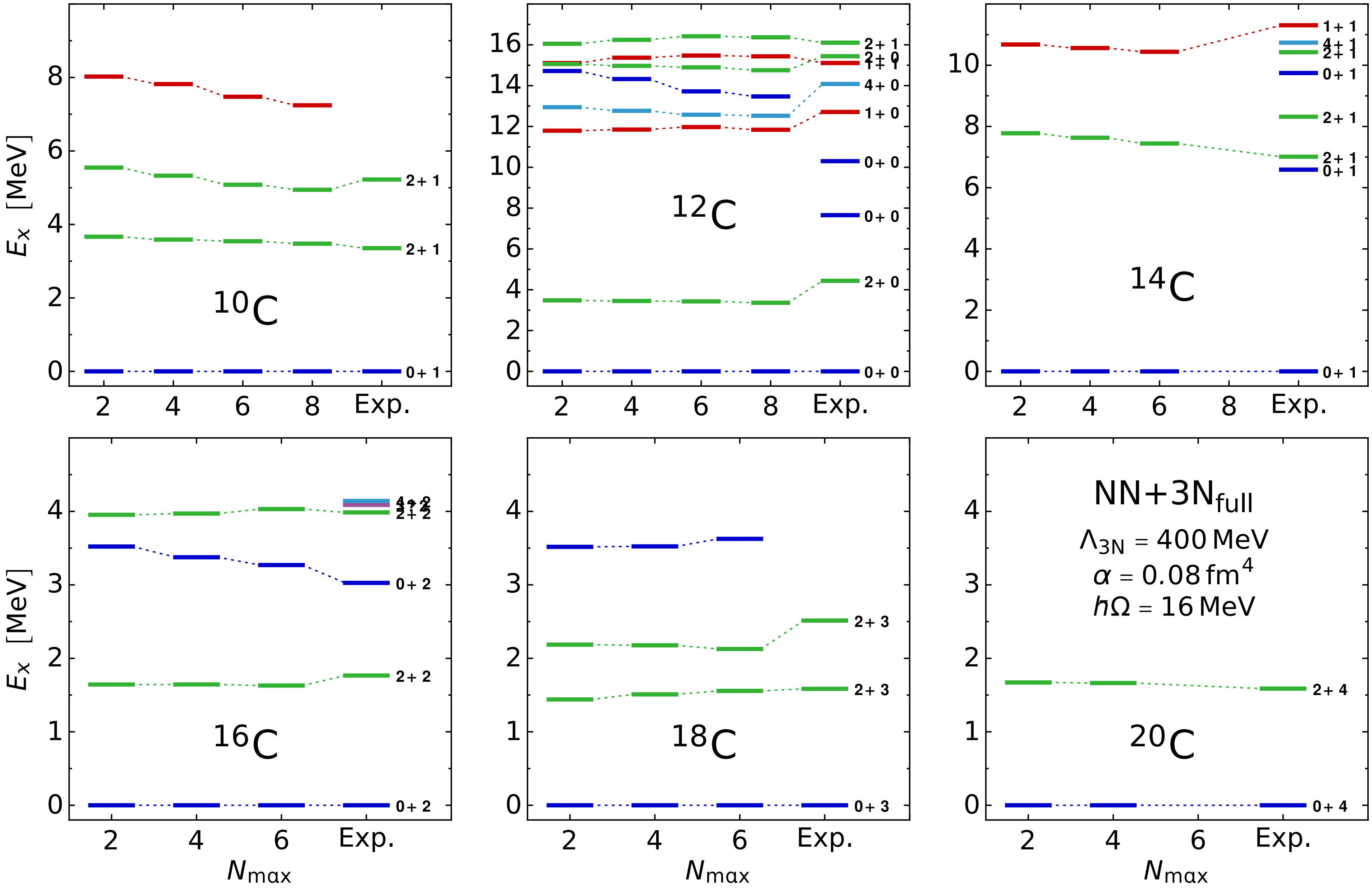
parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

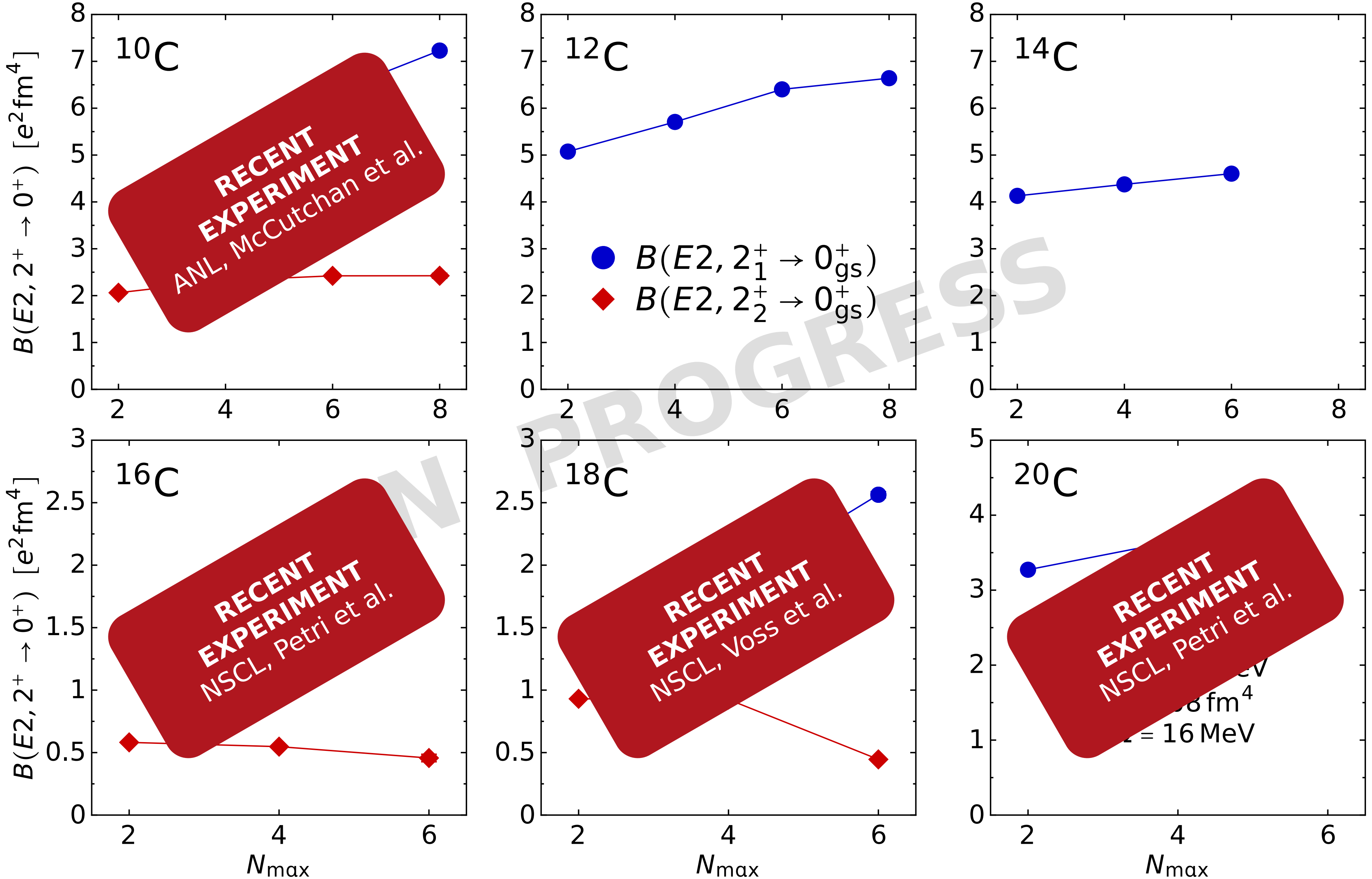
Λ_{3N} = 400 MeV, ... optimal $\hbar\Omega$

Spectroscopy of Carbon Isotopes

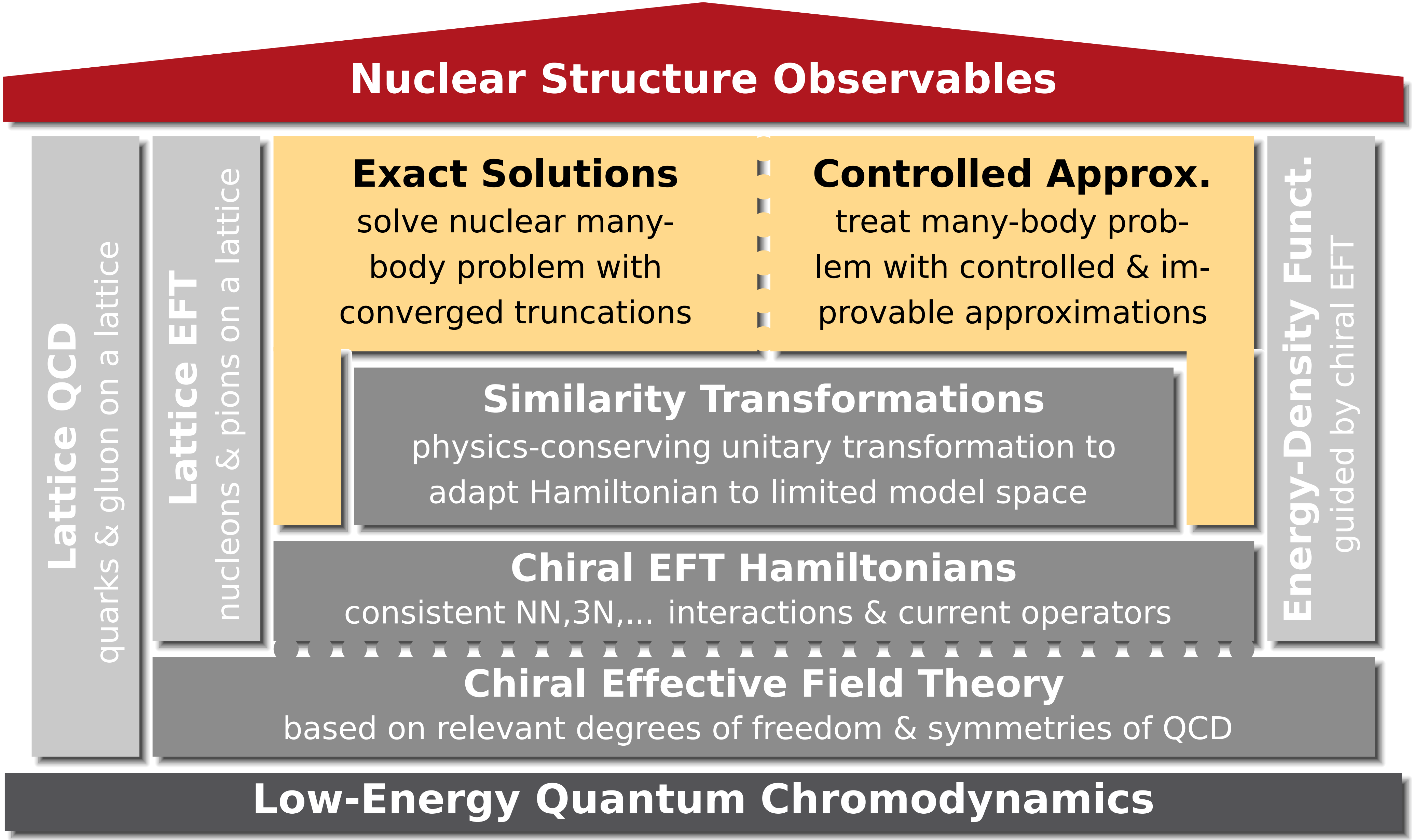
Forssen et al., JPG 40, 055105 (2013); Roth et al., in prep.



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 ... xponential 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...** ...ole 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, Cipollone,...

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

Inclusion of 3N Interactions

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

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

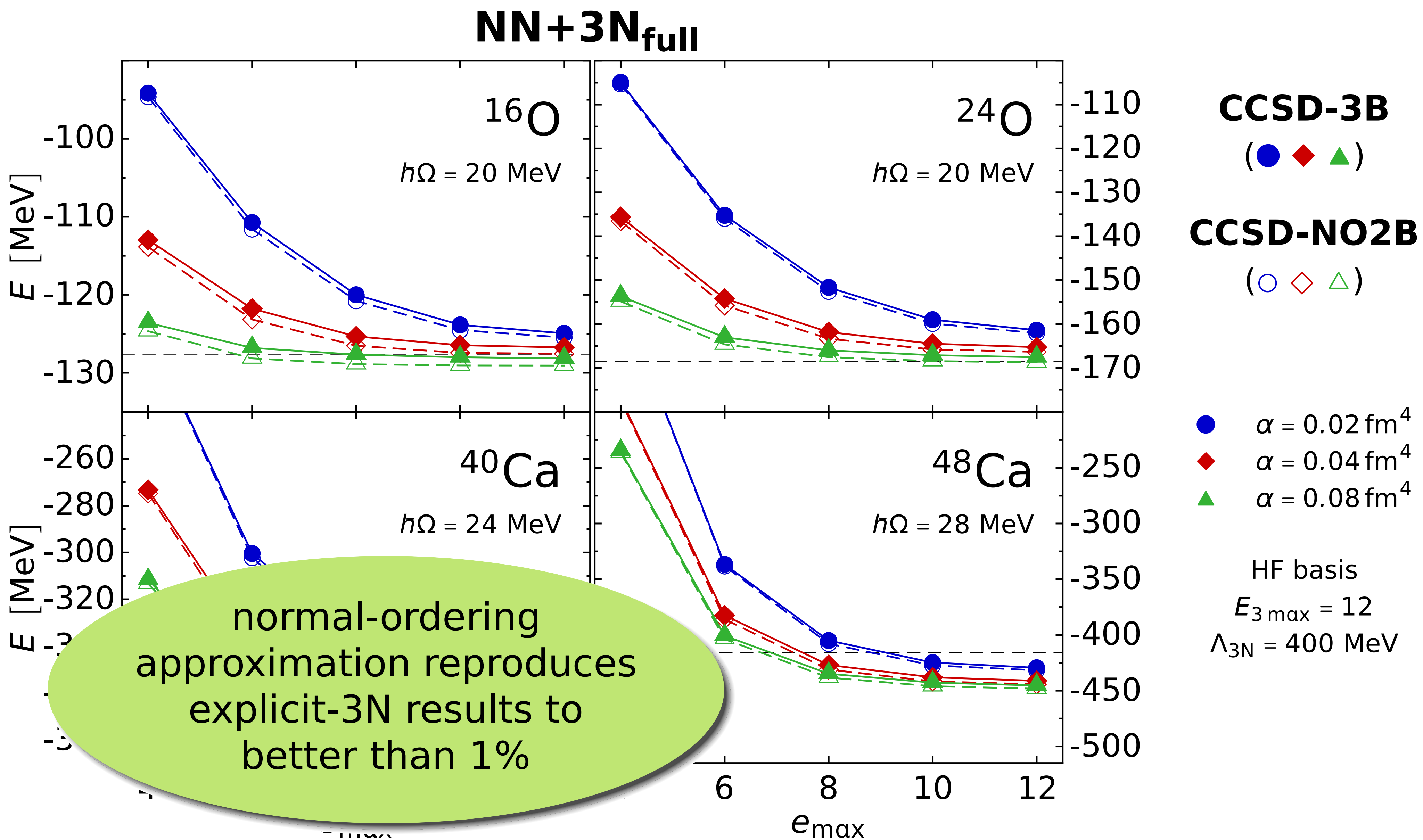
$$= W^{0B} + \sum W^{1B}_{\circ\circ}\, \{a^\dagger_\circ\, a_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ\}$$

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

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

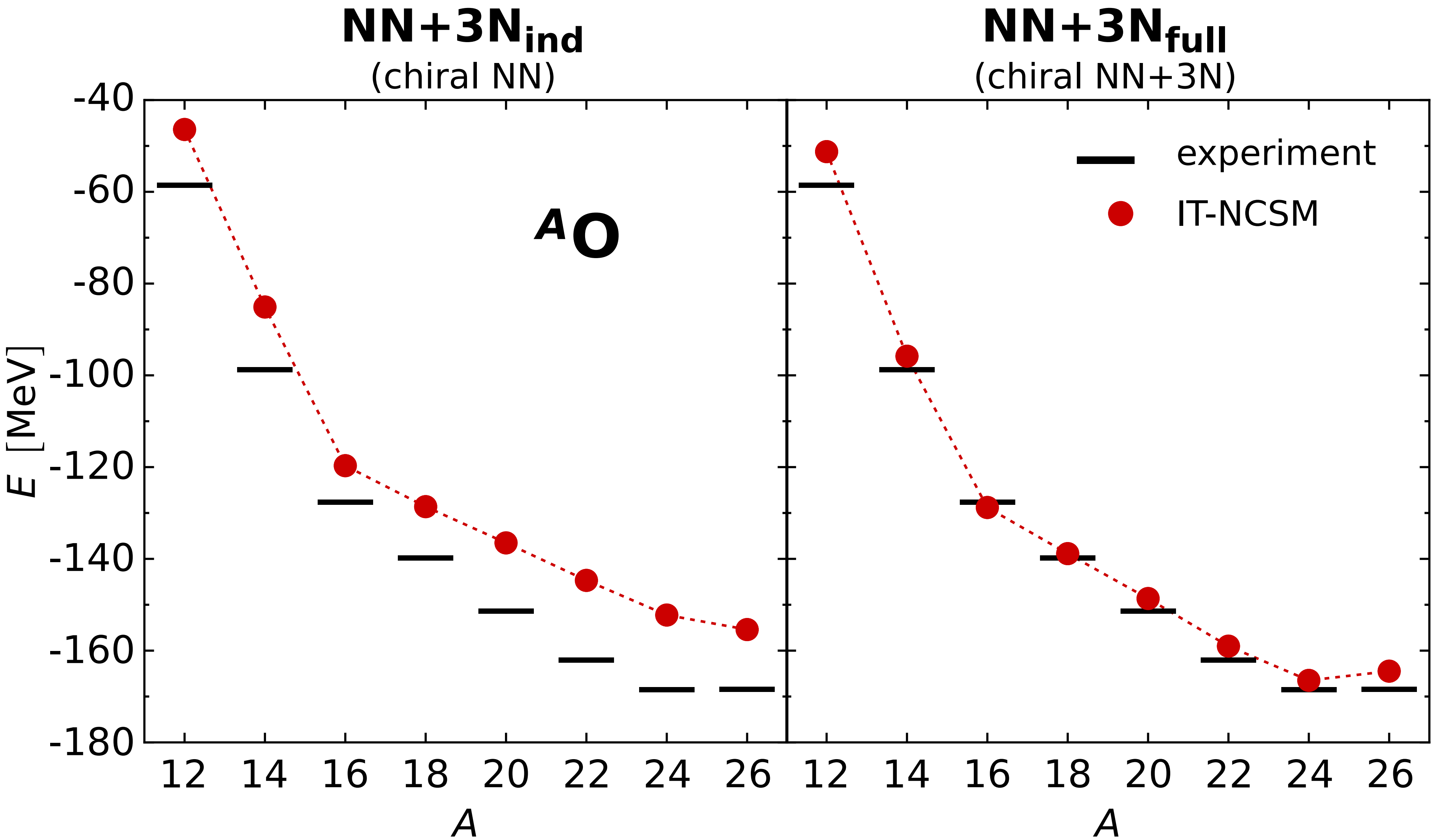
CCSD with Explicit 3N Interactions

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



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 $\hbar\Omega$

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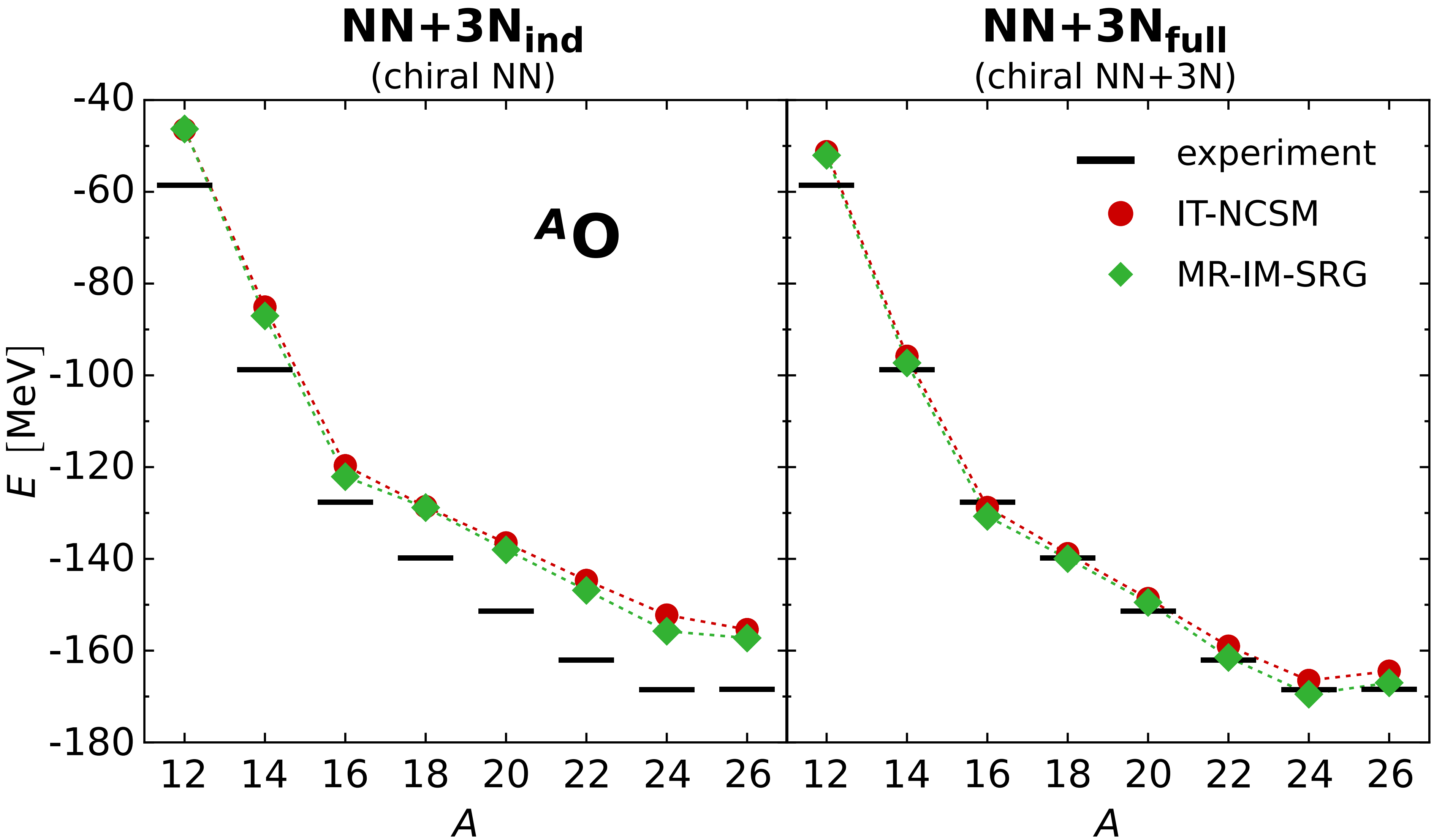

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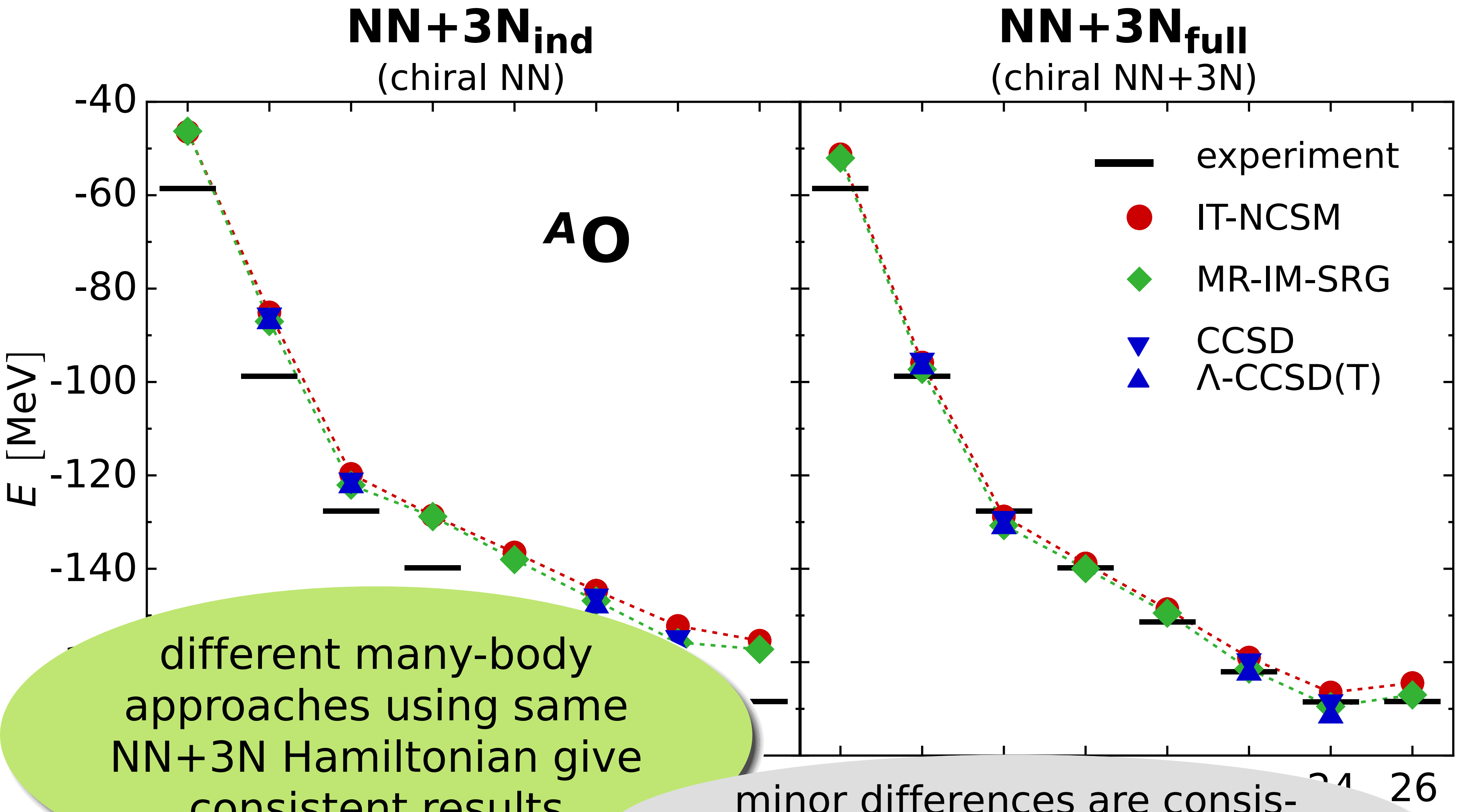

different many-body approaches using same NN+3N Hamiltonian give consistent results

minor differences are consistent with uncertainty analysis

Λ_{3N} = 400 MeV, α = 0.08 fm⁴, $E_{3\max}$ = 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)

computationally CC or IM-SRG can handle heavy nuclei, however, all technical truncations need to be revisited...

- **truncation of many-body model space**
  - truncation of underlying single-particle basis (e_{max})
  - truncation of excitation operators or corresponding diagrammatic truncations
- **truncation of many-body interactions**
  - normal-ordered 3N interaction truncated at the two-body level vs. explicit 3N
  - technical truncation of 3N matrix-element sets ($E_{3\,max}$)
  - truncation of model space for performing SRG evolution in 3N sector
  - omission of SRG-induced beyond-3N interactions
- **truncations in chiral EFT inputs**

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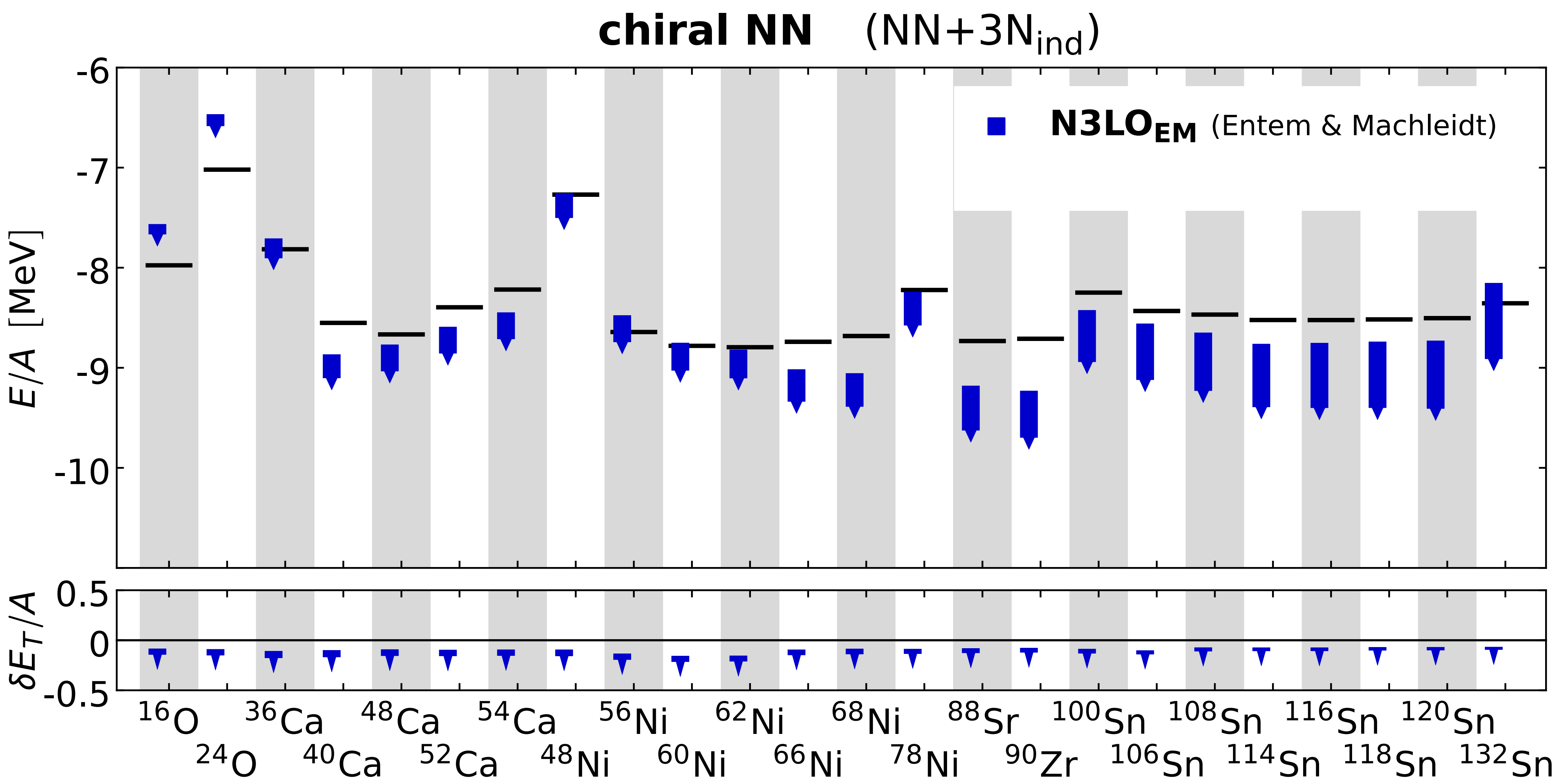
  - omission of SRG-induced beyond 3N interactions
- **truncations in chiral EFT**

...after lots of improvements

~ 2% uncertainty up to Sn isotopes

Towards Heavy Nuclei - Ab Initio

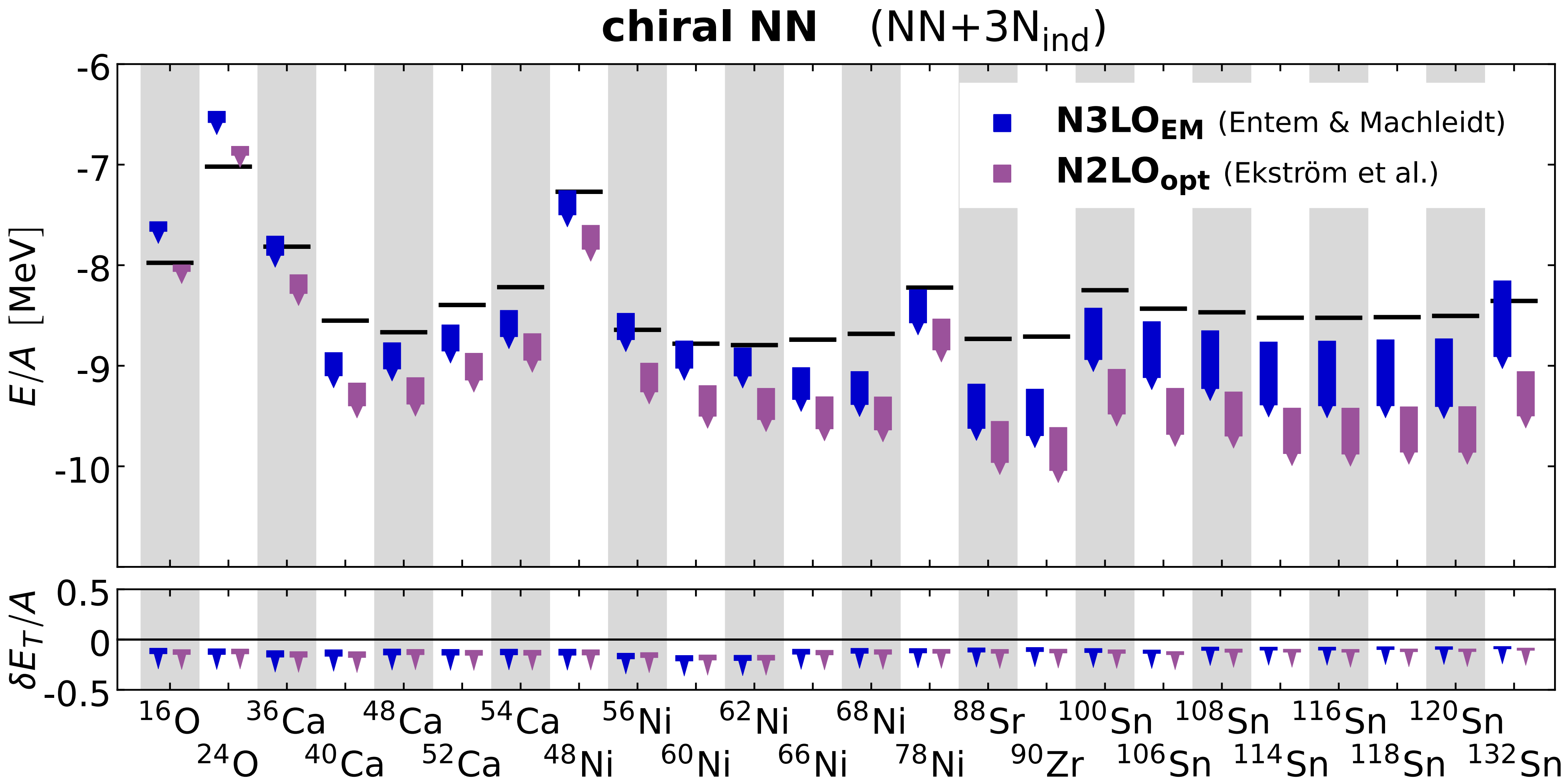
Binder et al., arXiv:1312.5685 (2013)



CR-CC(2,3), $\alpha = 0.08 \rightarrow 0.04\,\mathrm{fm}^4$, $E_{3\,\mathrm{max}} = 18$, optimal $\hbar\Omega$

Towards Heavy Nuclei - Ab Initio

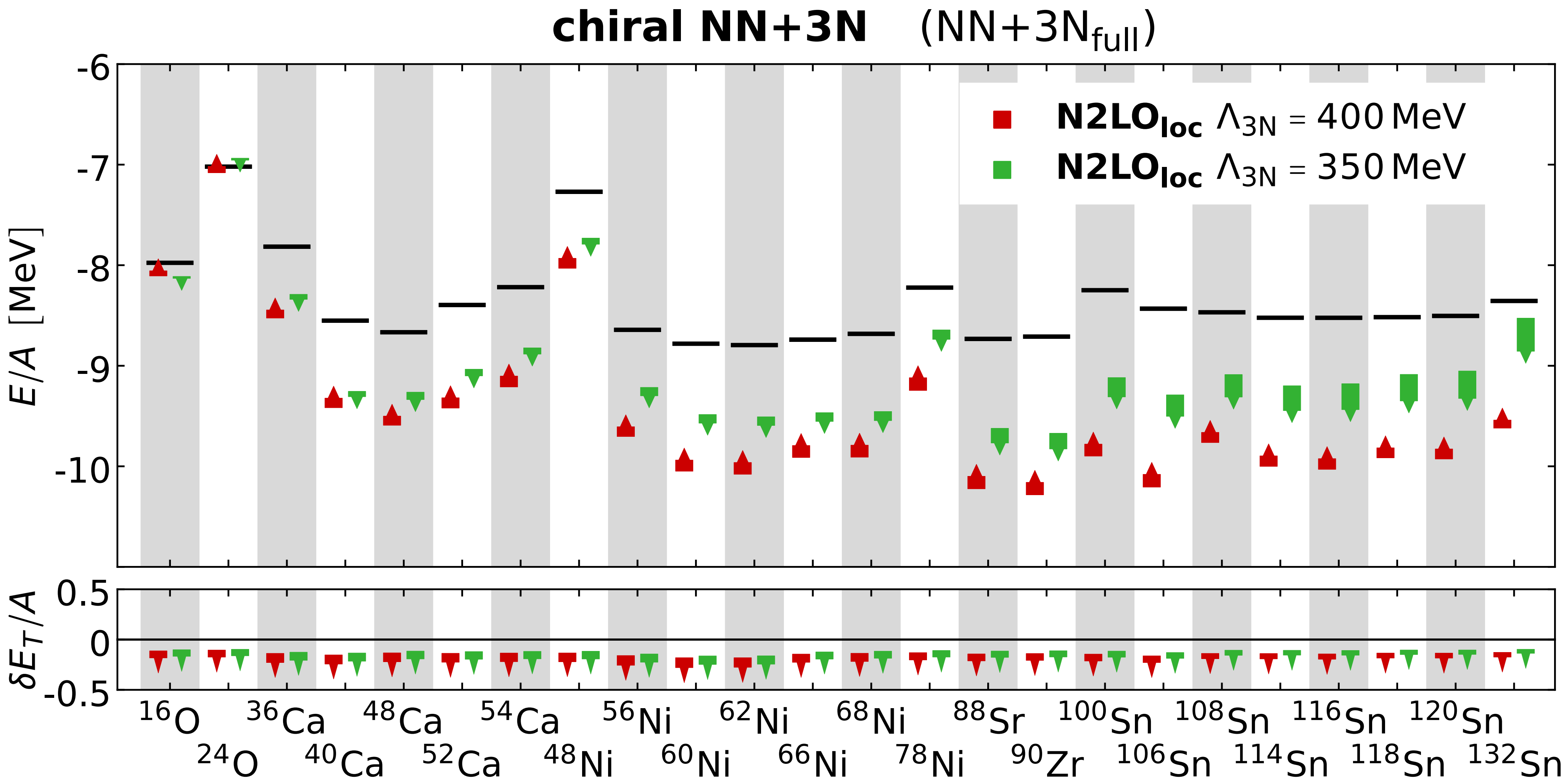
Binder et al., arXiv:1312.5685 (2013)



CR-CC(2,3), $\alpha = 0.08 \rightarrow 0.04\,\mathrm{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

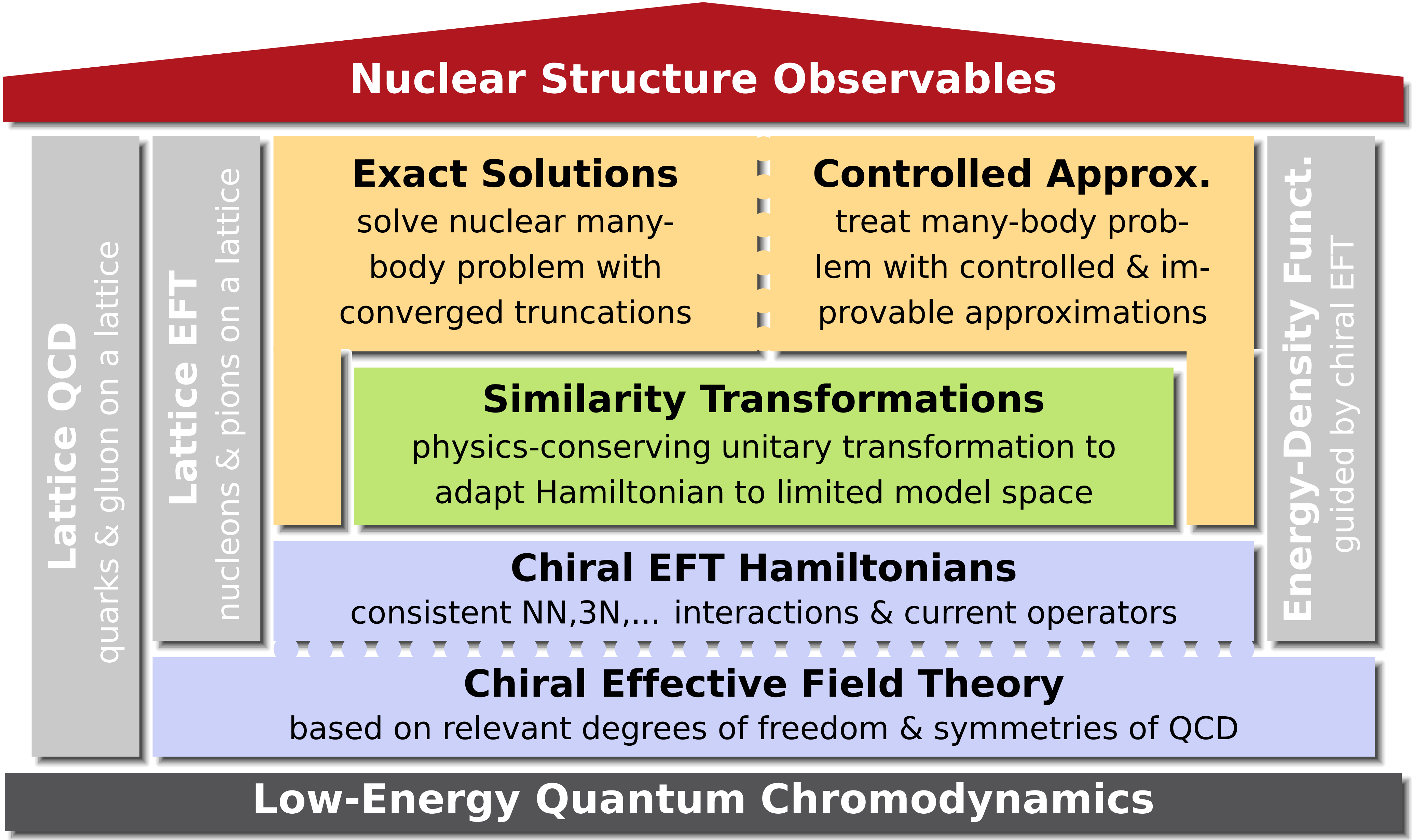
Towards Heavy Nuclei - Ab Initio

Binder et al., arXiv:1312.5685 (2013)

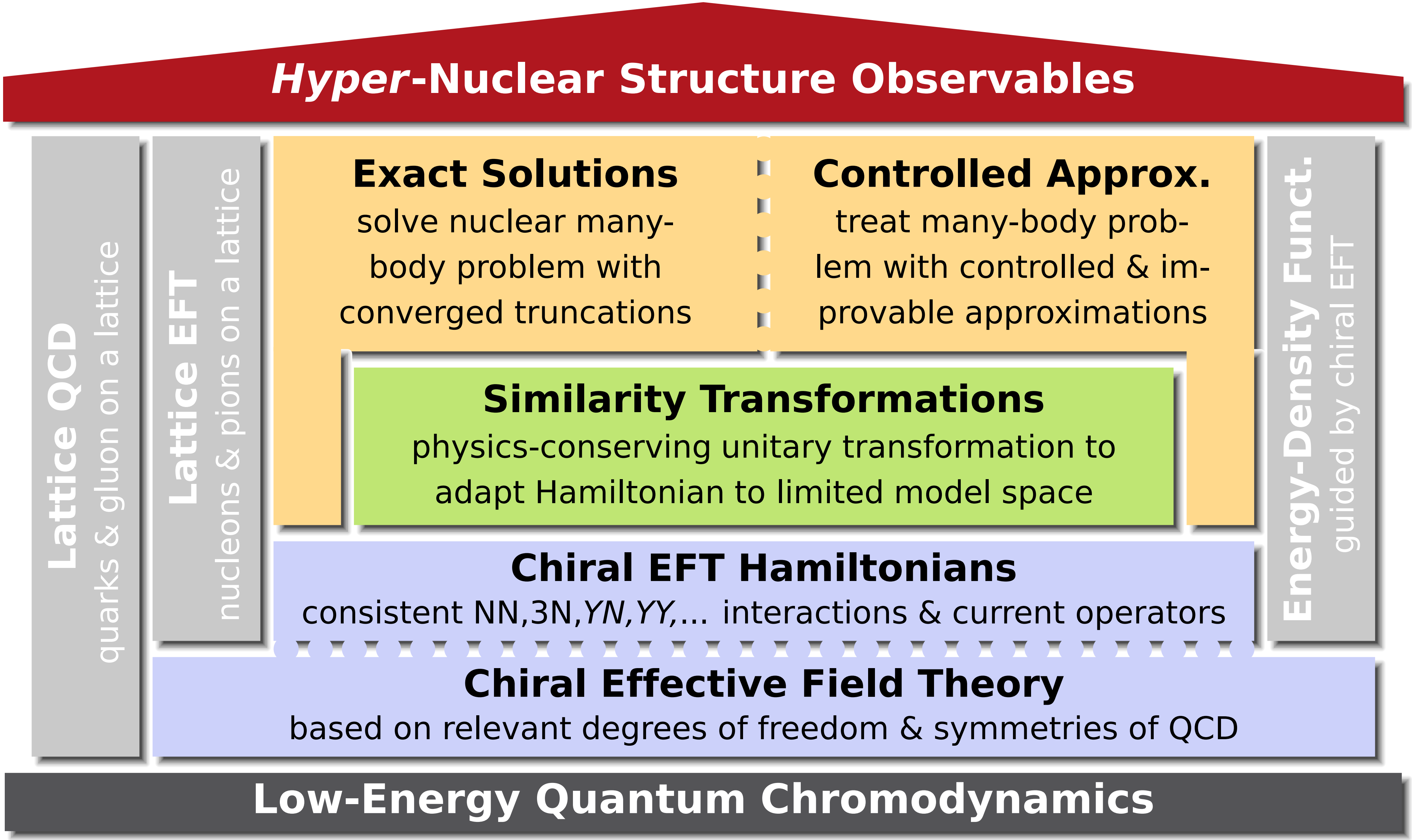


CR-CC(2,3), NN @ N3LO$_{EM}$, $\alpha = 0.08 \rightarrow 0.04\,\text{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

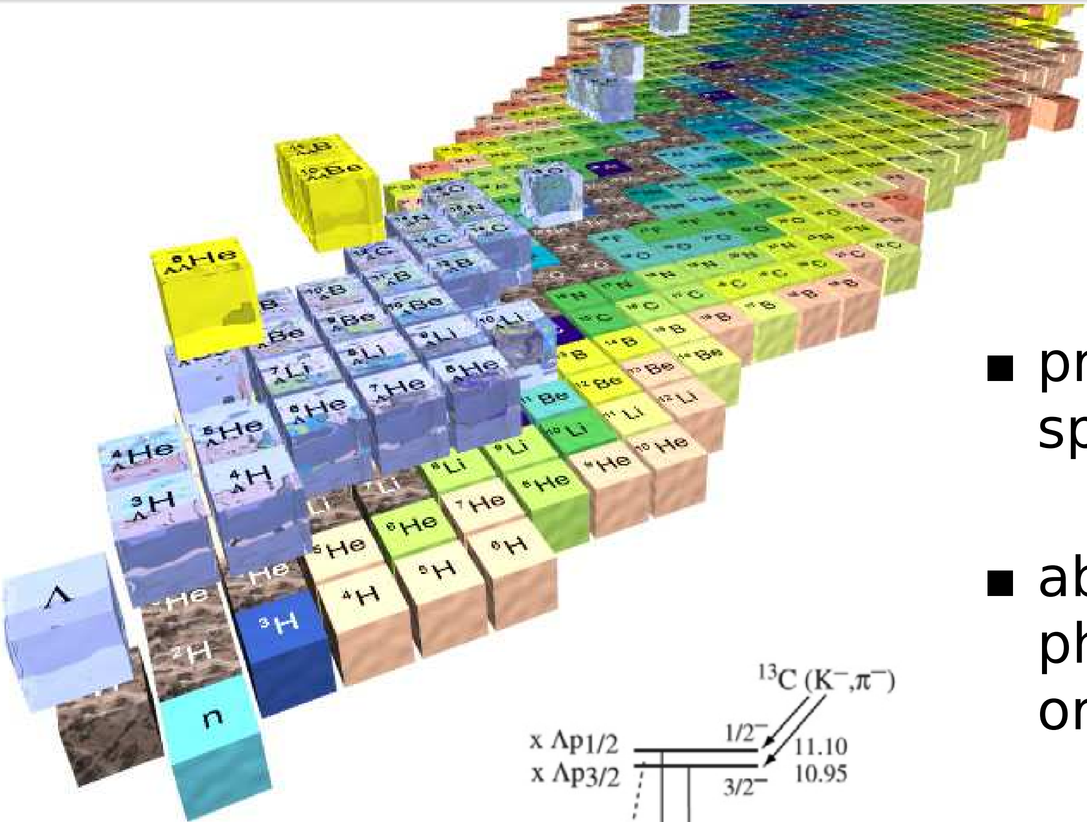
Ab Initio Nuclear Structure

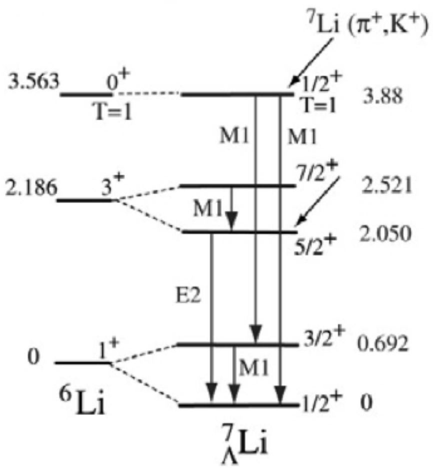


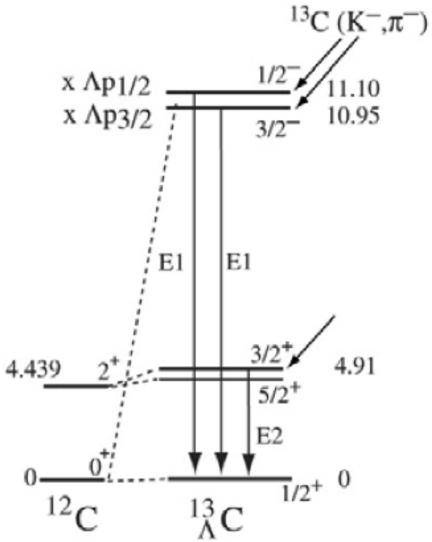
Ab Initio *Hyper*-Nuclear Structure



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

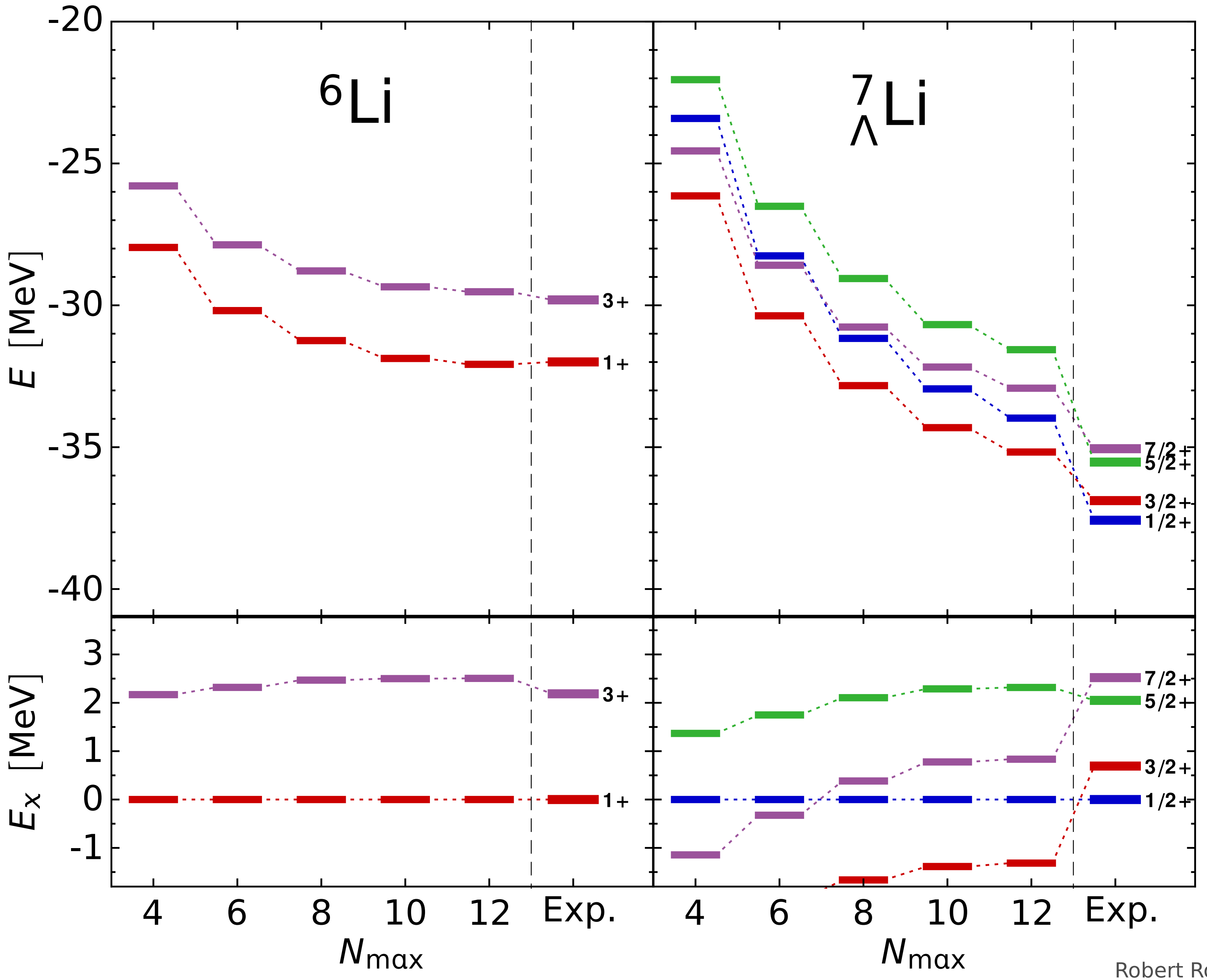
Similarity Renormalization Group

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



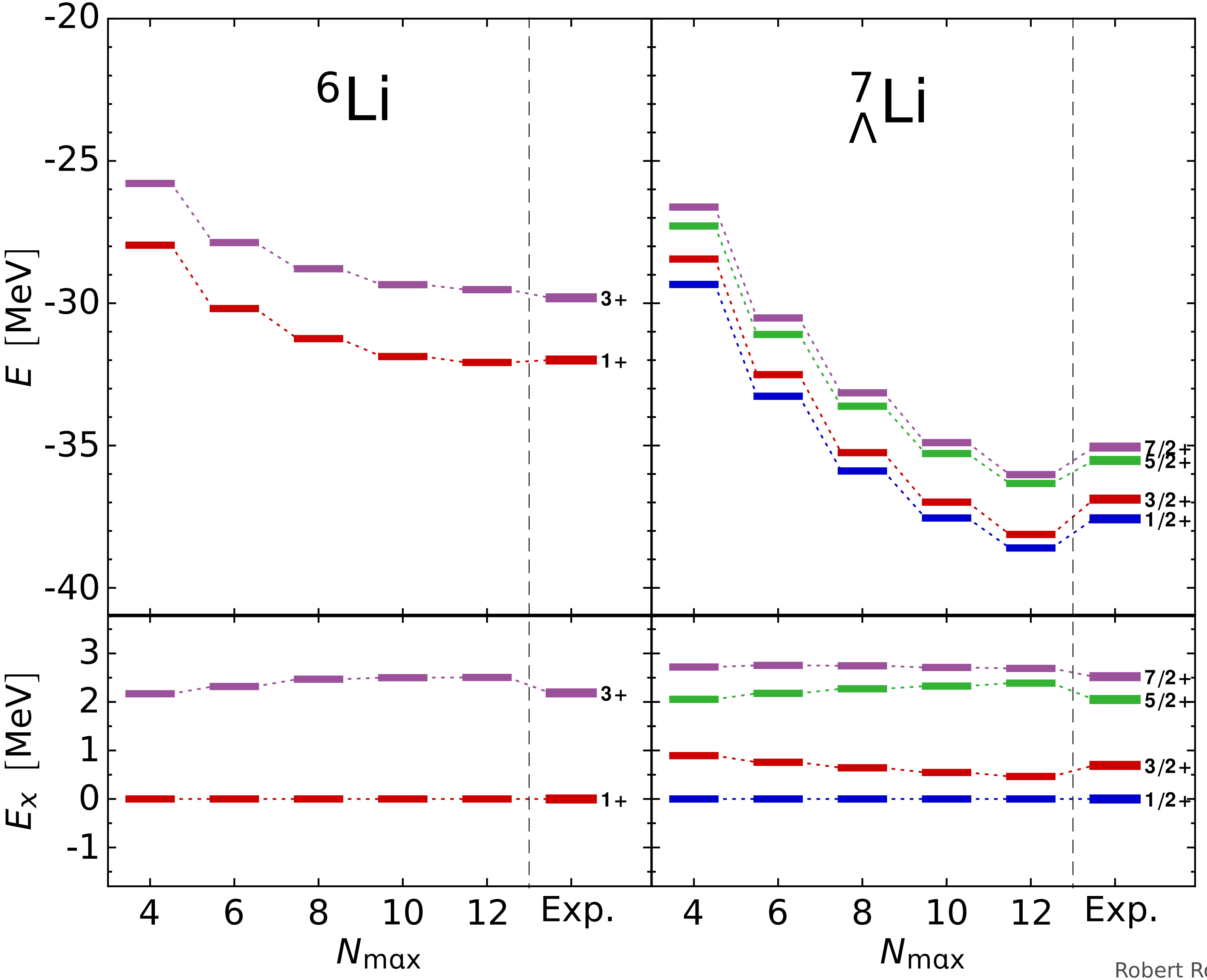
NN @ N3LO
$\Lambda_{NN} = 500$ MeV
Entem&Machleidt

3N @ N2LO
$\Lambda_{3N} = 500$ 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: ${}^{7}_{\Lambda}\mathrm{Li}$



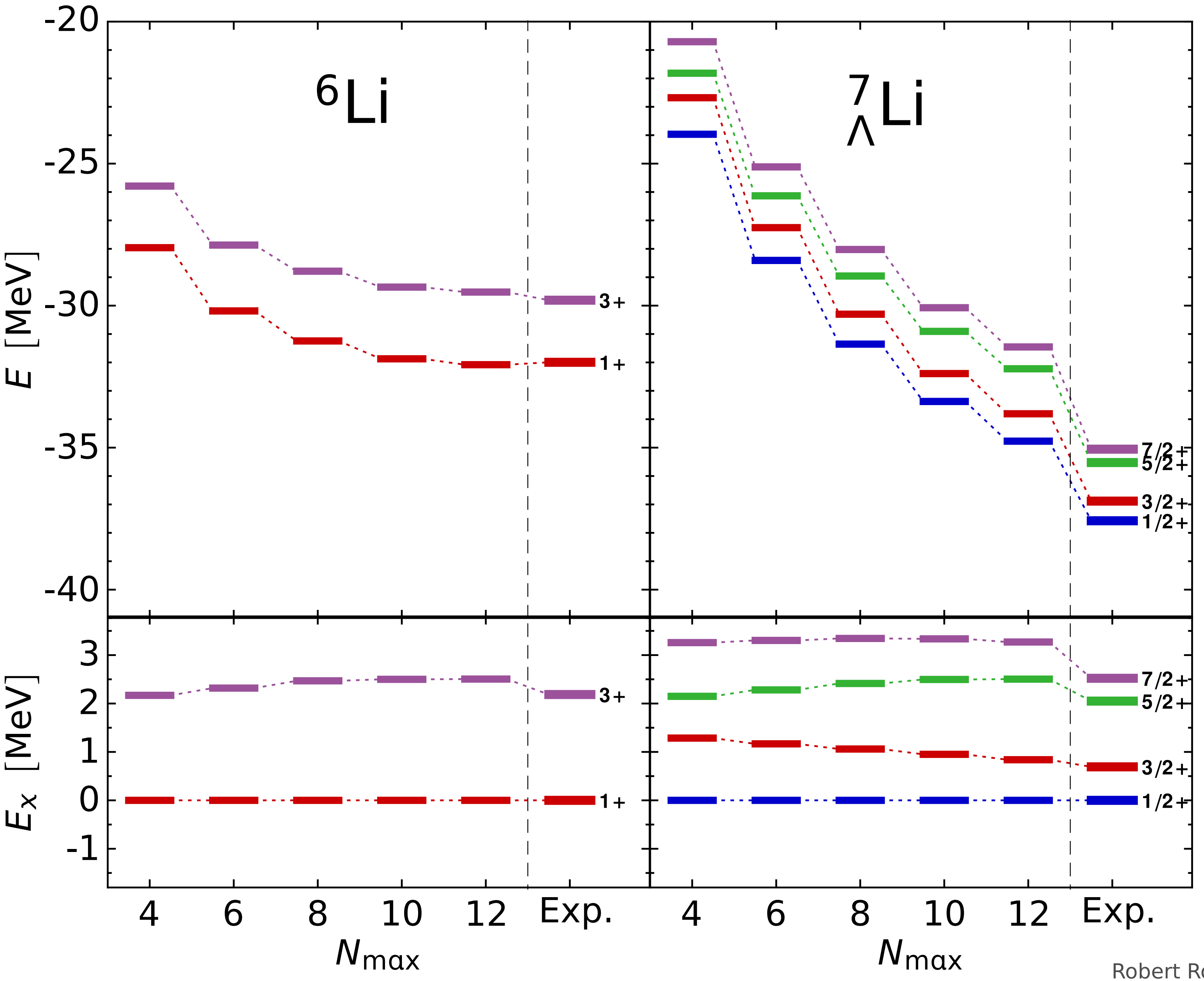
NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

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

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

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

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



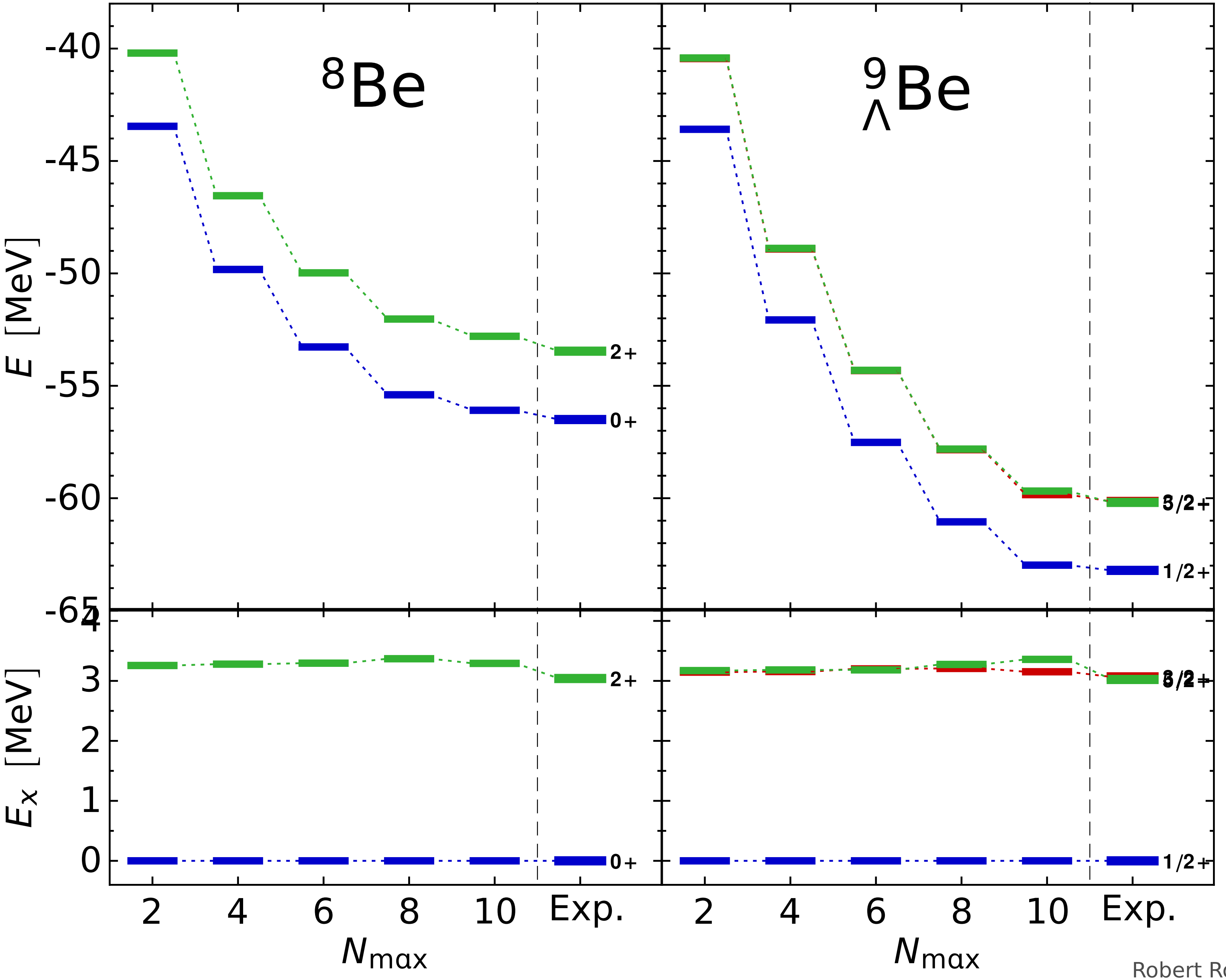
NN @ N3LO
$\Lambda_{NN} = 500$ MeV
Entem&Machleidt

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

YN @ LO
$\Lambda_{YN} = 700$ 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: $^{9}_{\Lambda}$Be



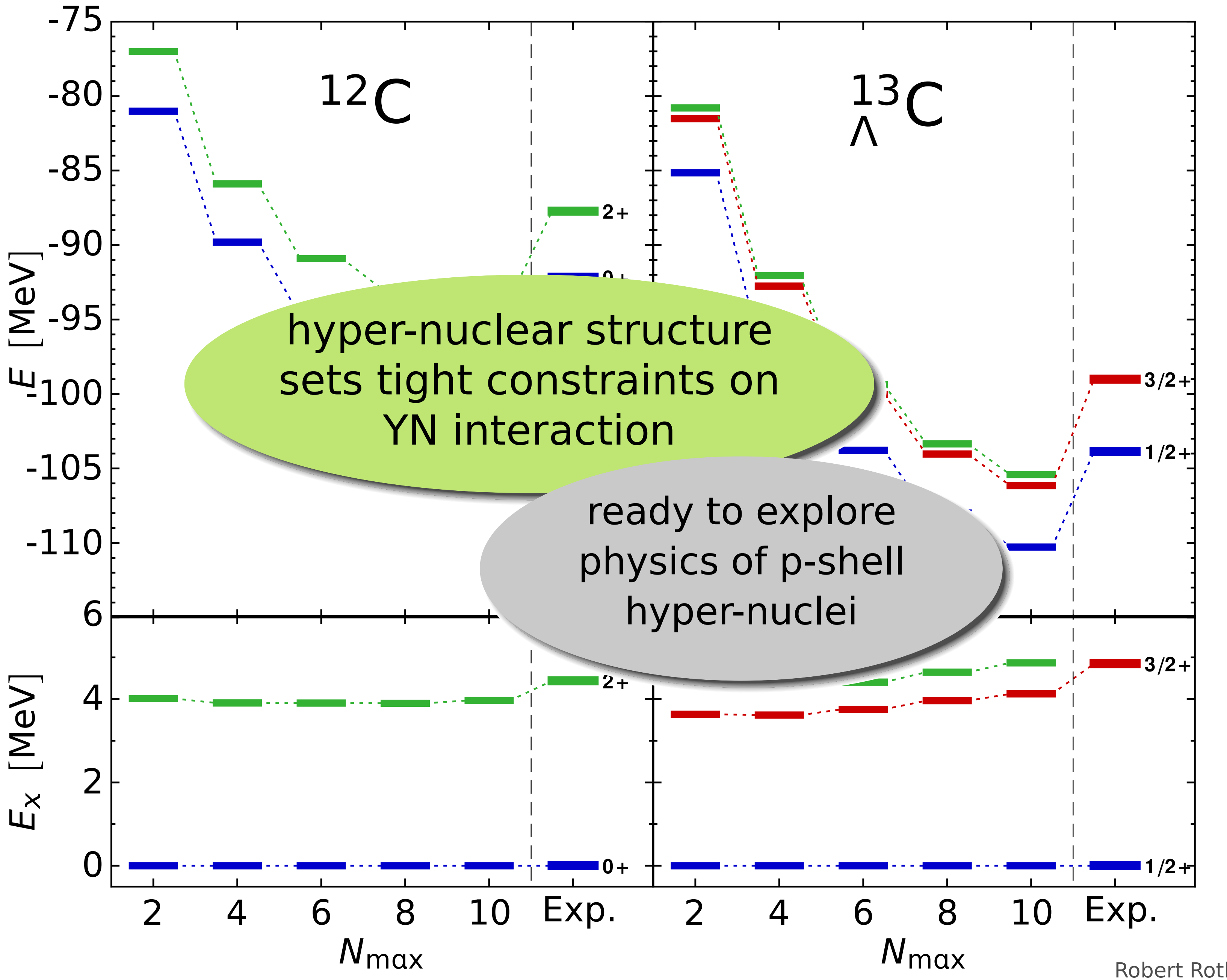
NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

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

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

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

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



NN @ N3LO
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3N @ N2LO
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$\alpha_{NN} = 0.08\,\mathrm{fm}^4$
$\alpha_{YN} = 0.00\,\mathrm{fm}^4$
$\hbar\Omega$ = 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 & reaction frontier**
    include continuum effects and reaction 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**
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