Ab Initio Nuclear Structure with Chiral NN+3N Hamiltonians

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

New Era of Low-Energy Nuclear Physics

Experiment

new facilities and experiments to produce nuclei far-off stability and study a range of observables

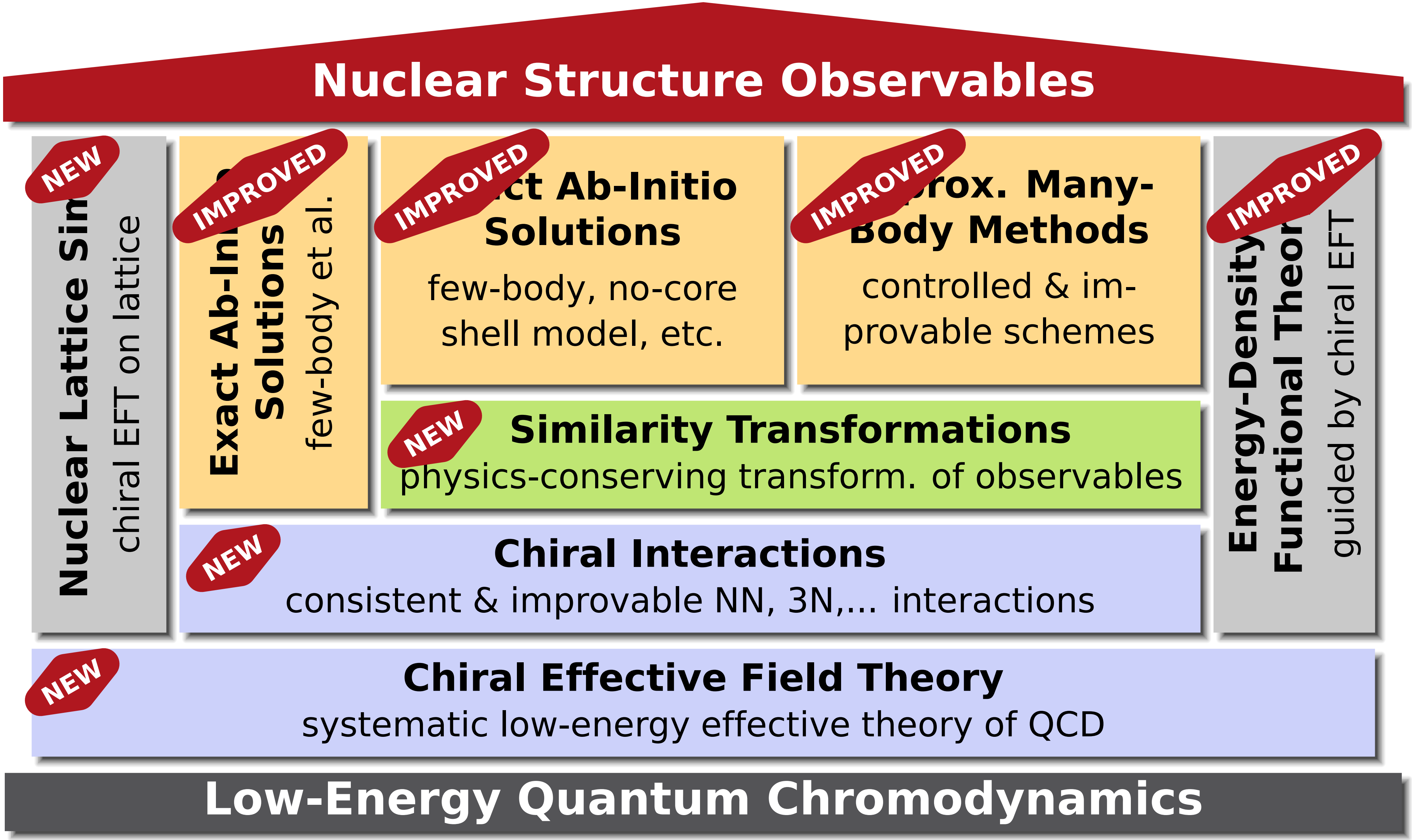
Quantum Chromodynamics

chiral effective field theory and lattice simulations access low-energy QCD and nuclear interactions

Nuclear Many-Body Theory

novel theoretical and computational methods allow for ab initio description of many more nuclei

Ab Initio Nuclear Structure



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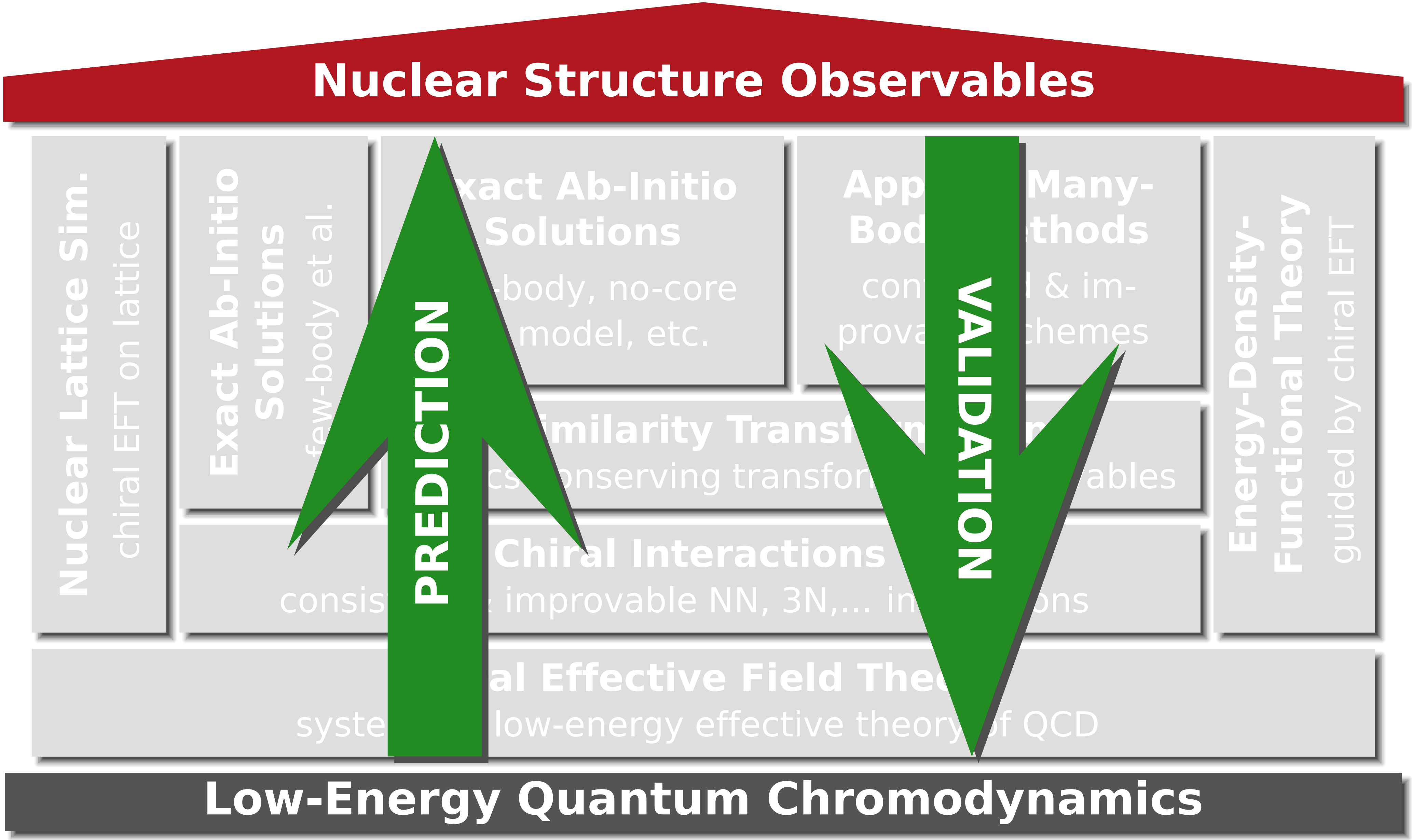

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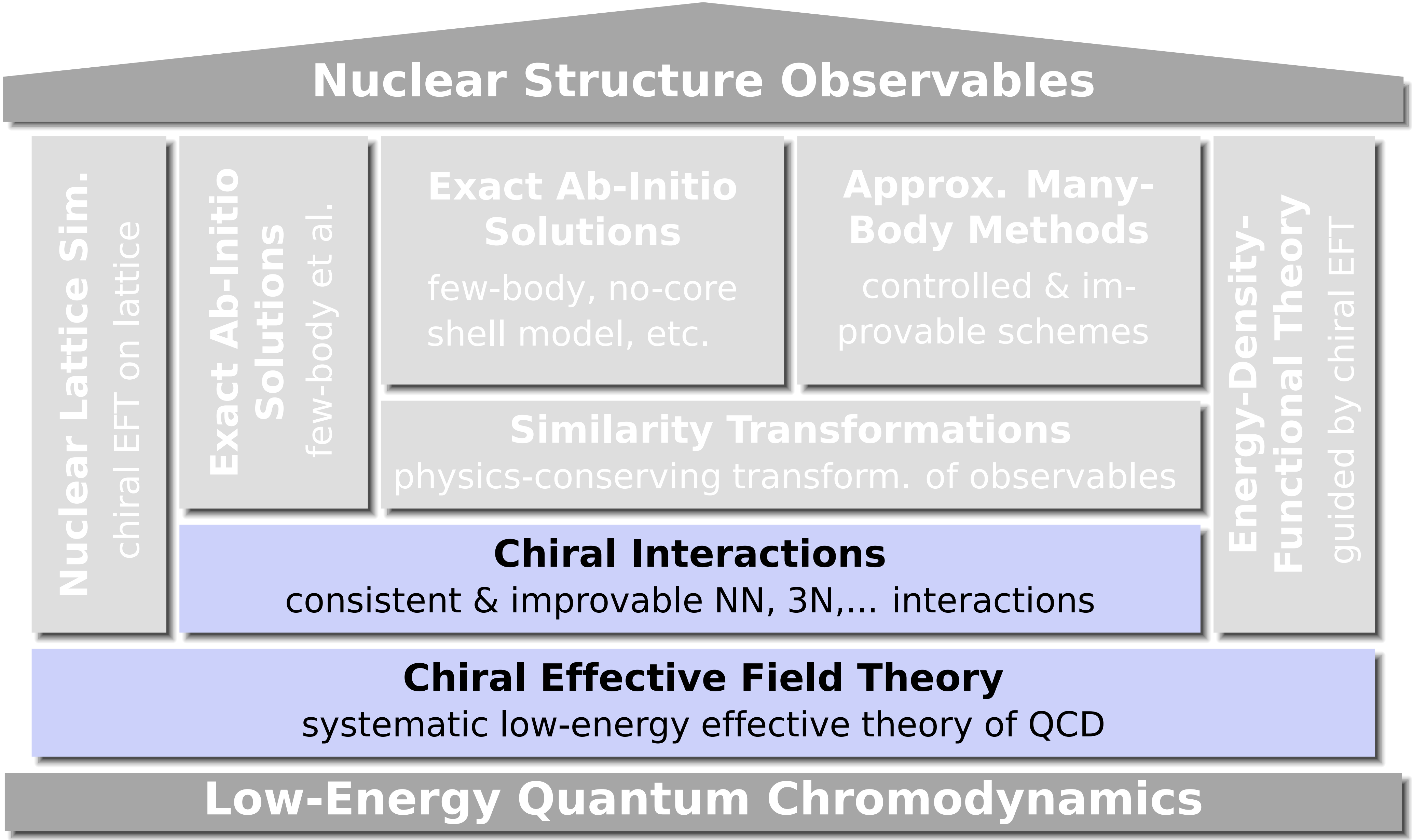
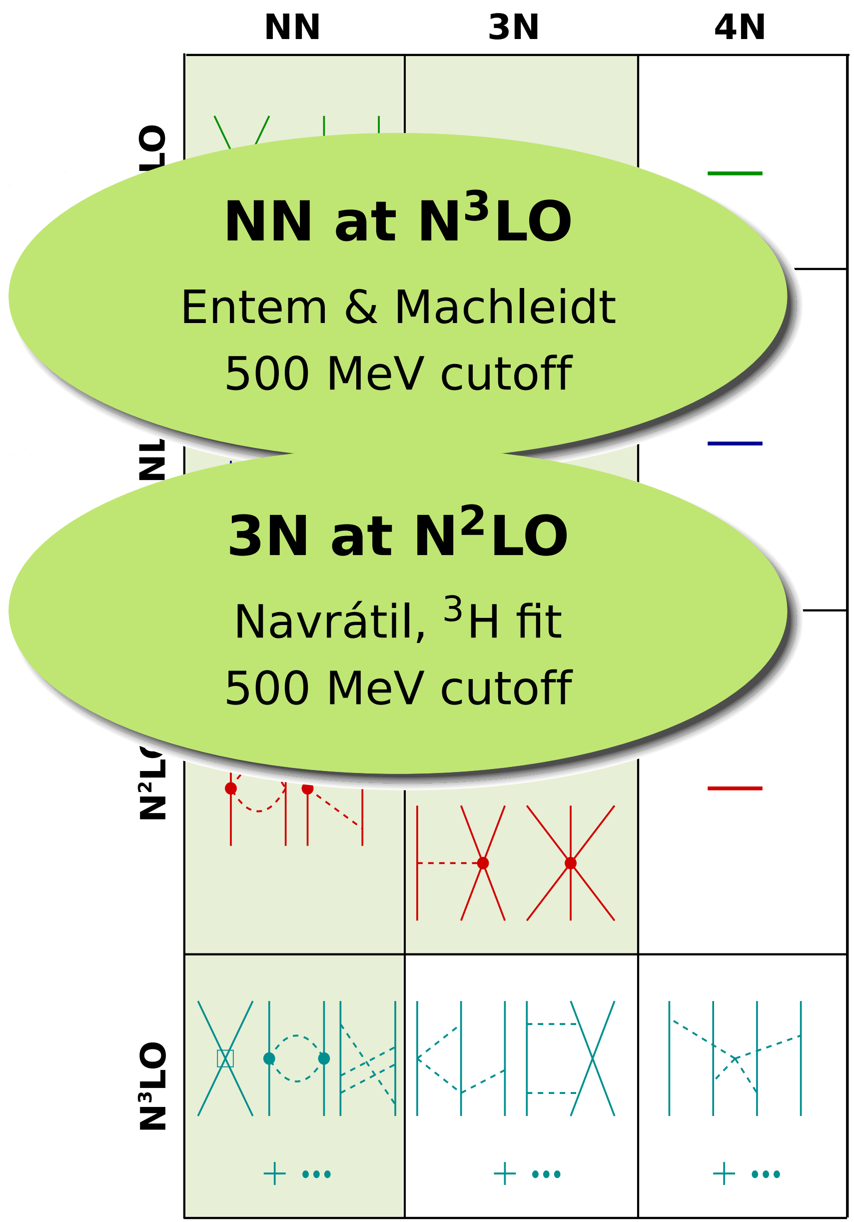


Nuclear Interactions from Chiral EFT

- 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 N^{3}LO
  - explicit inclusion of Δ-resonance
  - formal issues: power counting, renormalization, cutoff choice,...



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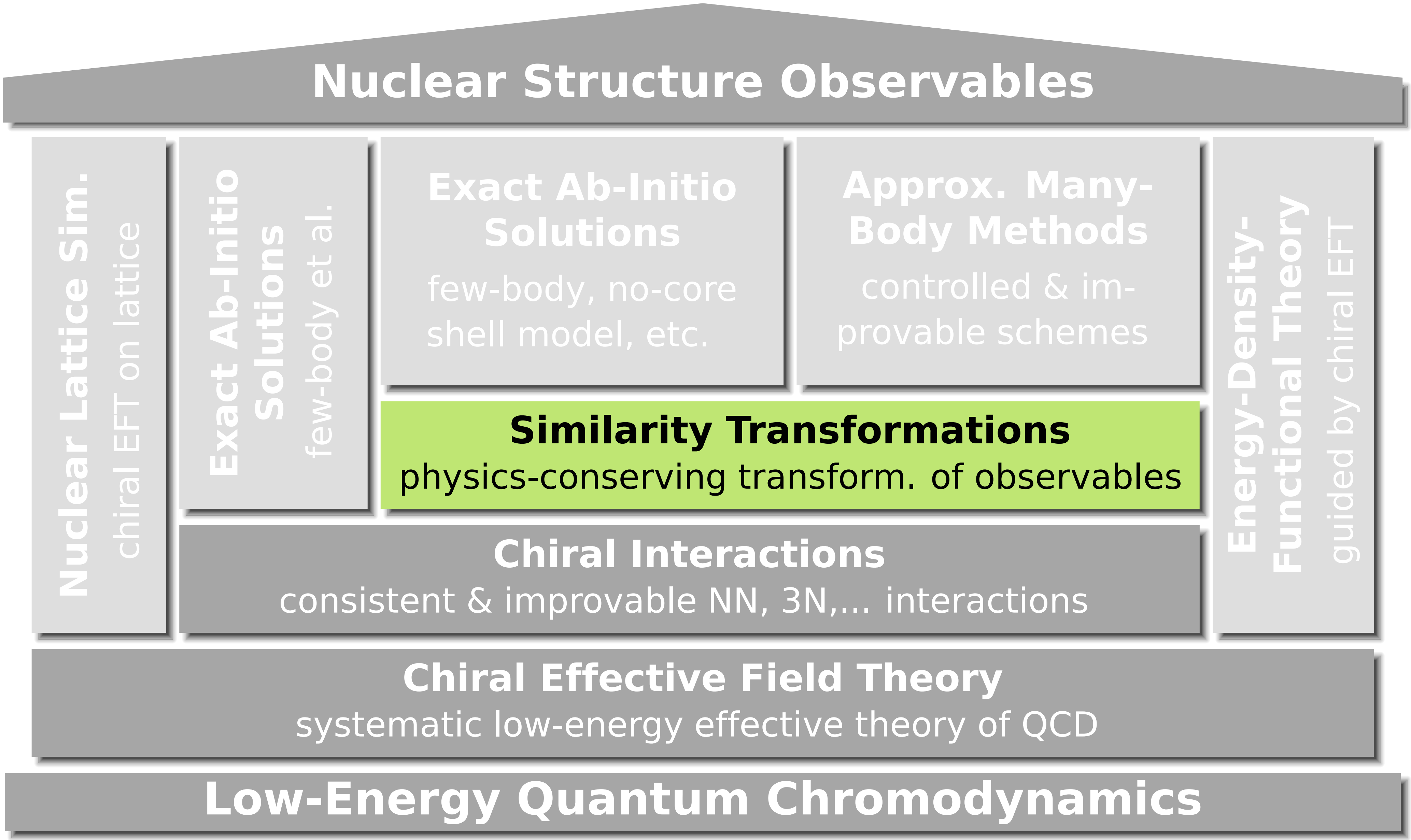


Similarity Renormalization Group

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

- **unitary transformation** of Hamil

$$\widetilde{H}_\alpha = U_\alpha^\dagger H U_\alpha$$

- **evolution equations** for $\widetilde{H}_\alpha$ and U

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha]$$

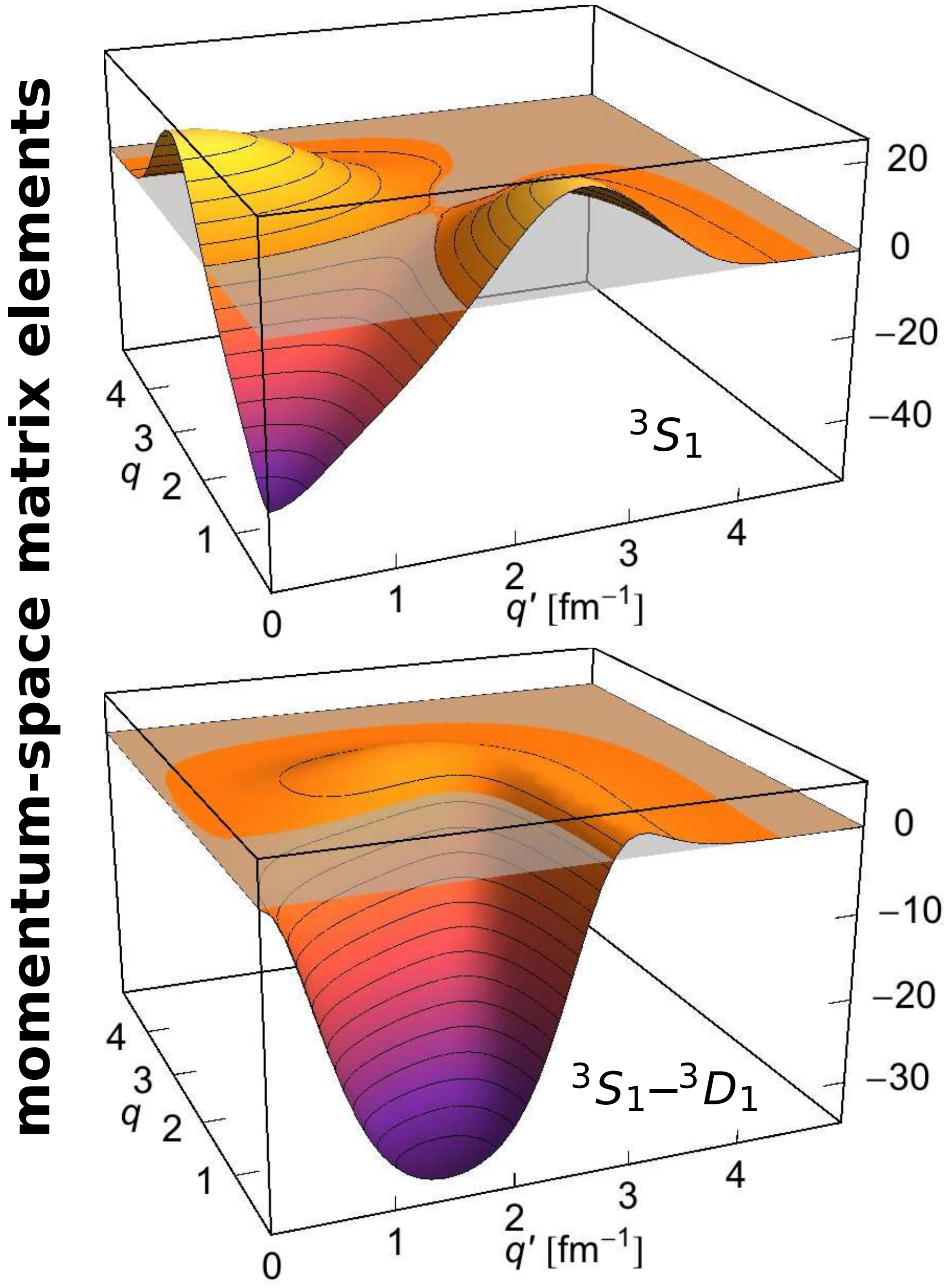
simplicity and flexibility are great advantages of the SRG approach

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

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

$$\eta_\alpha = (2\mu)^2 [T_{int}, \widetilde{H}_\alpha]$$

SRG Evolution in Two-Body Space

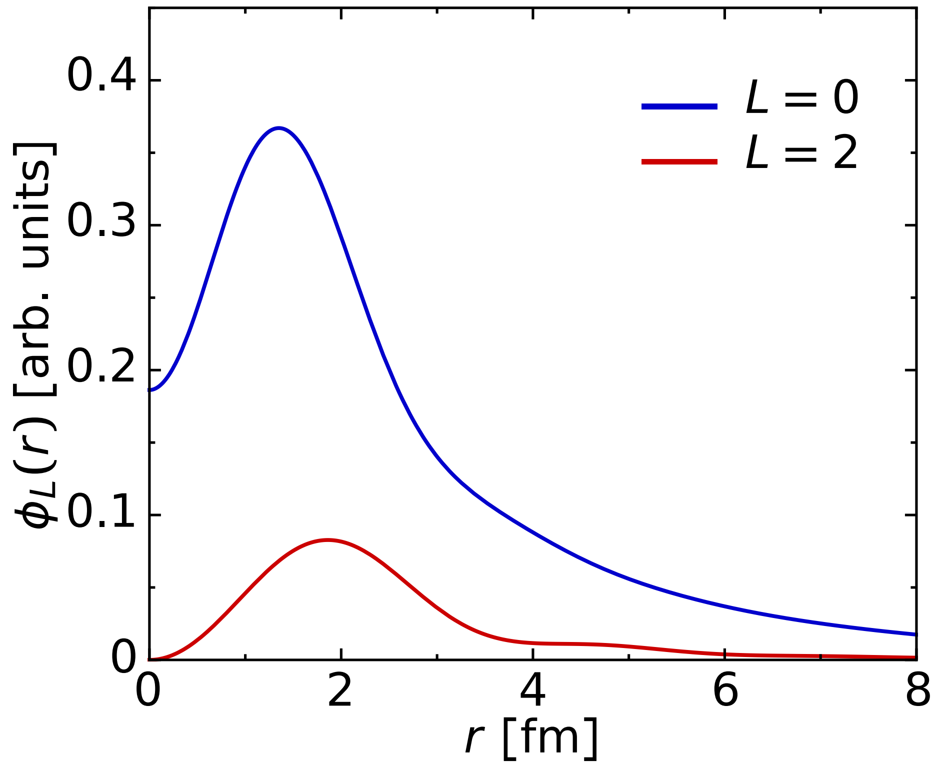


$$\alpha = 0.000\,\mathrm{fm}^4$$

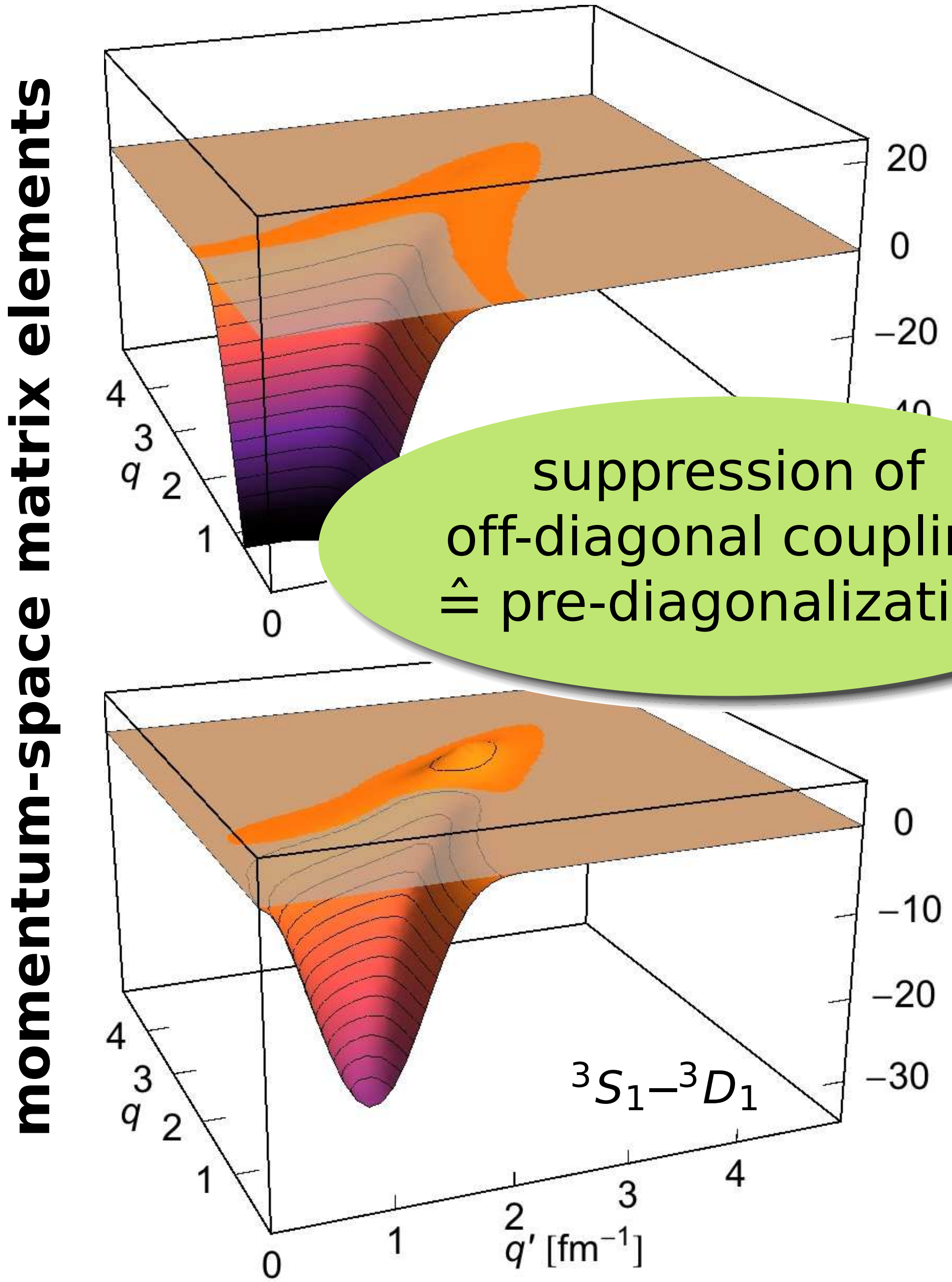
$\Lambda = \infty\,\mathrm{fm}^{-1}$

$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG Evolution in Two-Body Space



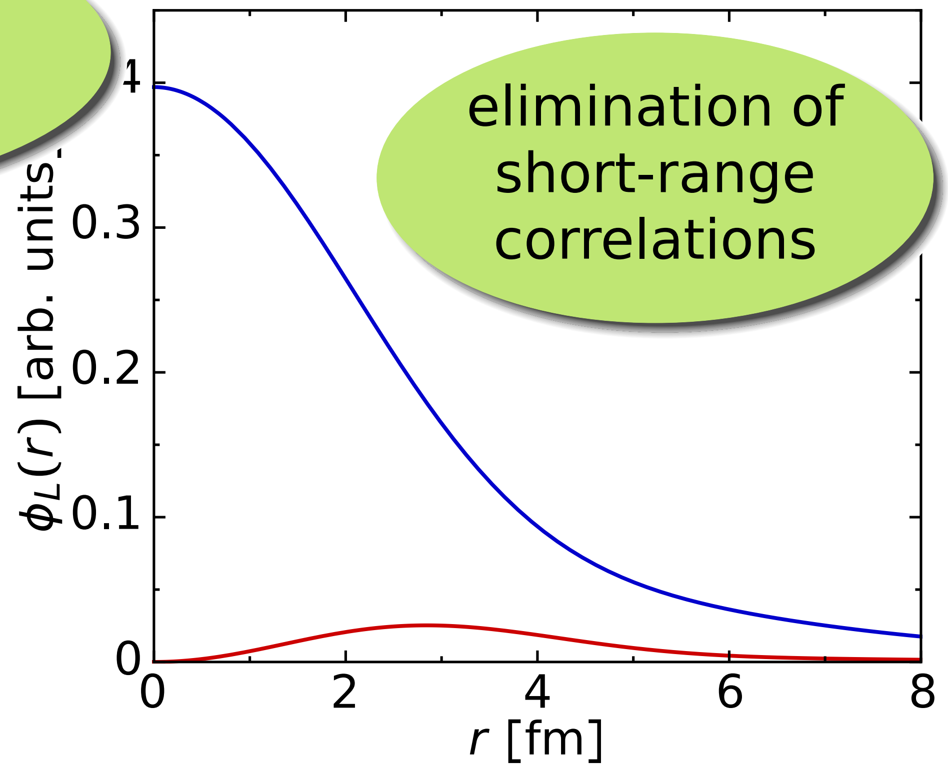
suppression of
off-diagonal coupling
≙ pre-diagonalization

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

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

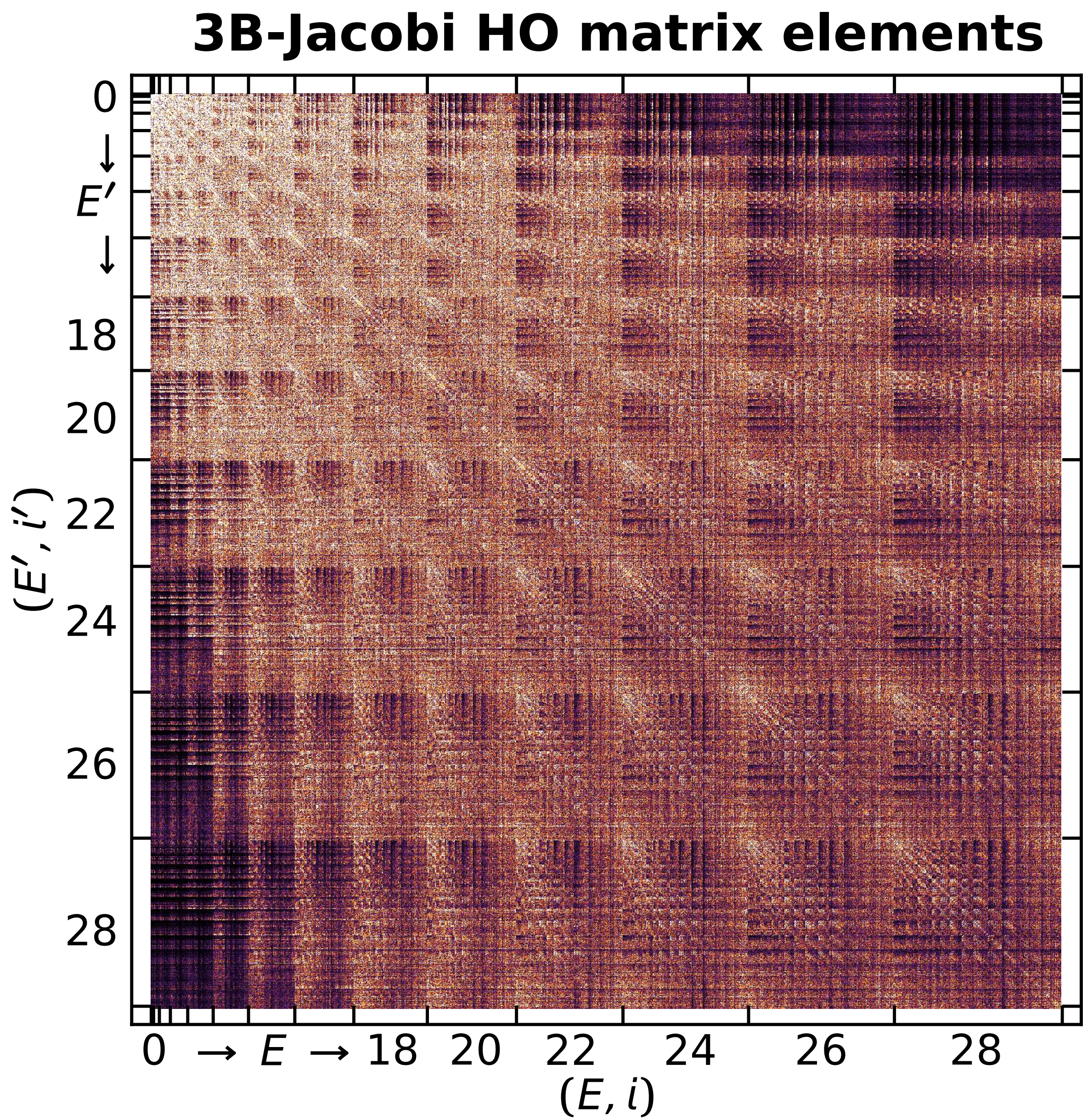
$J^\pi = 1^+, T = 0$

deuteron wave-function



elimination of
short-range
correlations

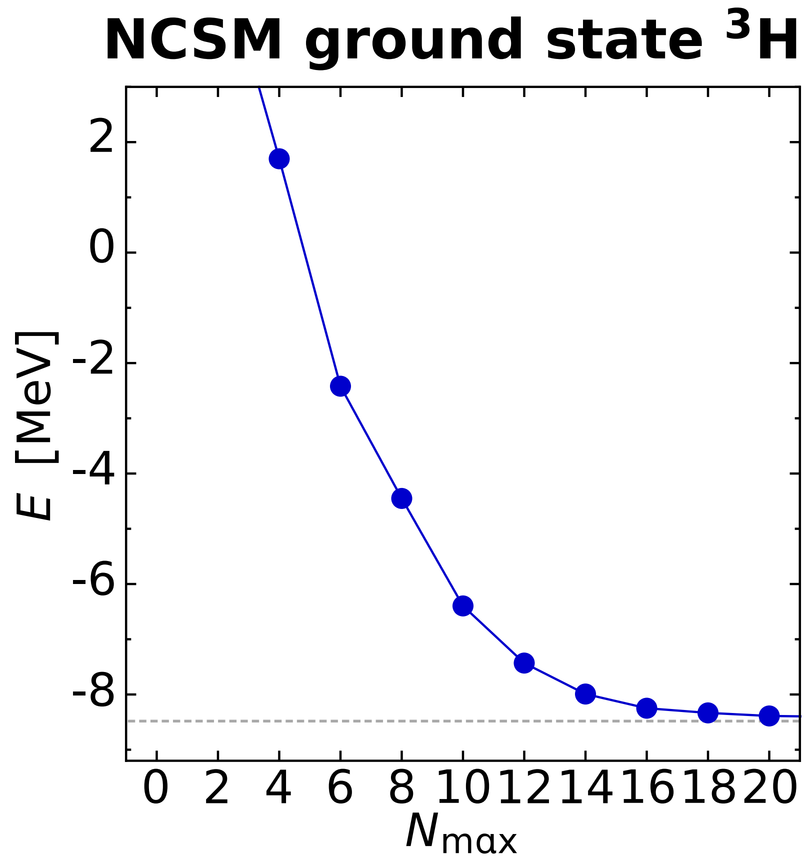
SRG Evolution in Three-Body Space



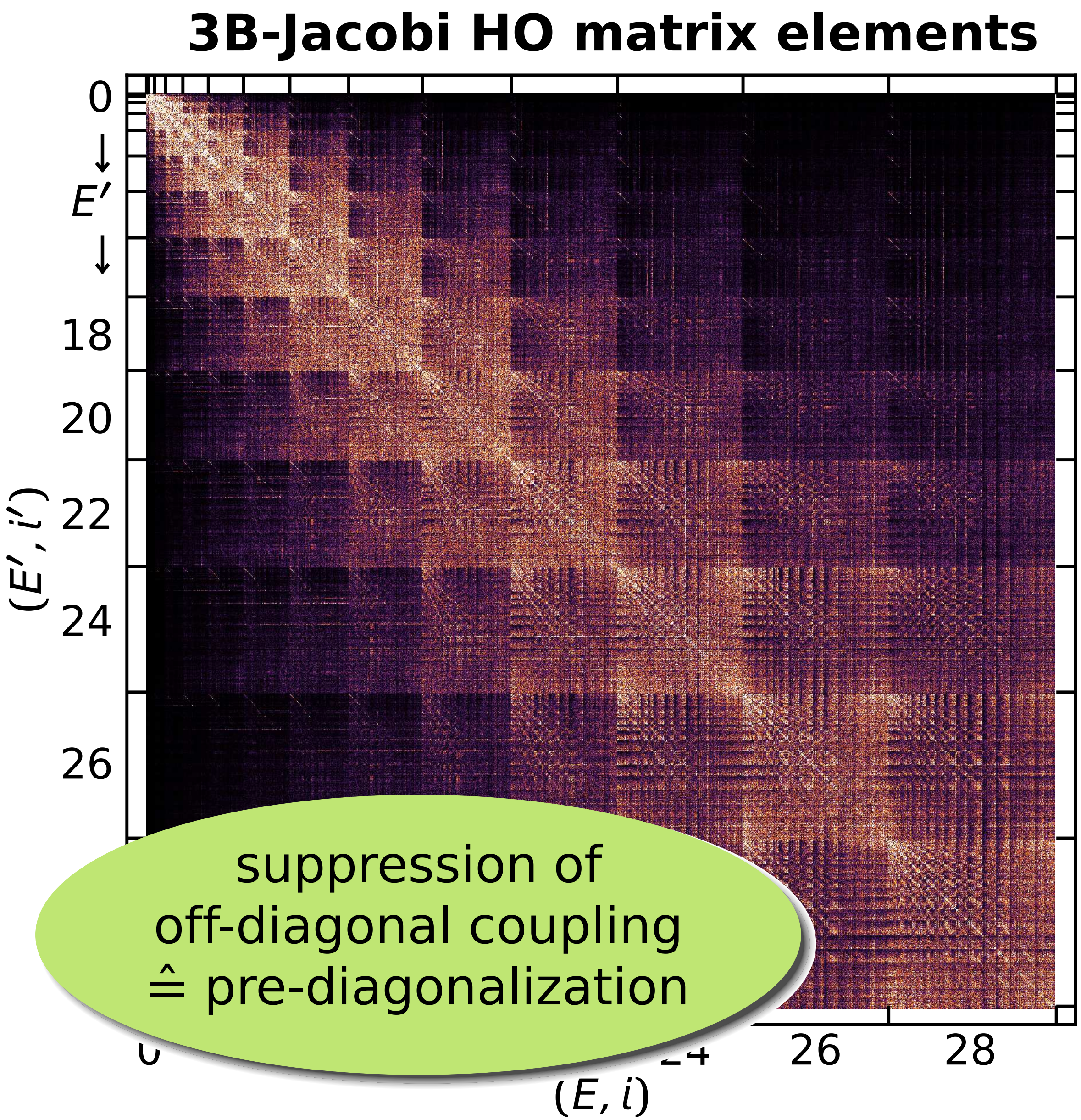
$\alpha = 0.000\,\mathrm{fm}^4$

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

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



SRG Evolution in Three-Body Space



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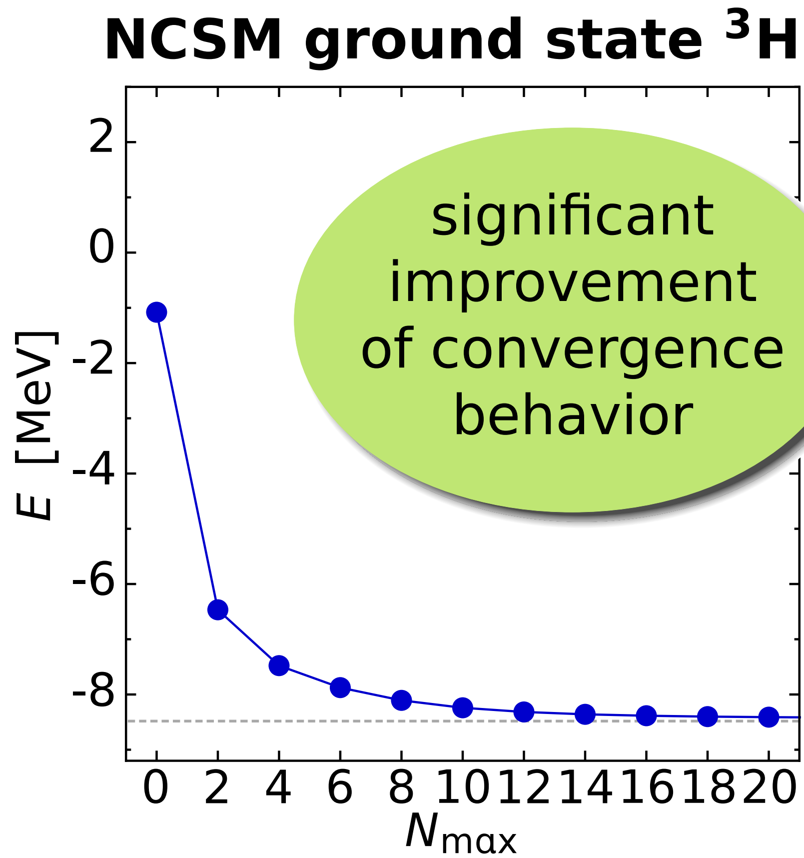


significant
improvement
of convergence
behavior

Calculations in *A*-Body Space

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

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

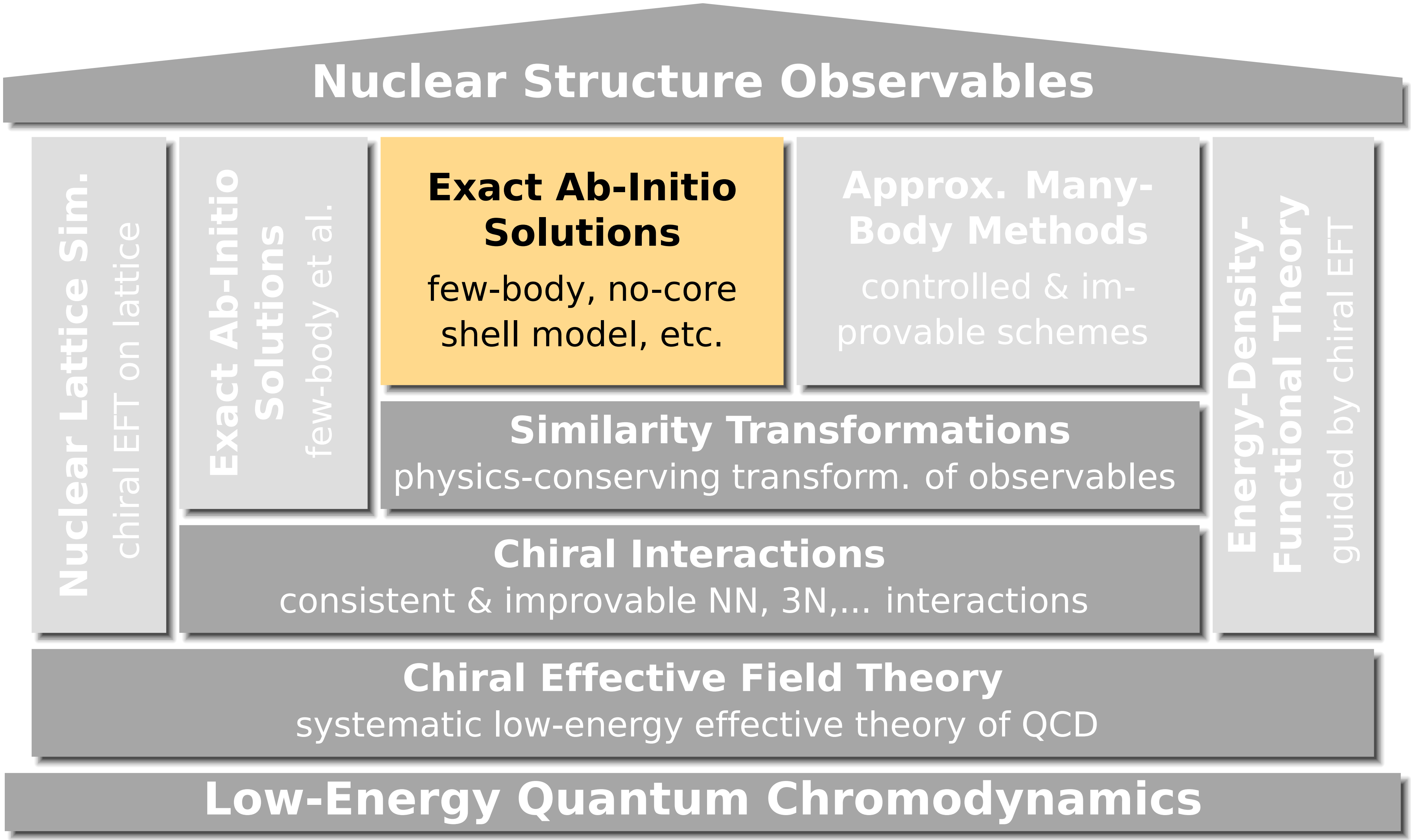
- truncation of cluster series inevitable — formally destroys unitarity and invariance of energy eigenvalues (independence of α)

Three SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Ham… keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3… and all three-body terms

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

Ab Initio Nuclear Structure



Importance Truncated NCSM

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

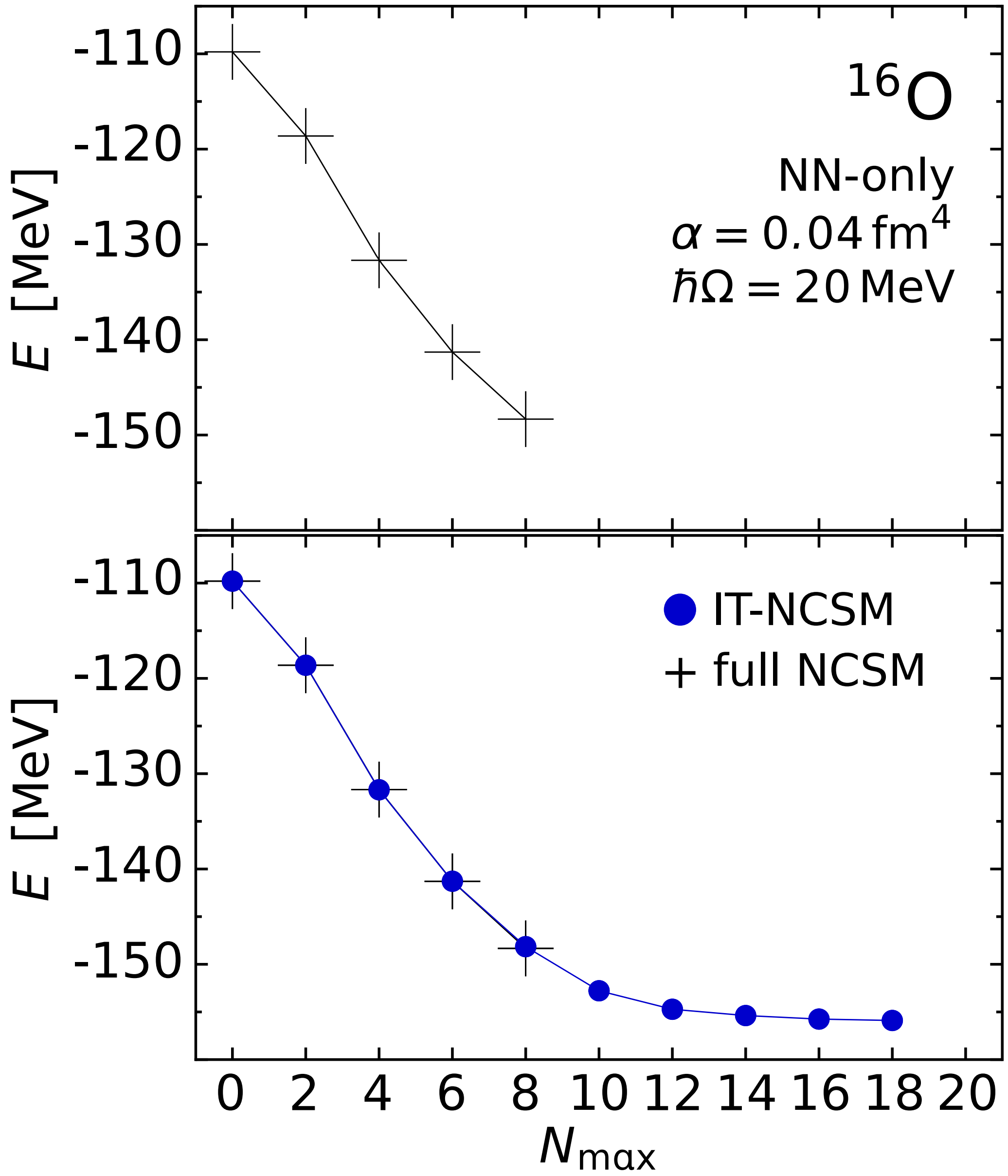
- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range 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
- we have developed a **parallelized IT-NCSM/NCSM code** capable of handling 3N matrix elements up to $E_{3\max} = 16$

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for ^{16}O getting 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



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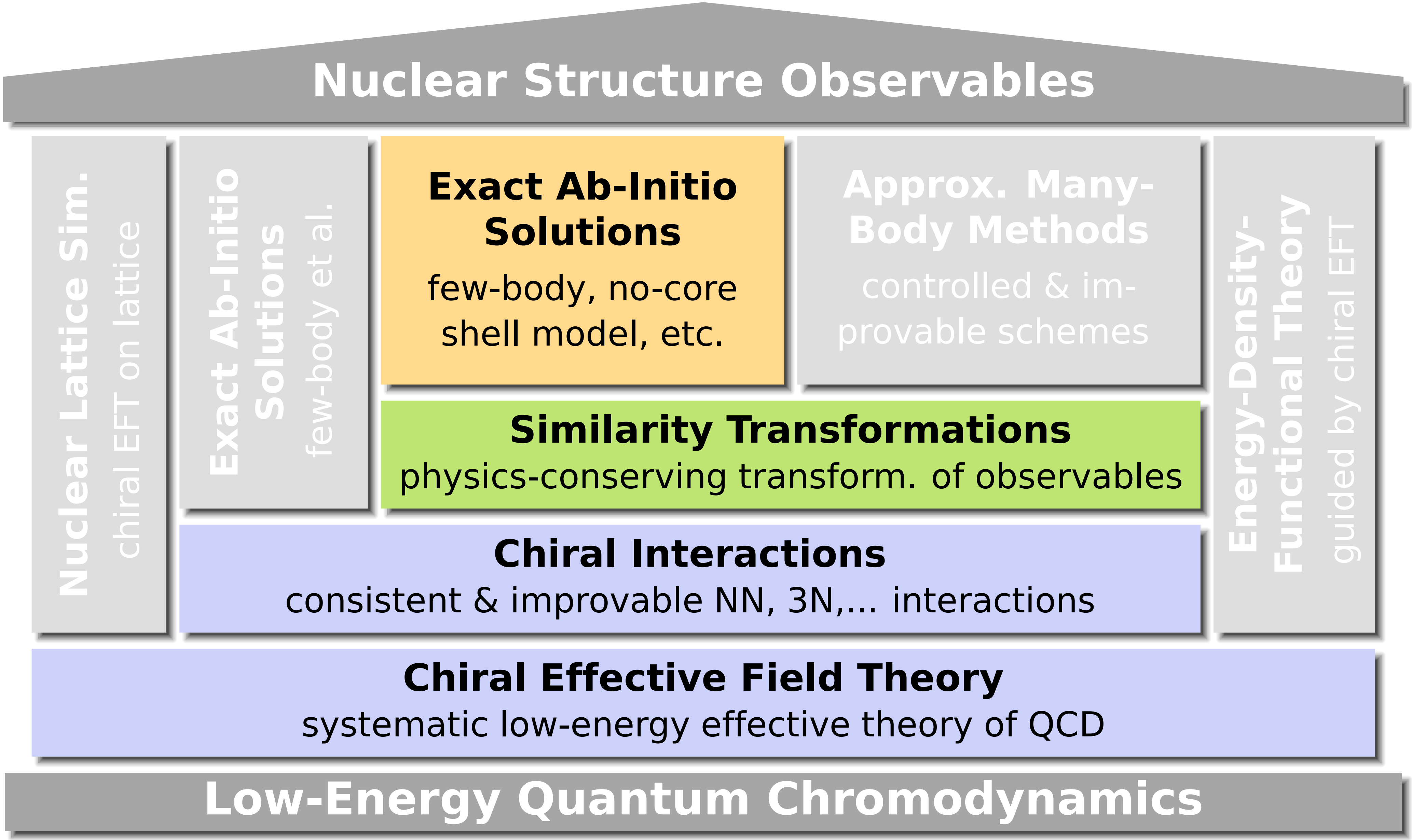
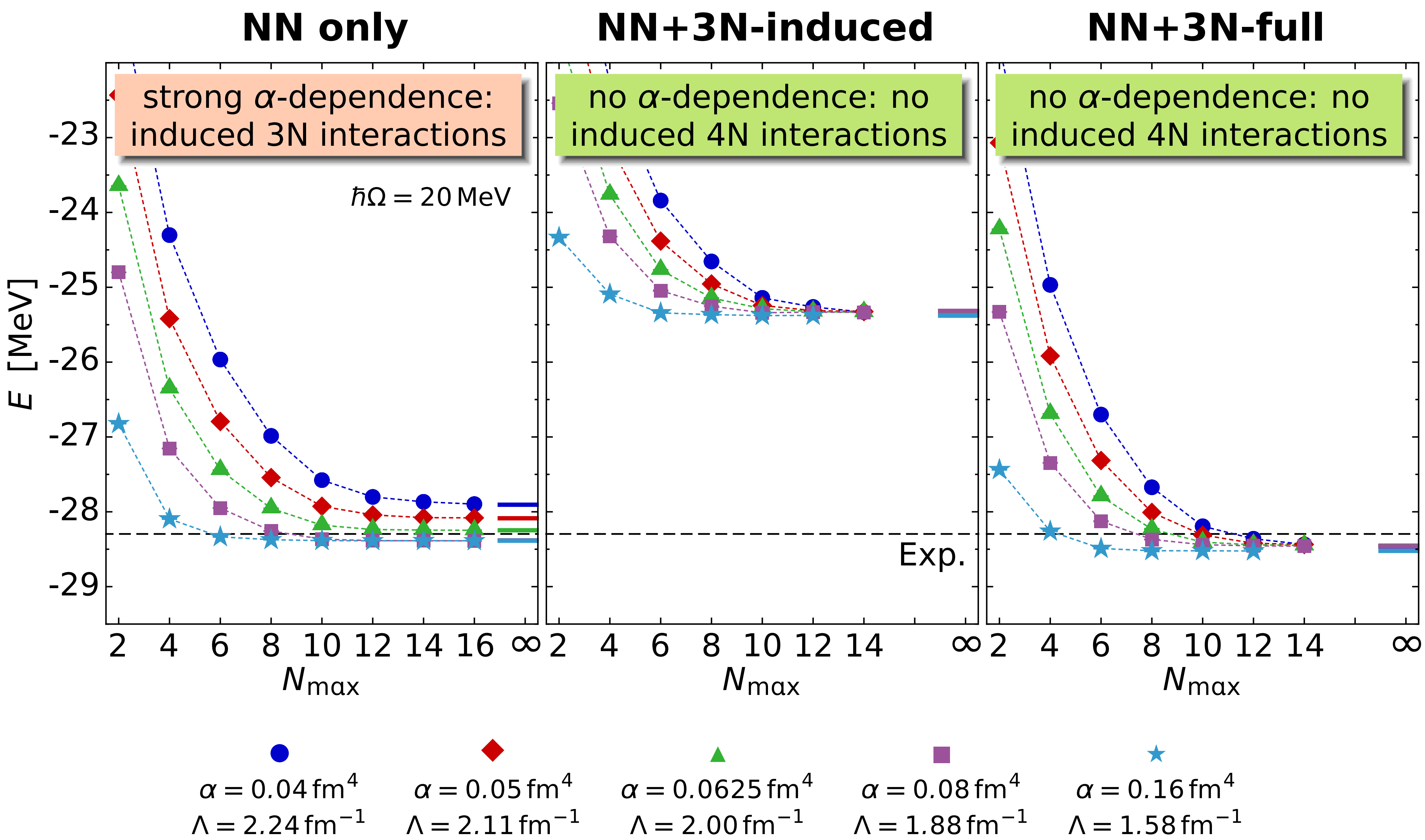
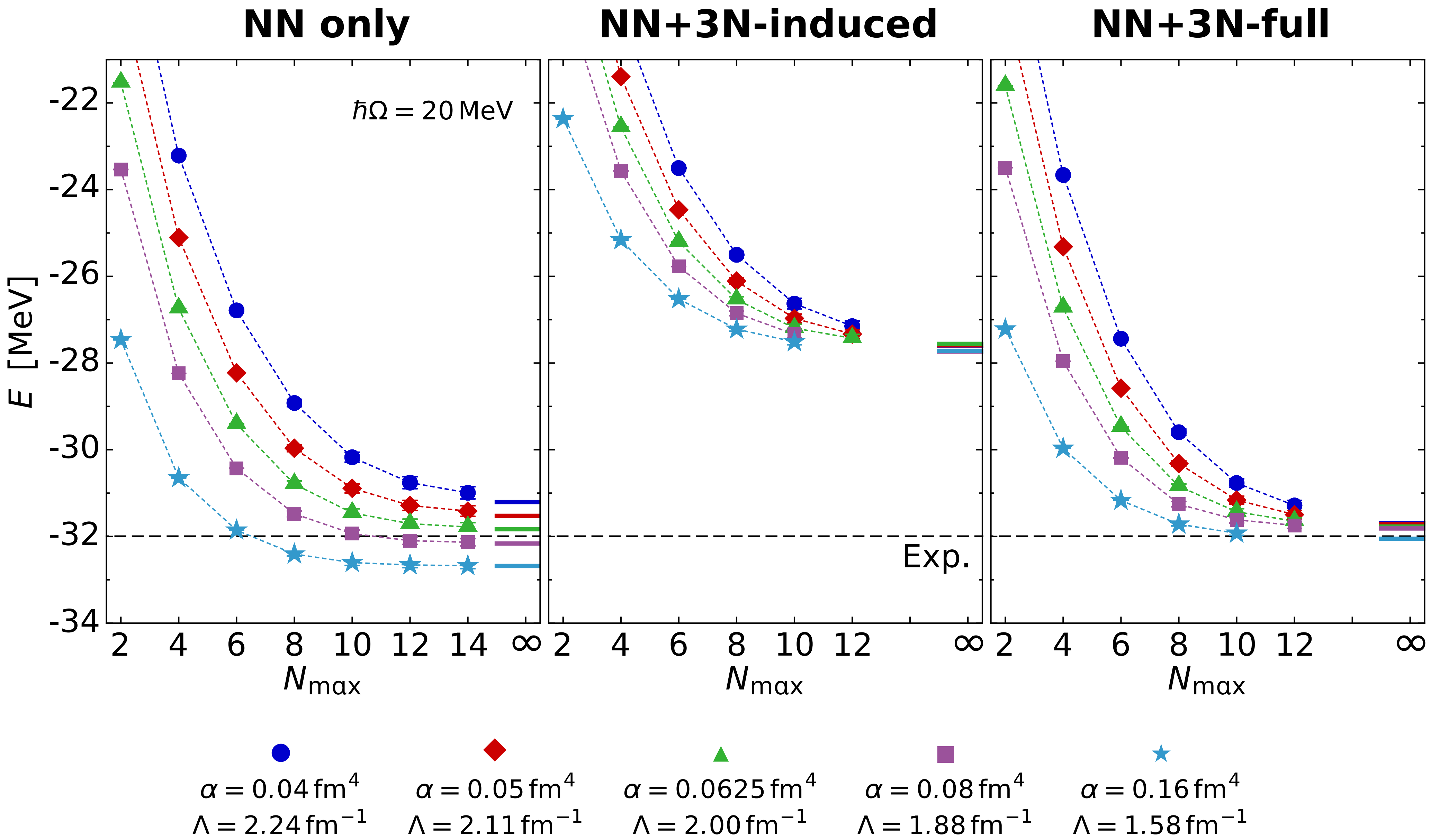


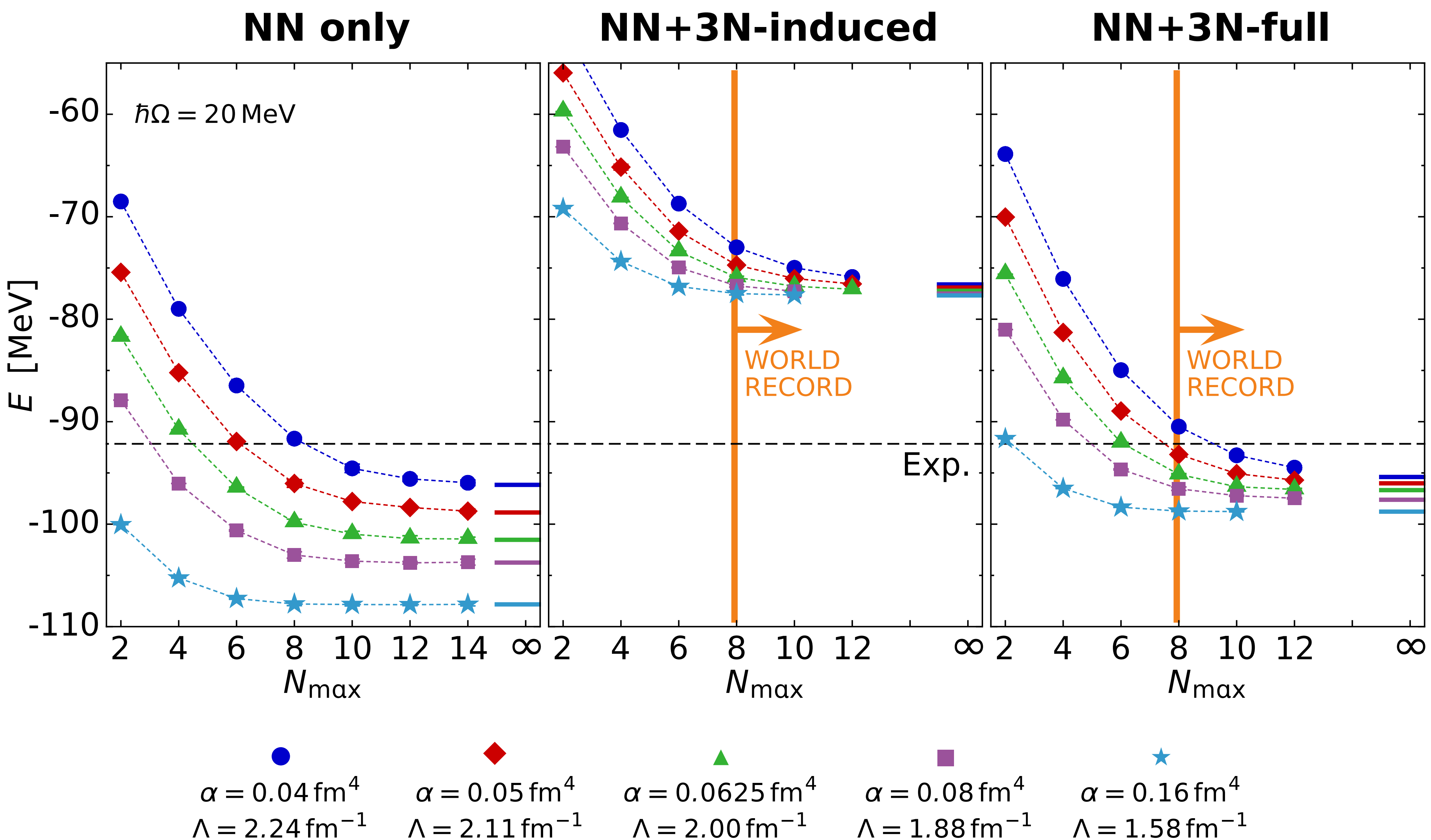
^{4}He: Ground-State Energies



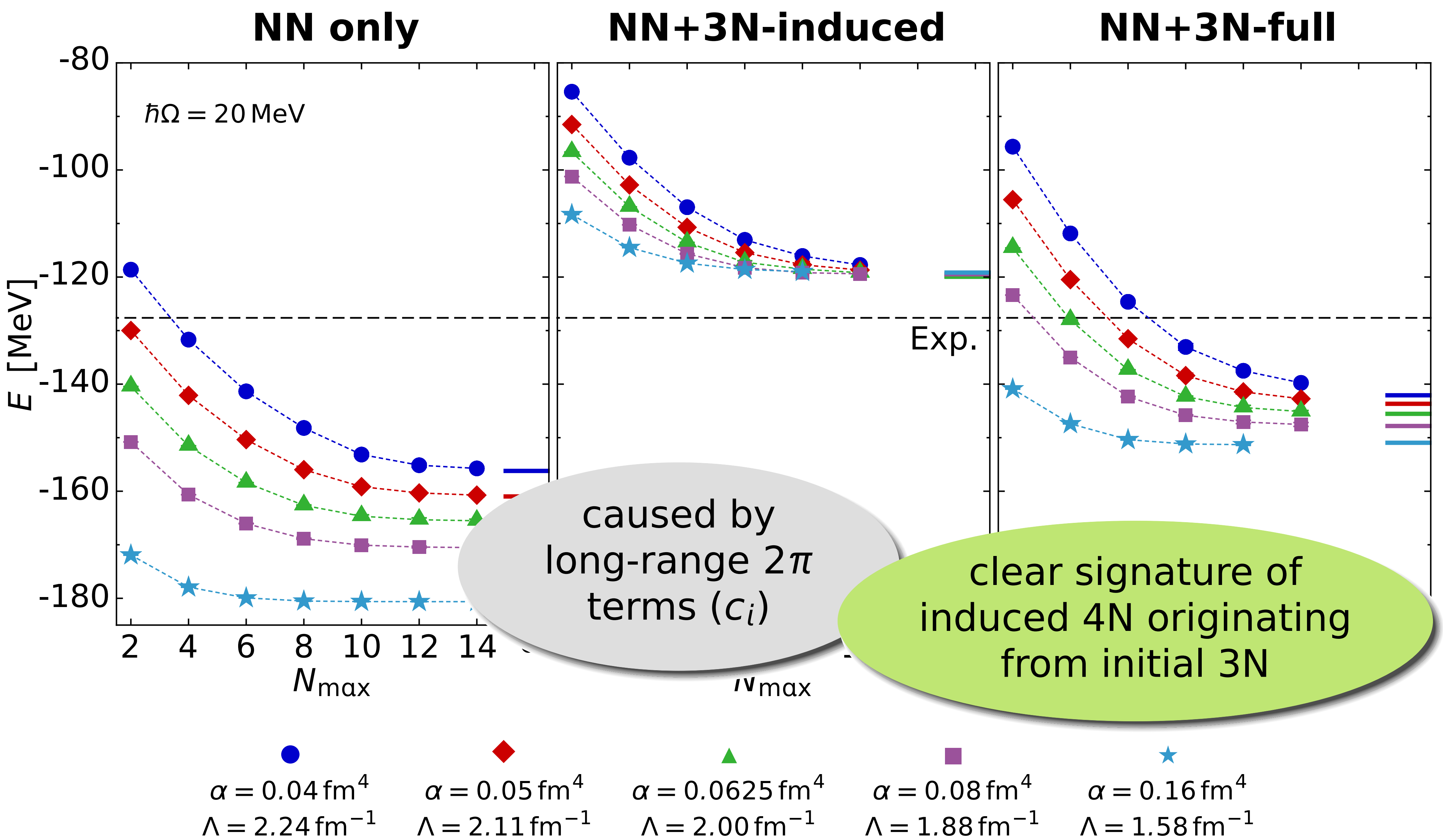
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies



^{16}O: Ground-State Energies



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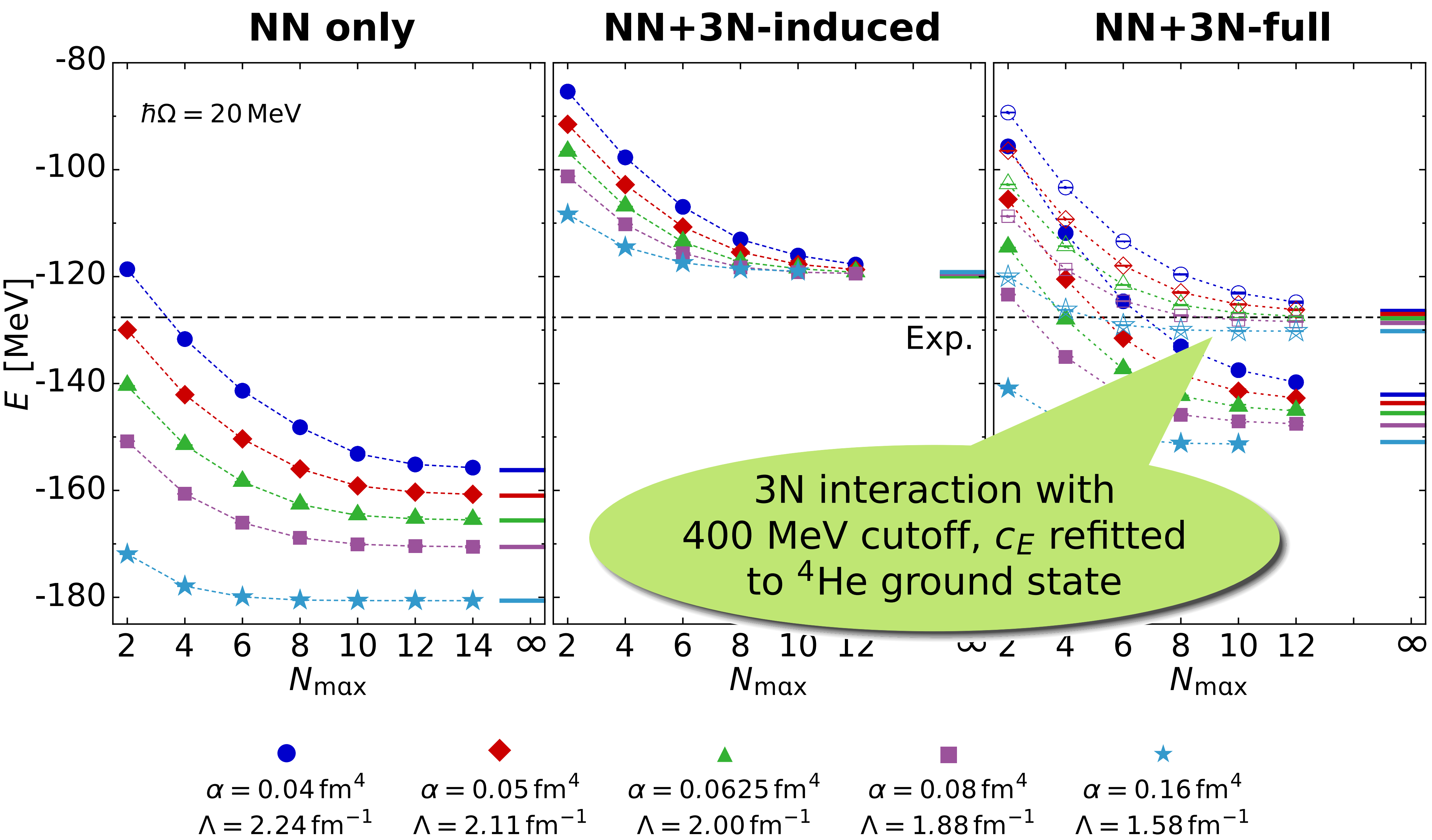
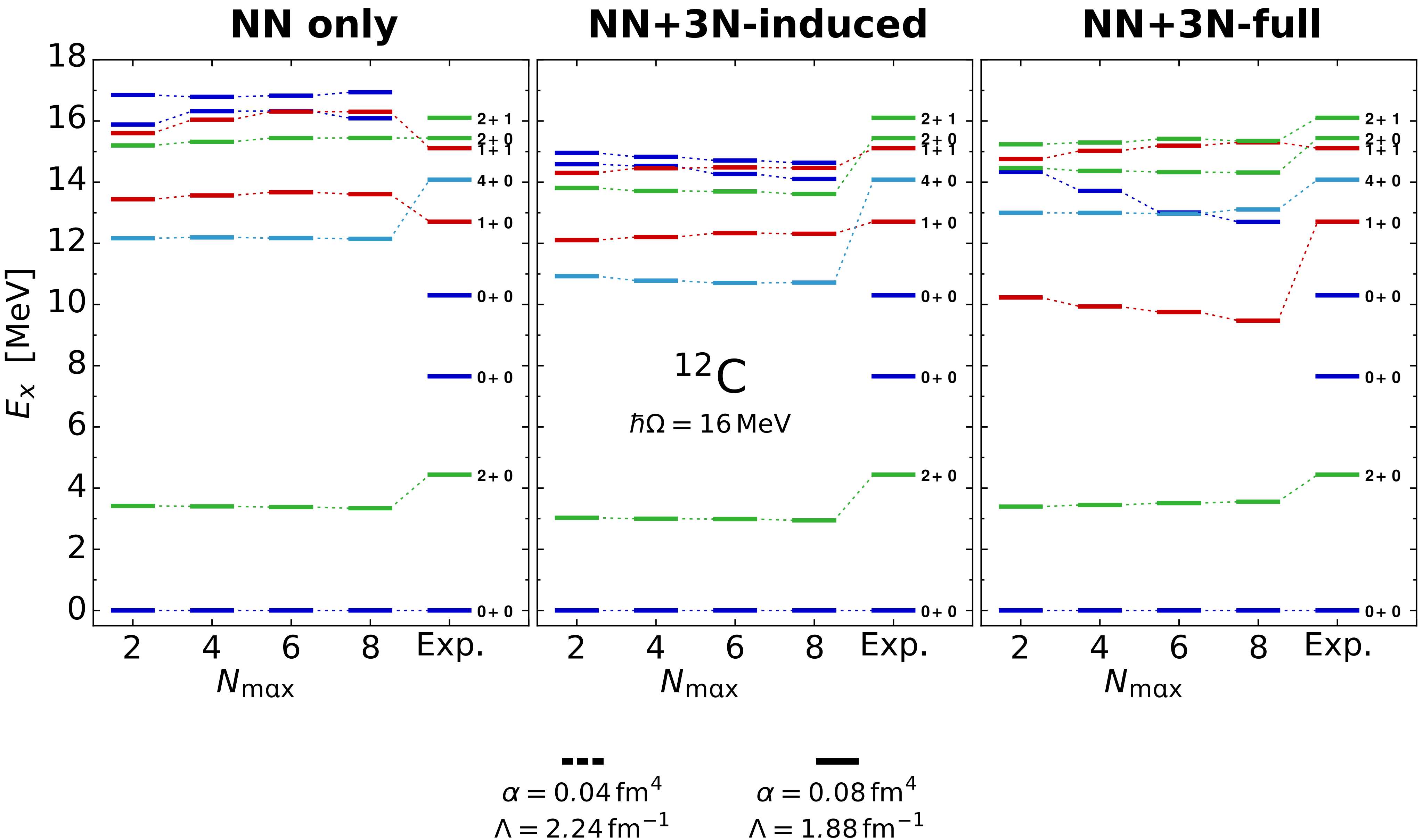


Spectroscopy of ^{12}C



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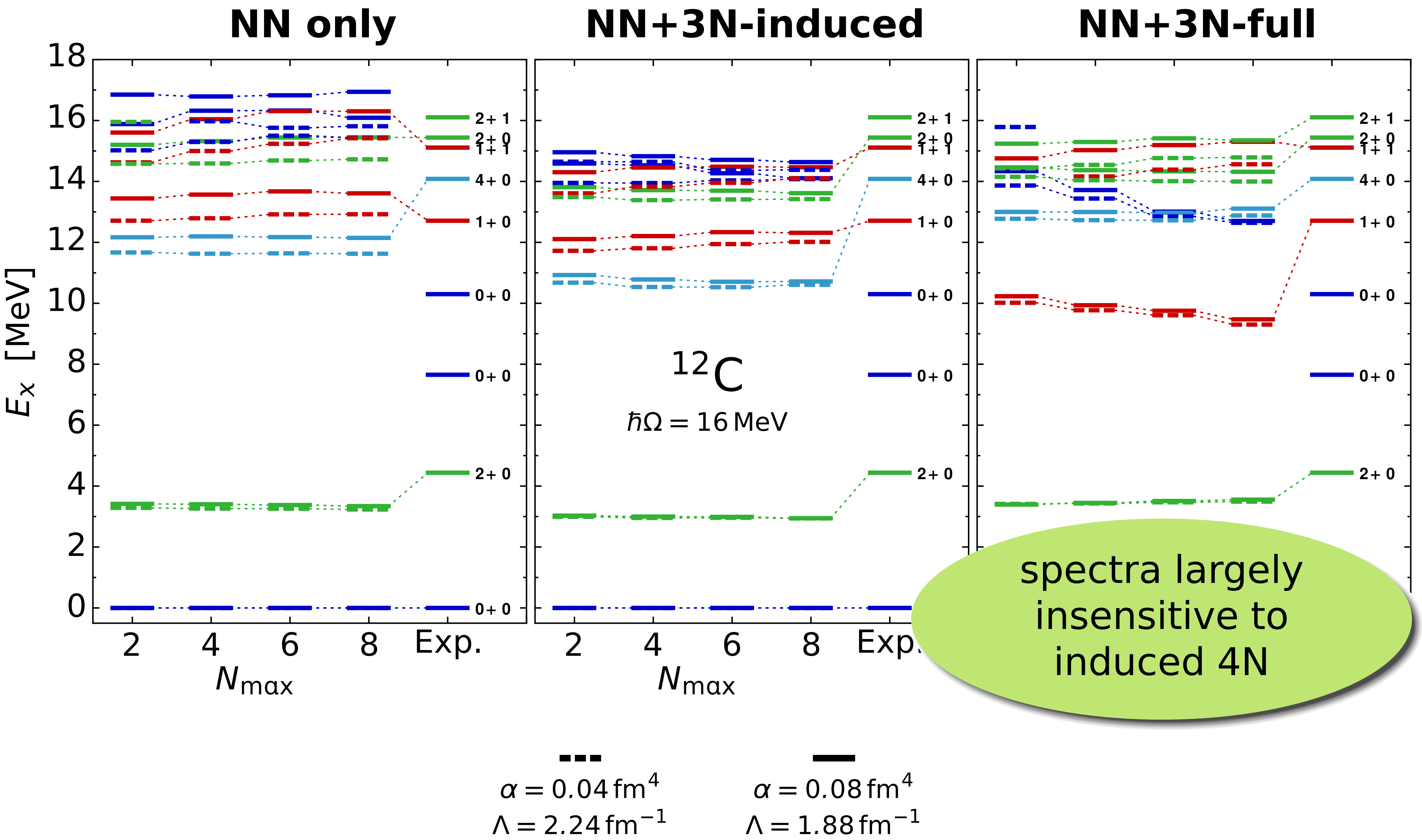


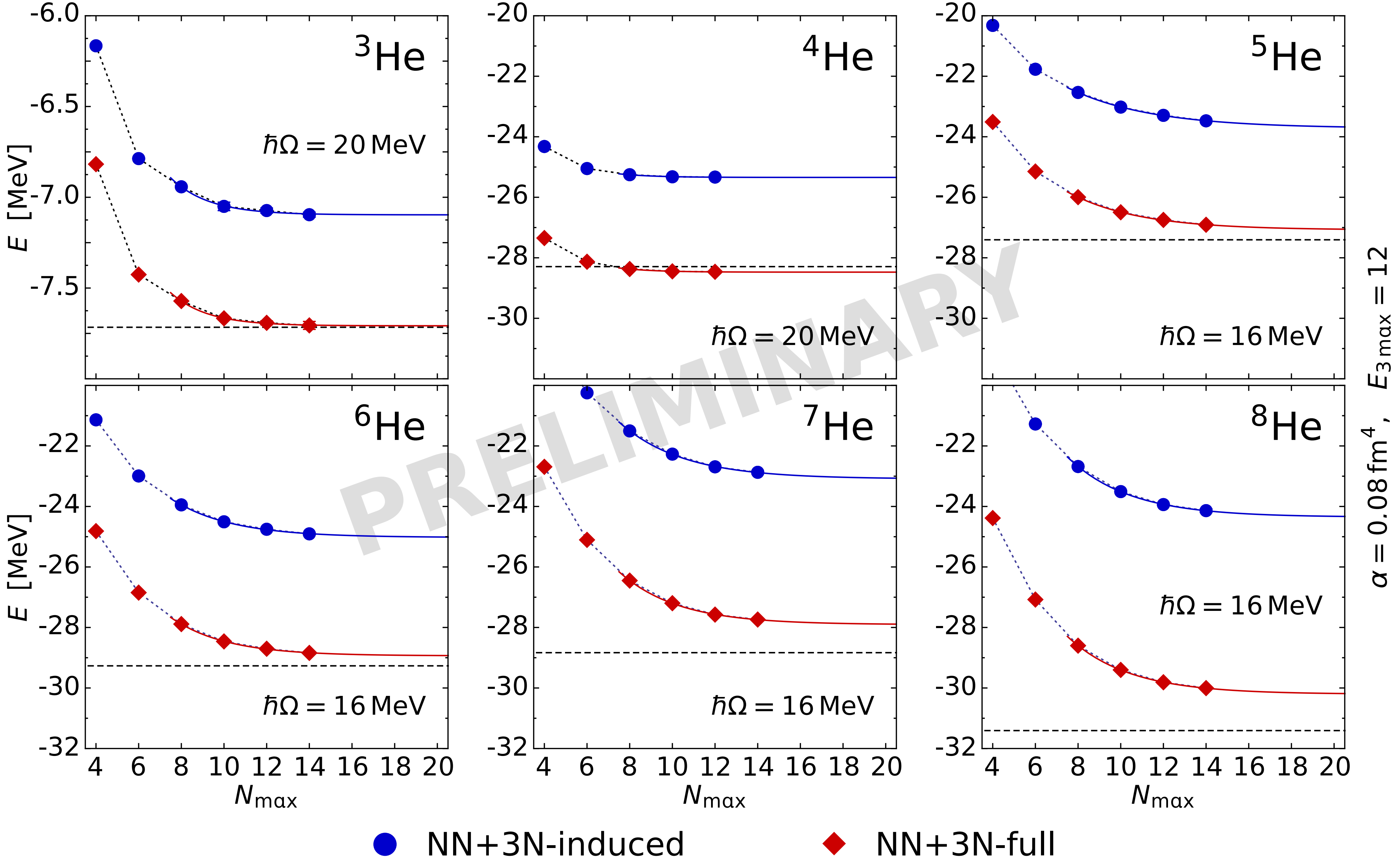
spectra largely insensitive to induced 4N

The Bottom Line...

- beyond the lightest nuclei, **SRG-induced 4N contributions** affect the absolute energies (but not the excitation energies)
- with the inclusion of the leading 3N interaction we already obtain a **good description** of spectra (and ground states)
- **breakthrough** in computation, transformation and management of 3N matrix-elements

- **next-generation SRG**: can we find new SRG-generators that do not induce as much 4N but still give good convergence?
- **next-generation chiral 3N**: how will N3LO or Δ-full chiral 3N interactions affect the picture?
- **applications**: which experiment-related applications are in reach with the present framework?

Outlook: Ground-States of Helium Isotopes



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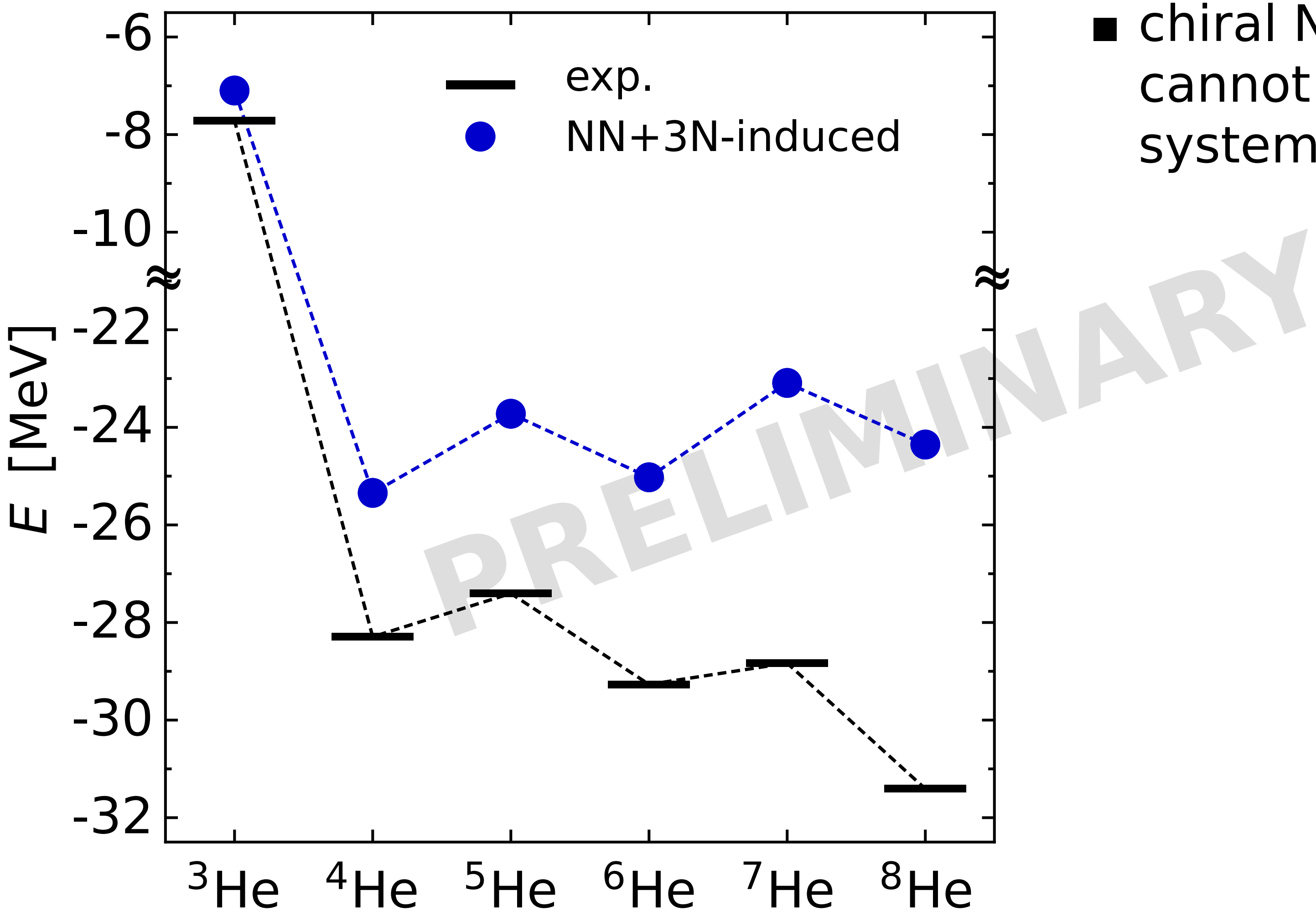

$\alpha = 0.08\,\text{fm}^4,\ E_{3\,\text{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics

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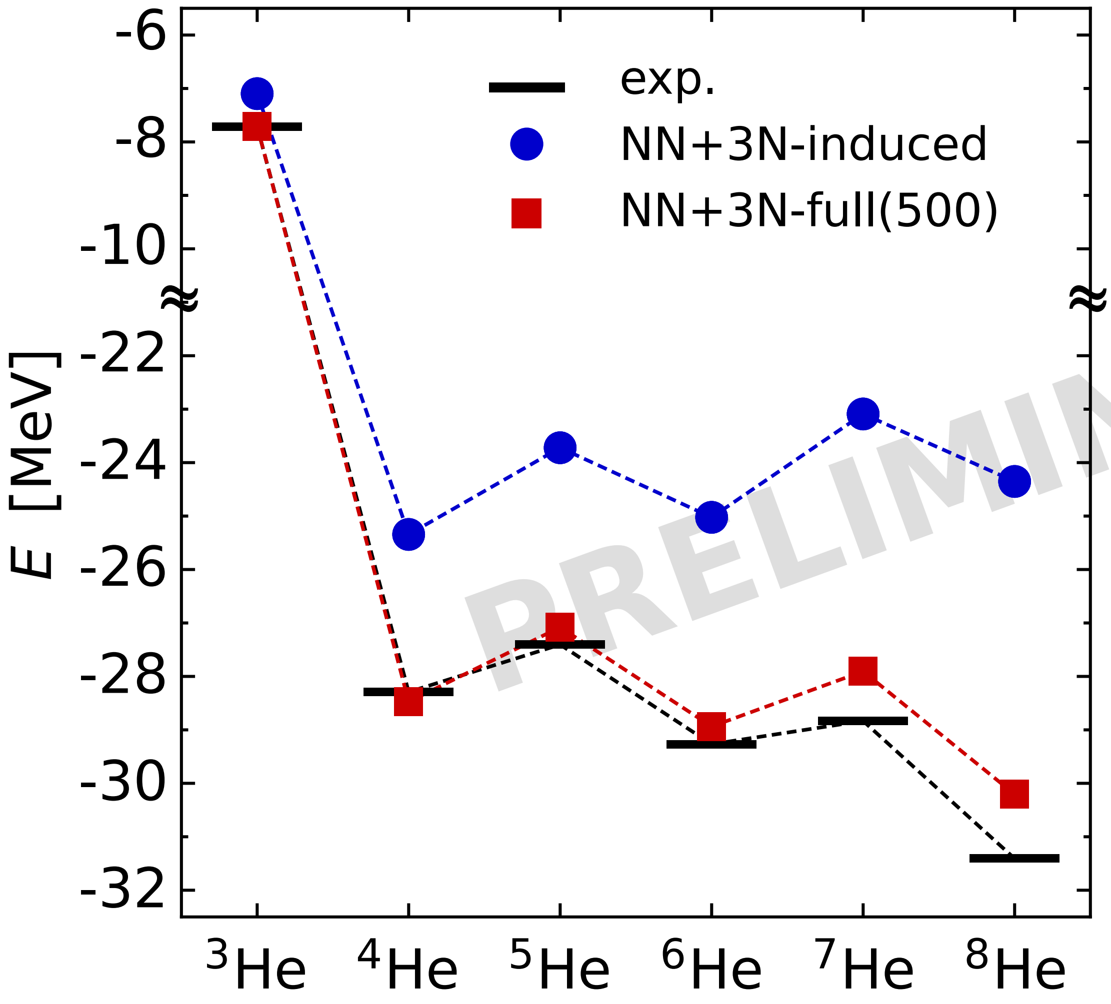

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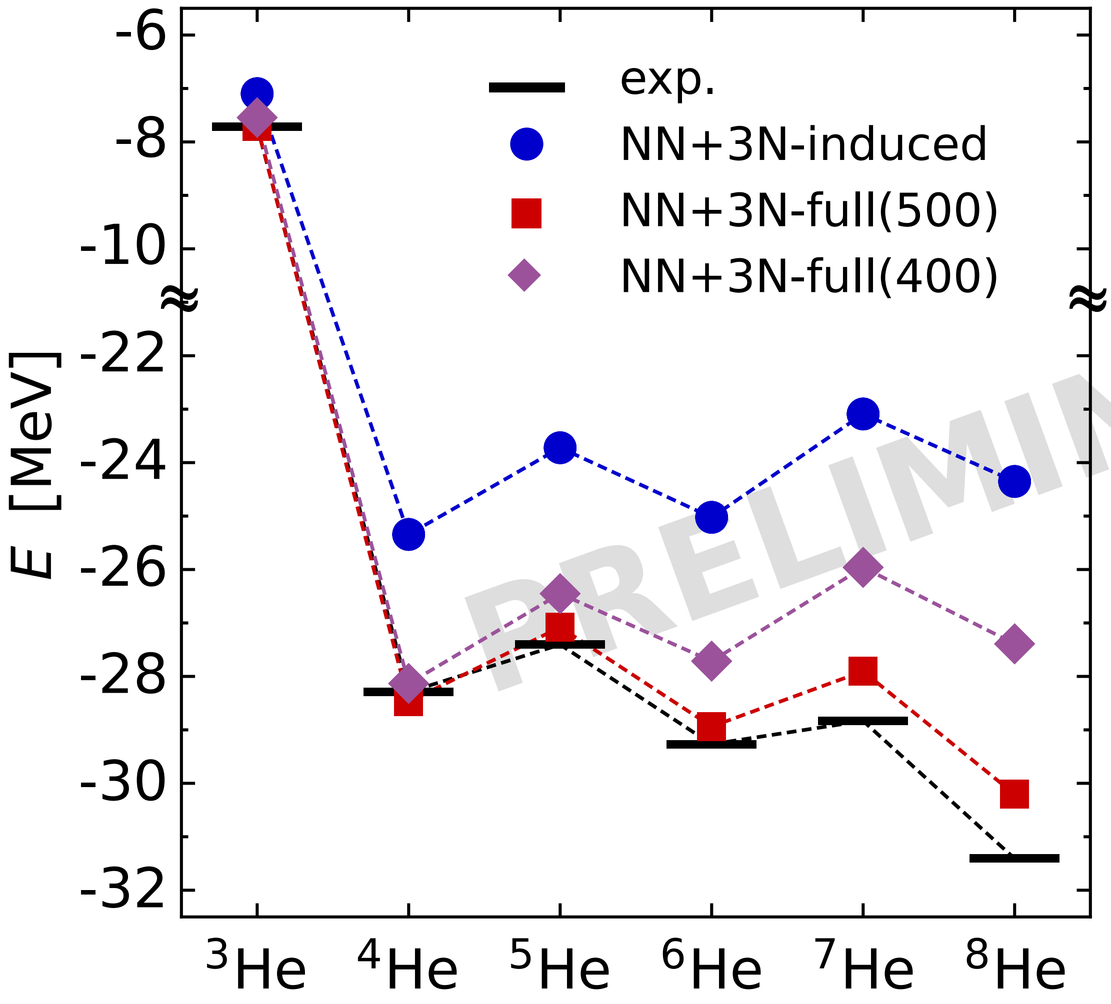
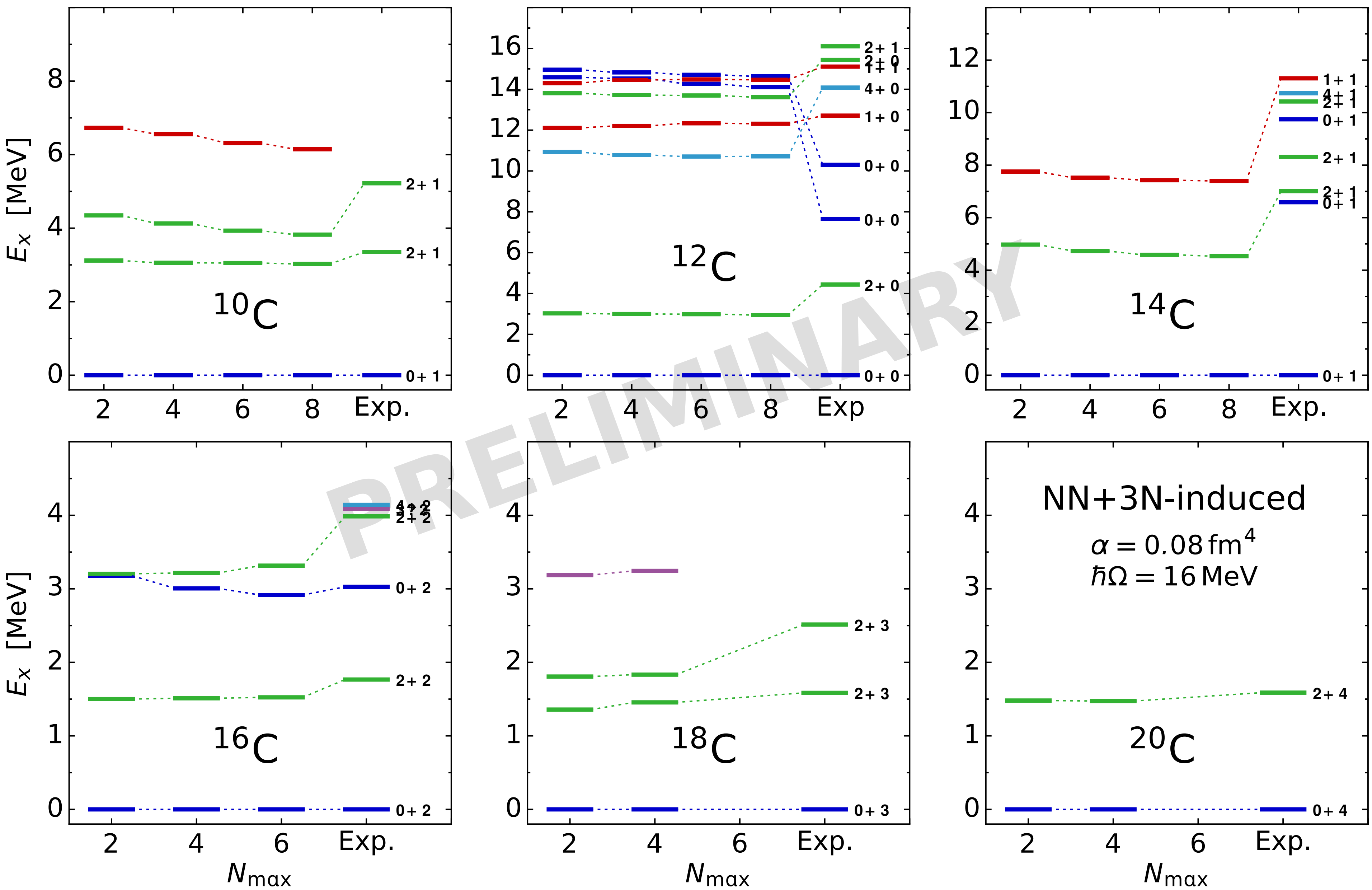


$\alpha = 0.08\,\mathrm{fm}^4,\ E_{3\,\mathrm{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics
- inclusion of chiral 3N gives a **very good systematic agreement**
- sensitive to details of the initial 3N interaction, e.g. the cutoff
- next: **consistent coupling to continuum** within NCSMC

Outlook: Carbon Isotopic Chain



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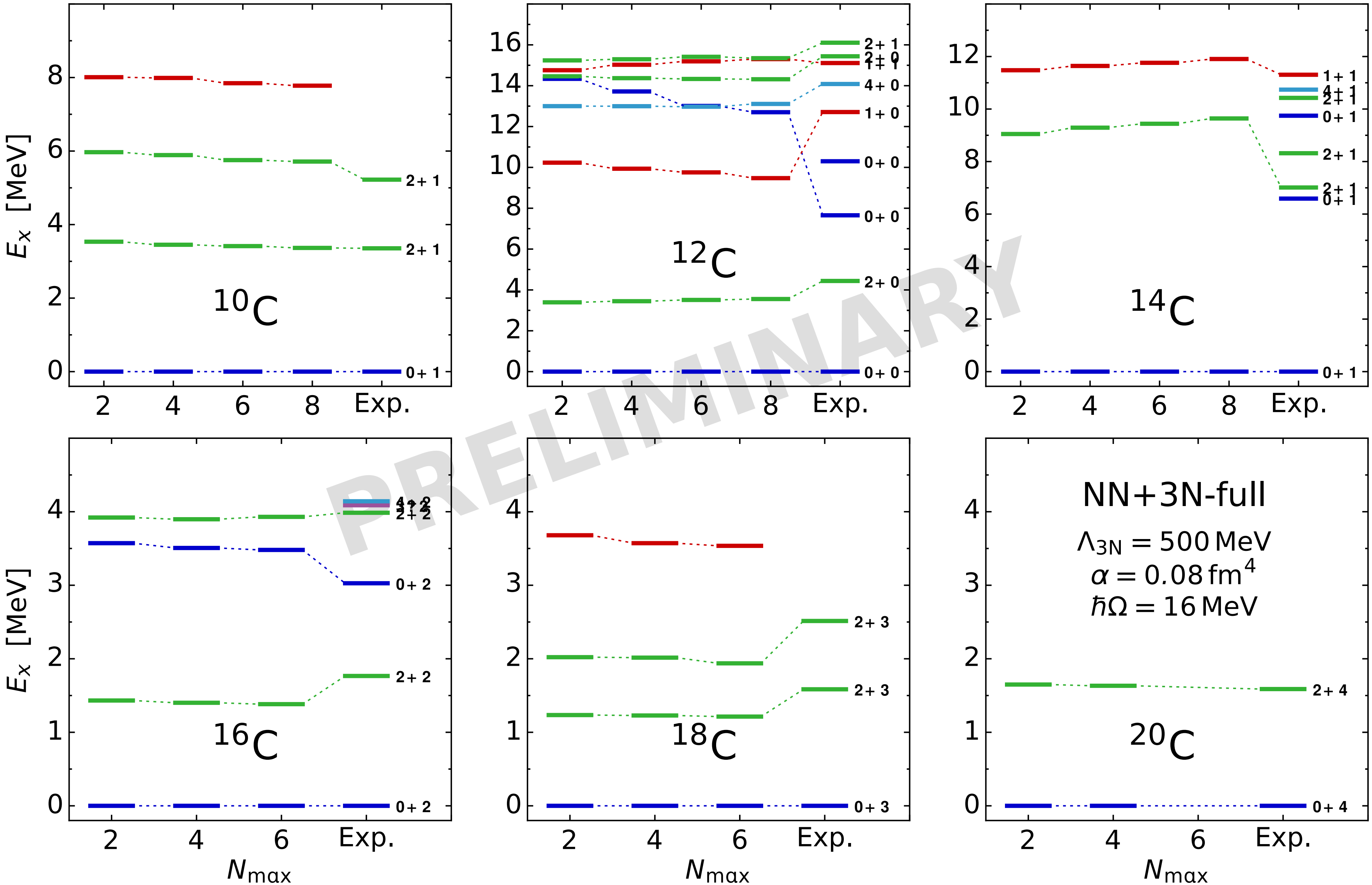

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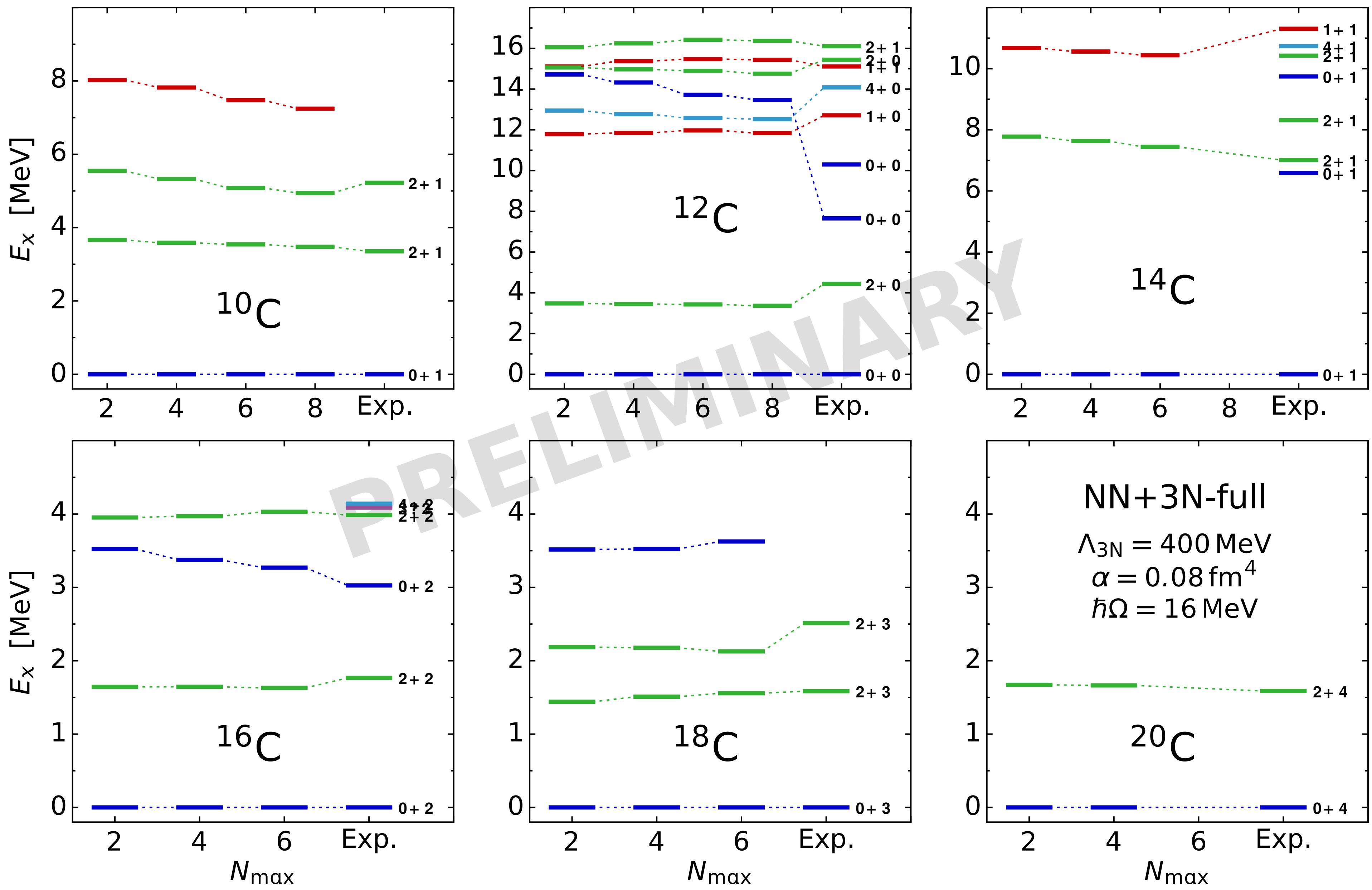

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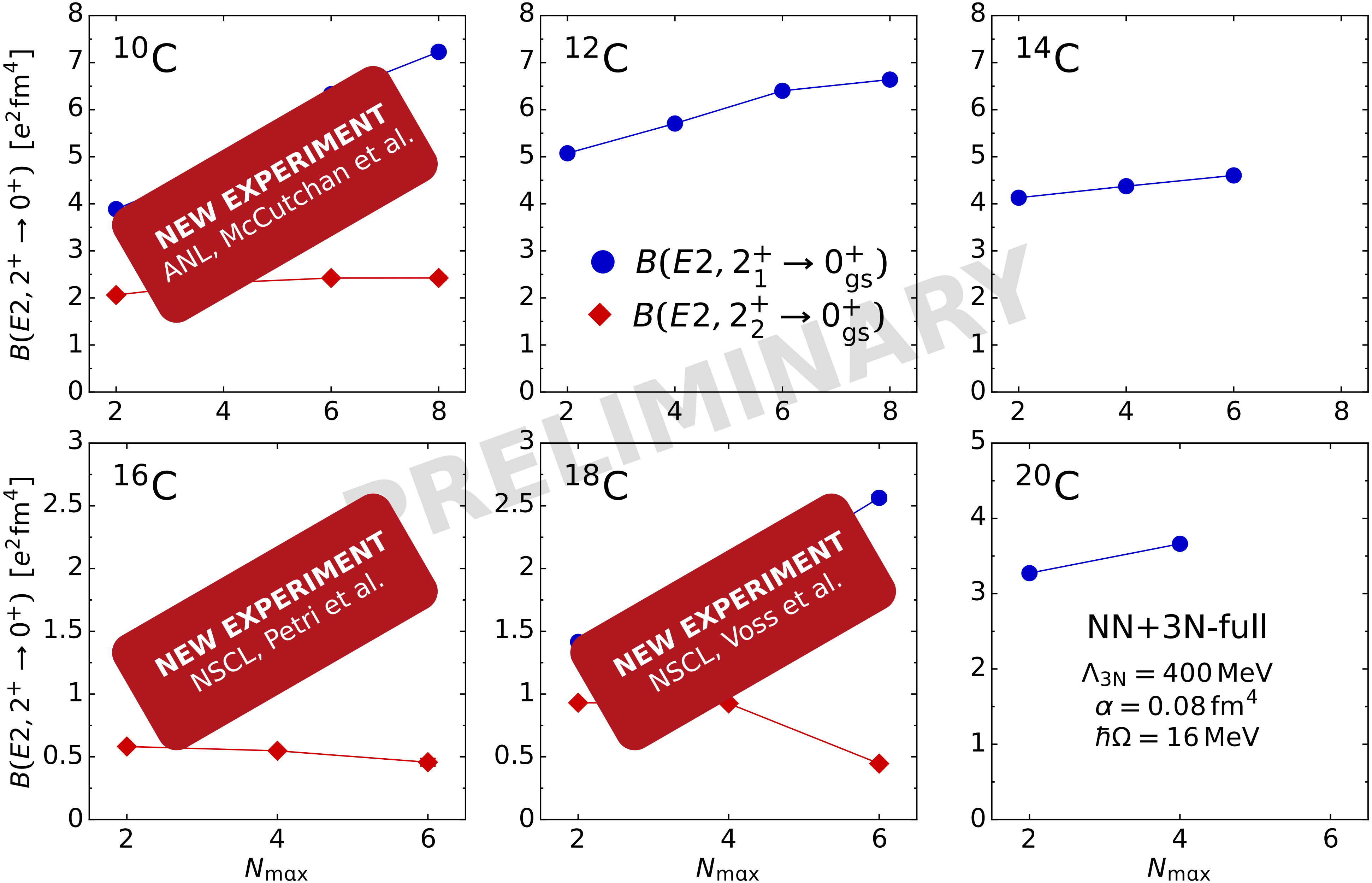

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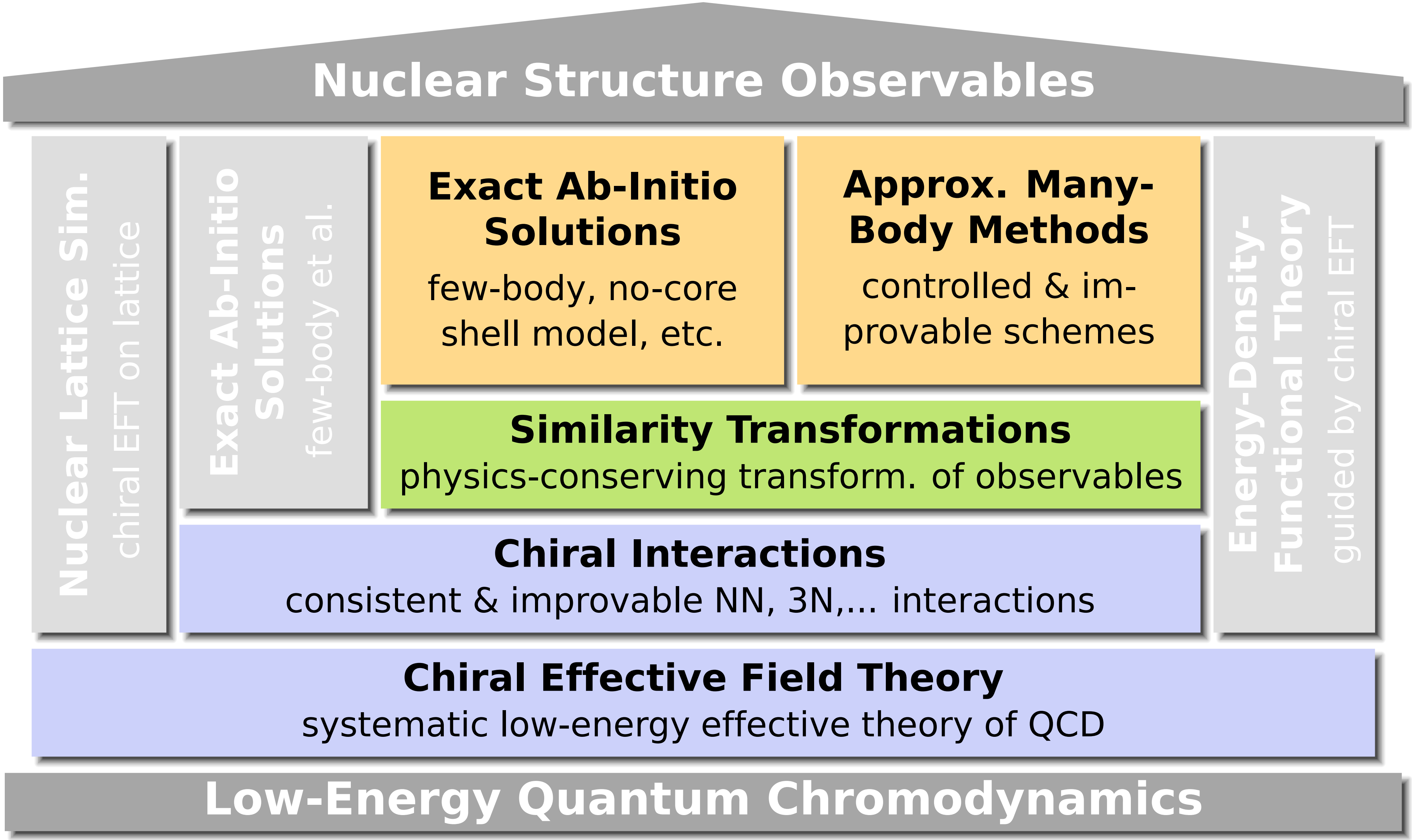
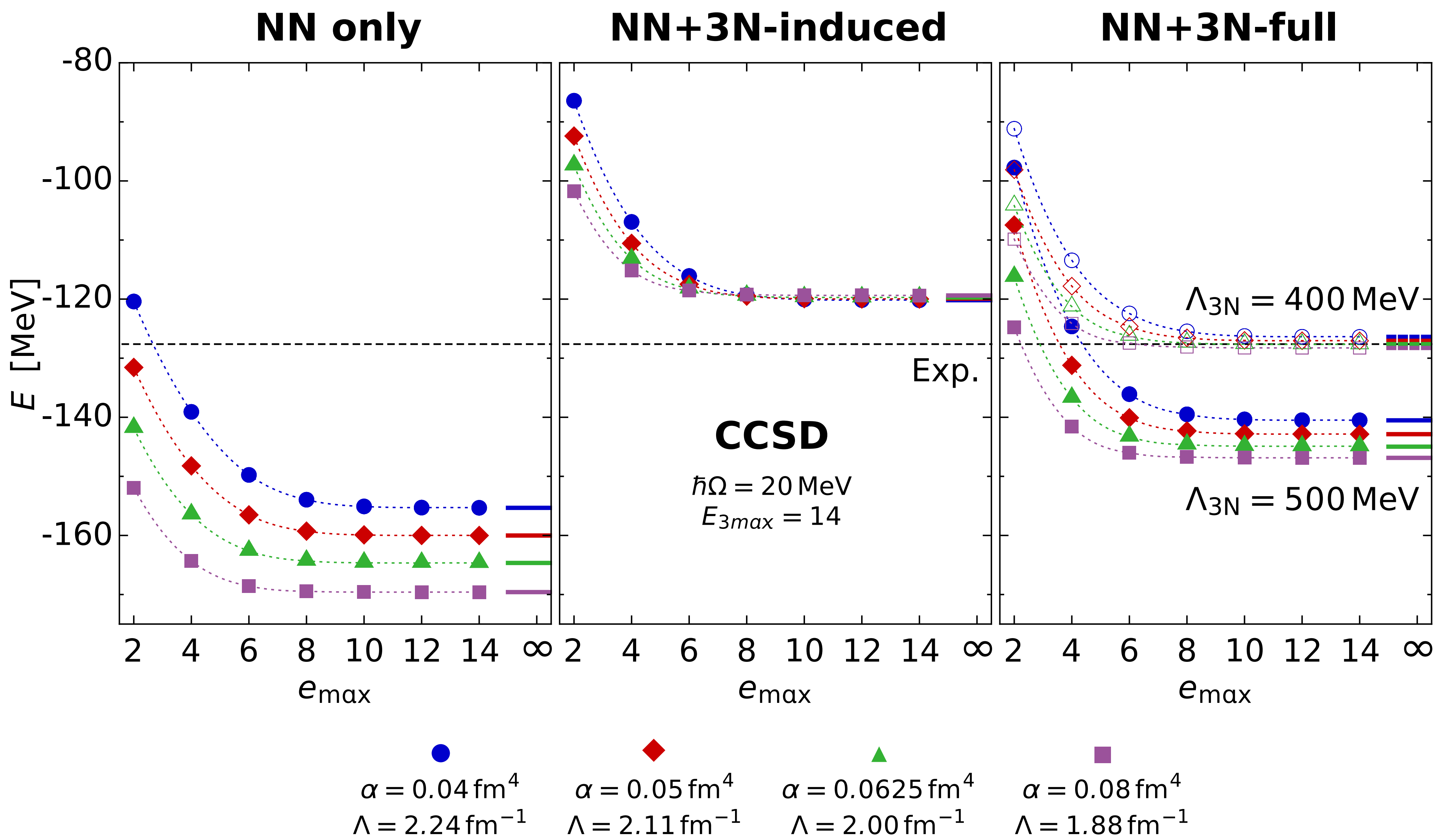


Heavy Nuclei with 3N Interactions

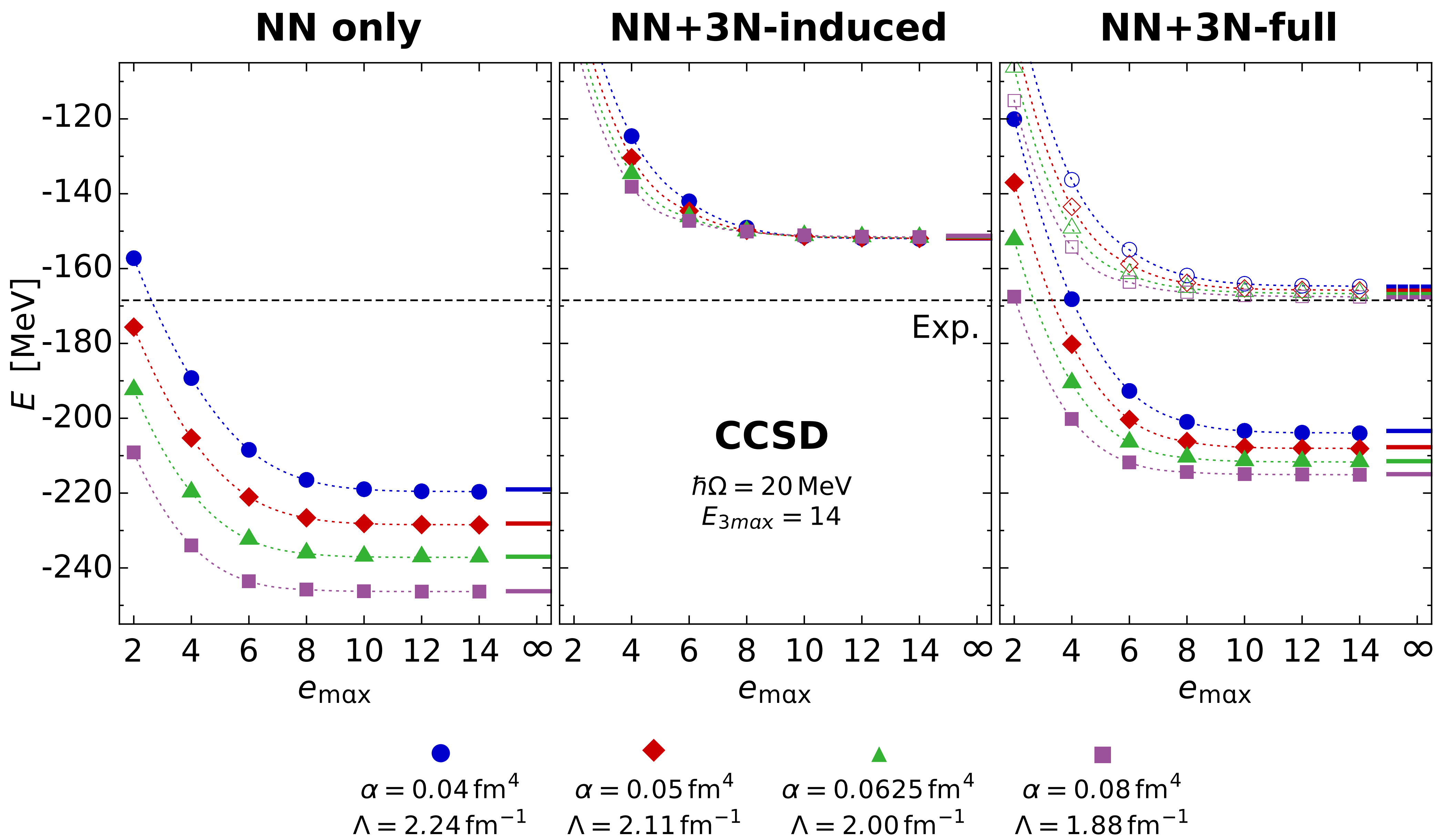
'ab initio' calculations for heavier nuclei require alternative many-body tools and approximate treatment of 3N interactions

- **coupled-cluster method** for ground states of closed-shell nuclei
  - exponential ansatz for many-body states using singles and doubles excitations (CCSD)
- **normal-ordering approximation** of the 3N interaction truncated at the two-body level
  - summation over reference state converts part of 3N interaction to zero-, one- and two-body terms
- both approximations are controlled and systematically improvable

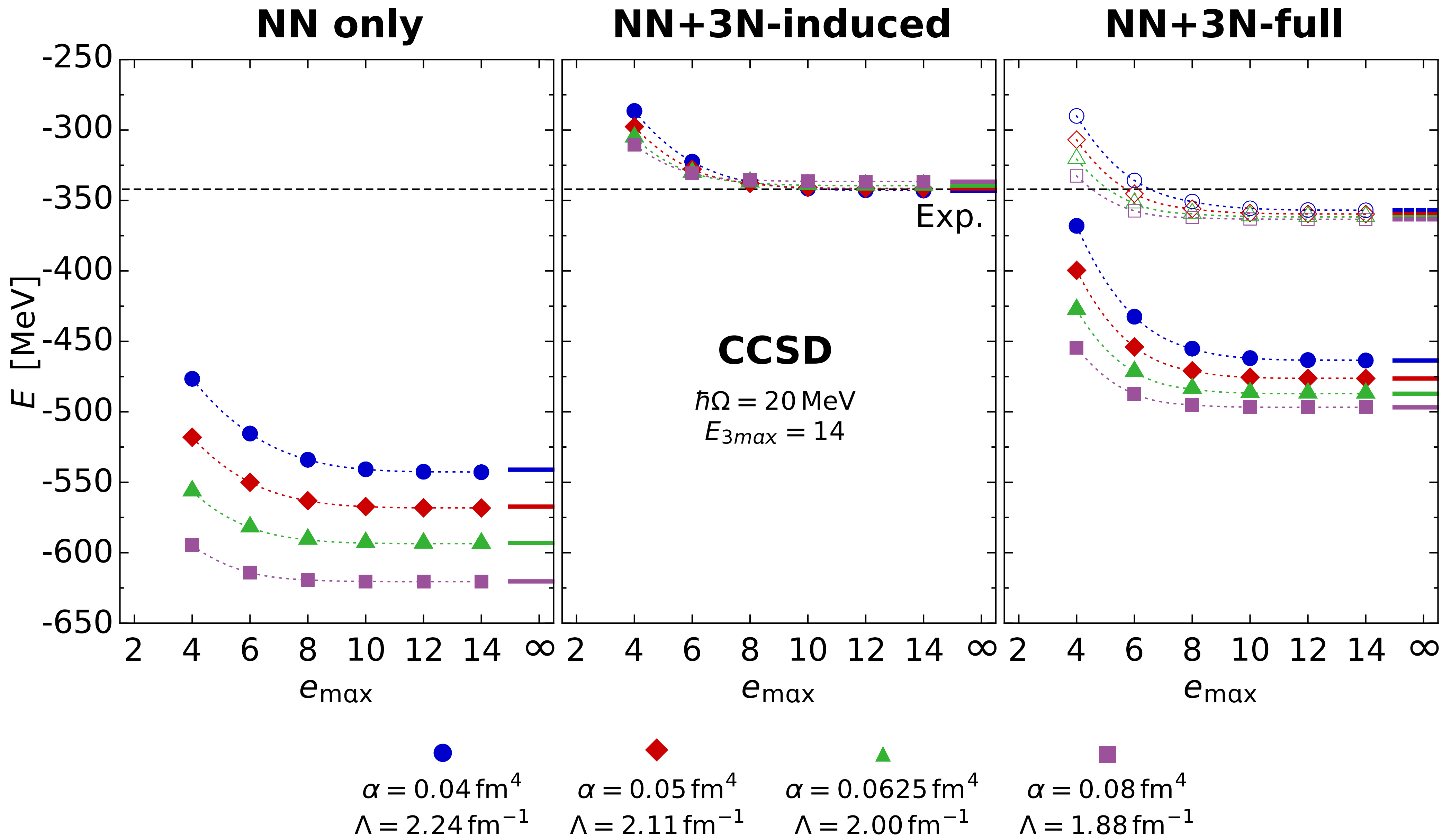
^{16}O: Coupled-Cluster with $3N_{NO2B}$



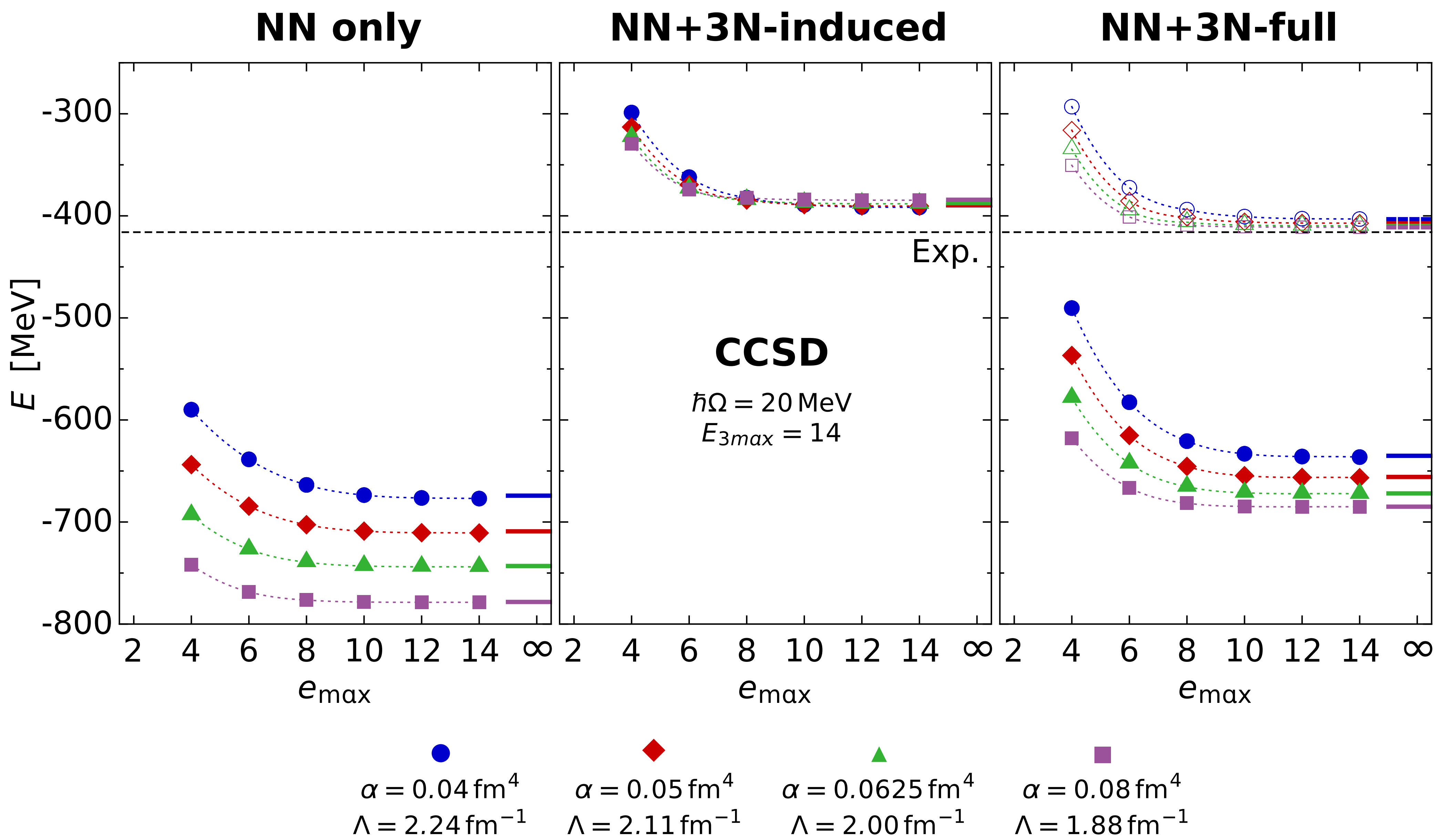
^{24}O: Coupled-Cluster with $3N_{NO2B}$



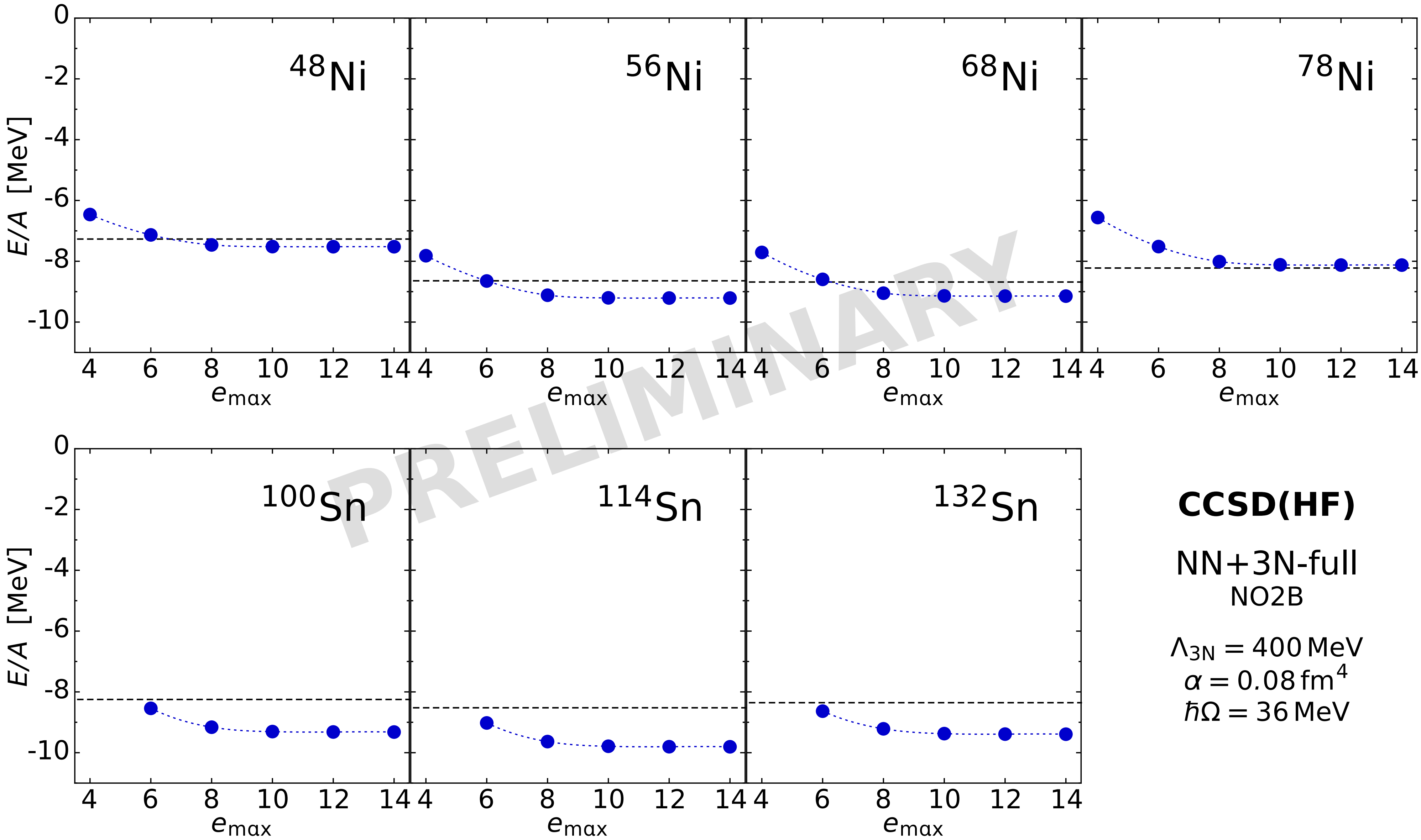
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



^{48}Ca: Coupled-Cluster with $3N_{NO2B}$



Outlook: Chiral 3N for Heavy Nuclei



CCSD(HF)

NN+3N-full
NO2B

$\Lambda_{3N} = 400\,\text{MeV}$
$\alpha = 0.08\,\text{fm}^4$
$\hbar\Omega = 36\,\text{MeV}$

Conclusions

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some issues remain
- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
  - breakthrough in computation & handling of 3N 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**
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LOEWE-CSC — CSC Center for Scientific Computing Frankfurt
HOPPER — NERSC

COMPUTING TIME

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HIC for FAIR Helmholtz International Center
LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz
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