New Horizons in Ab Initio Nuclear Structure Theory

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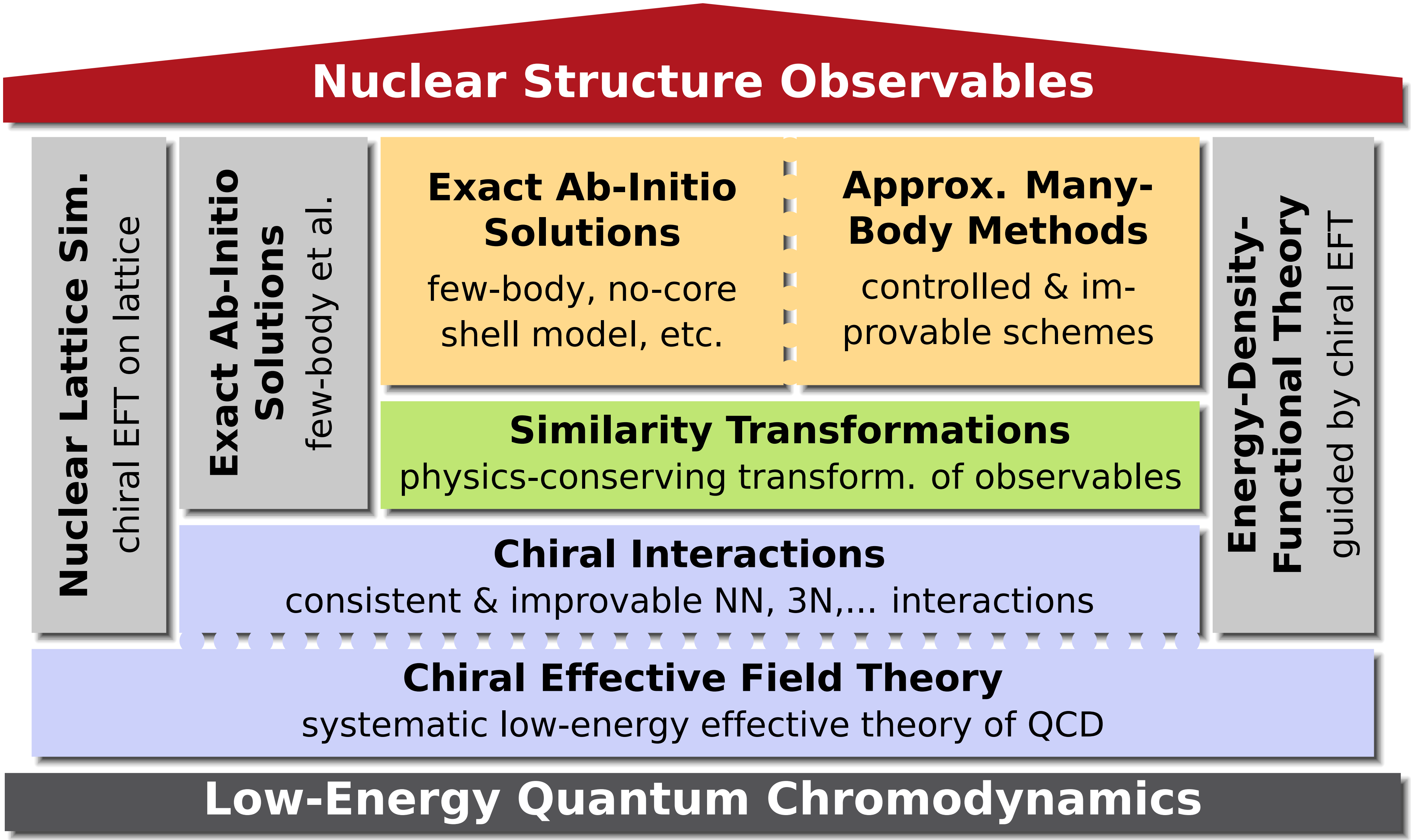
Ab Initio Nuclear Structure



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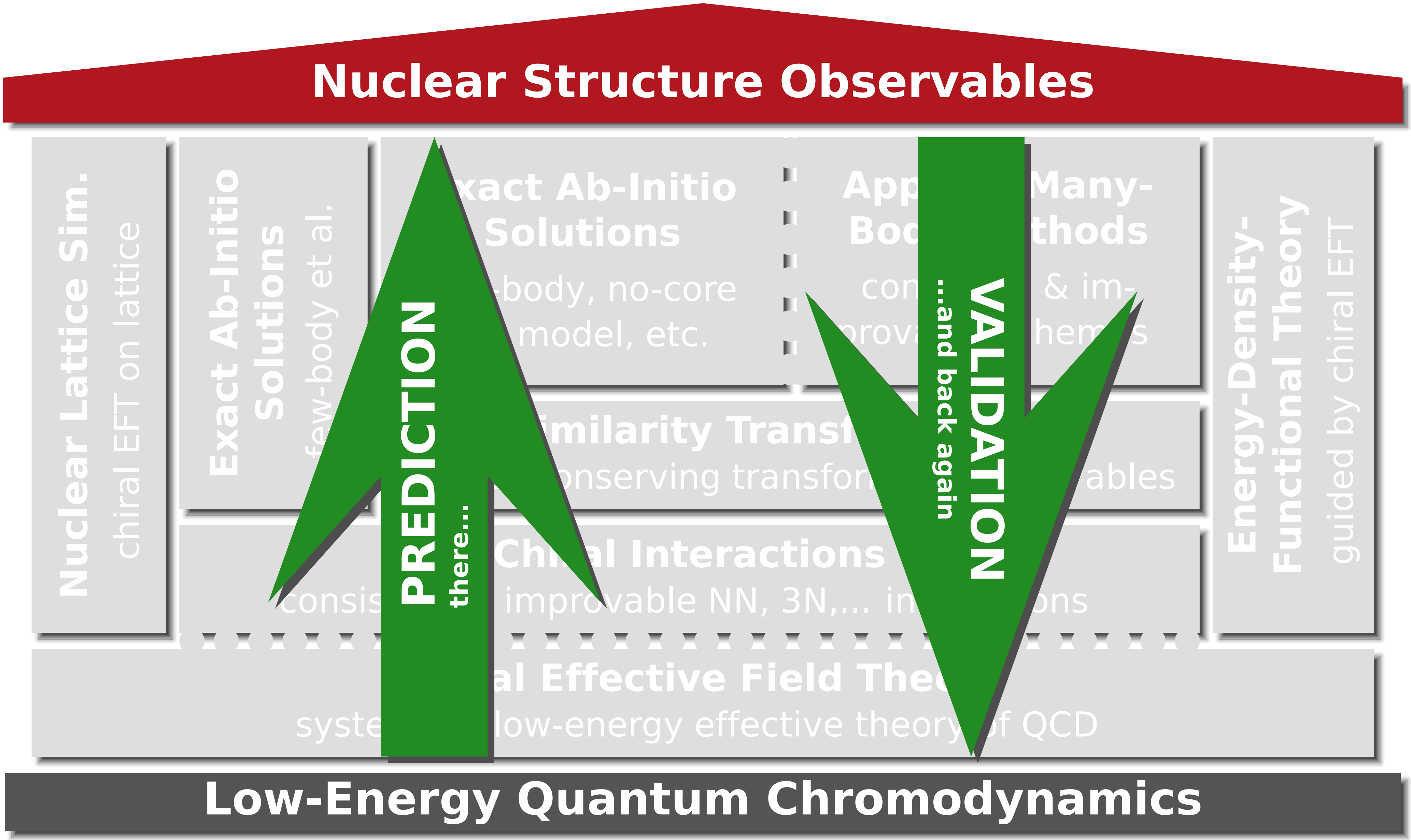
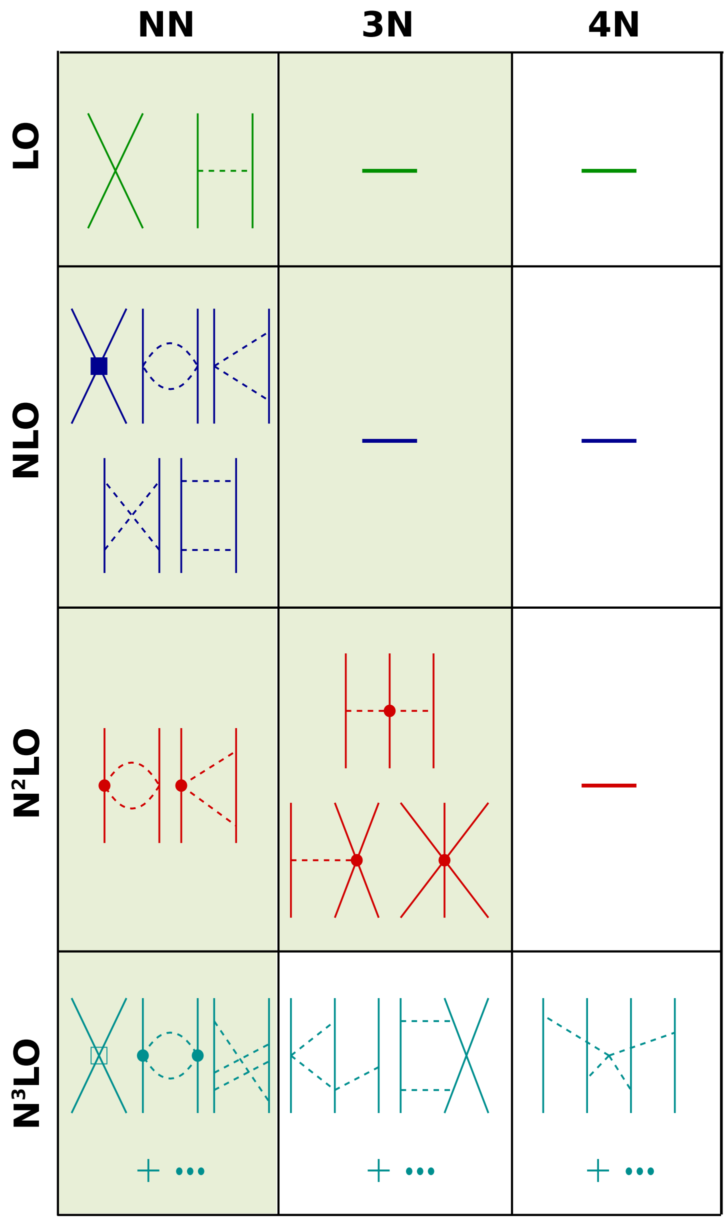


Nuclear Interactions from Chiral EFT

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**, low-energy constants fitted to experiment (NN, πN,...)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at N3LO, N4LO,...
  - explicit inclusion of Δ-resonance
  - YN- & YY-interactions
  - formal issues: power counting, renormalization, cutoff choice,...



Chiral NN+3N Hamiltonians

- **standard Hamiltonian:**
  - NN at N3LO: Entem / Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, local, 500 MeV cutoff, fit to $T_{1/2}(^3\mathrm{H})$ and $E(^3\mathrm{H}, {}^3\mathrm{He})$
- **standard Hamiltonian with modified 3N:**
  - NN at N3LO: Entem / Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, local, with modified LECs and cutoffs, refit to $E(^4\mathrm{He})$
- **consistent N2LO Hamiltonian:**
  - NN at N2LO: Epelbaum et al., 450,...,600 MeV cutoff
  - 3N at N2LO: Epelbaum et al., nonlocal, 450,...,600 MeV cutoff
- **consistent N3LO Hamiltonian:**
  - coming soon...

Similarity Renormalization Group

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Roth, Reinhardt, Hergert — Phys. Rev. C 77, 064033 (2008)
Hergert, Roth — Phys. Rev. C 75, 051001(R) (2007)

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

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

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

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

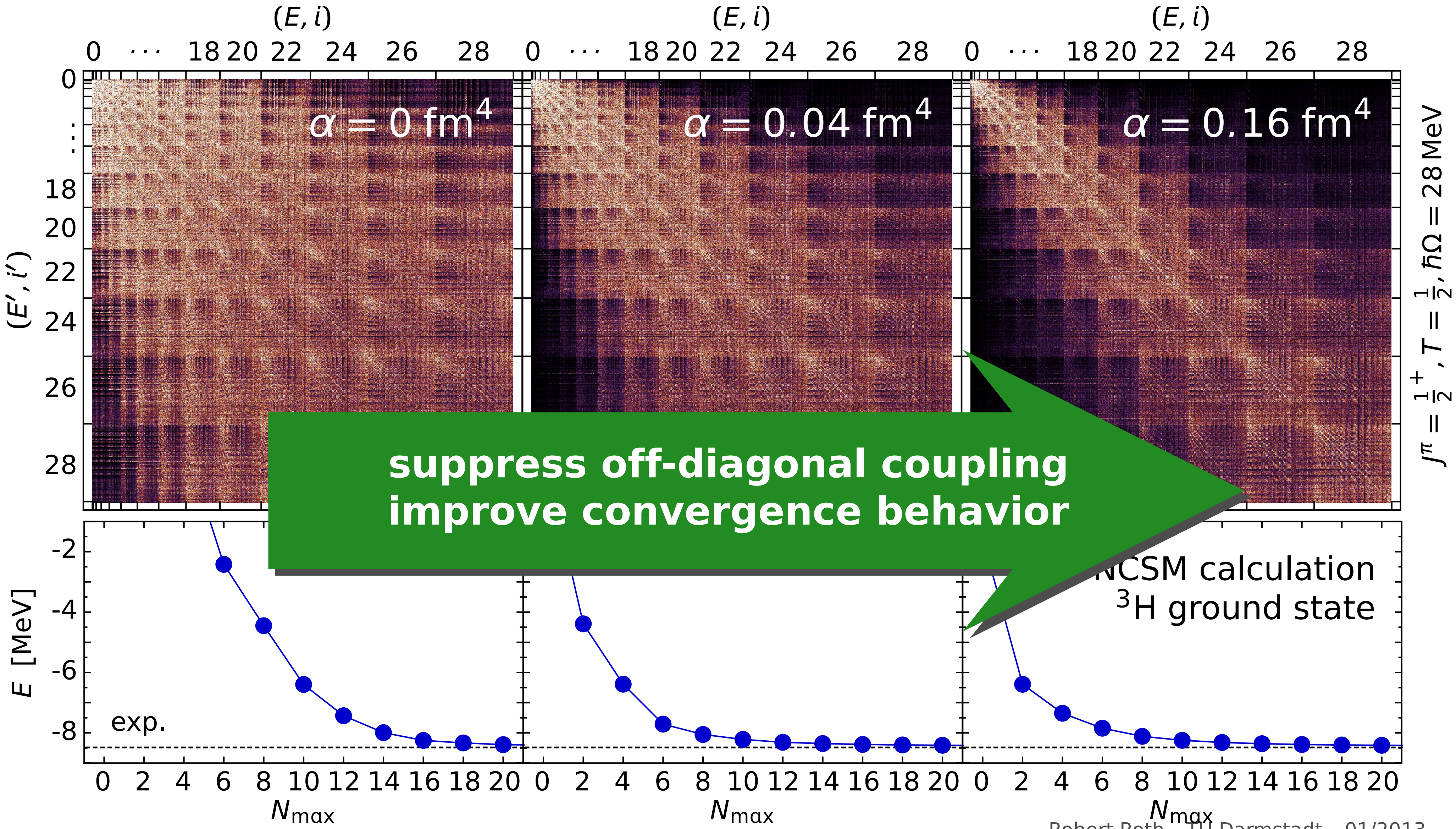
$$\frac{d}{d\alpha}\tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha]$$

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

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

SRG Evolution in Three-Body Space

- perform SRG evolution for **three-body Jacobi-HO** matrix elements



Hamiltonian 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)

SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamilt[...] 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

Importance Truncated No-Core Shell Model

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth, Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

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
- we have developed a **parallelized IT-NCSM/NCSM code** capable of handling 3N matrix elements up to $E_{3\max} = 16$

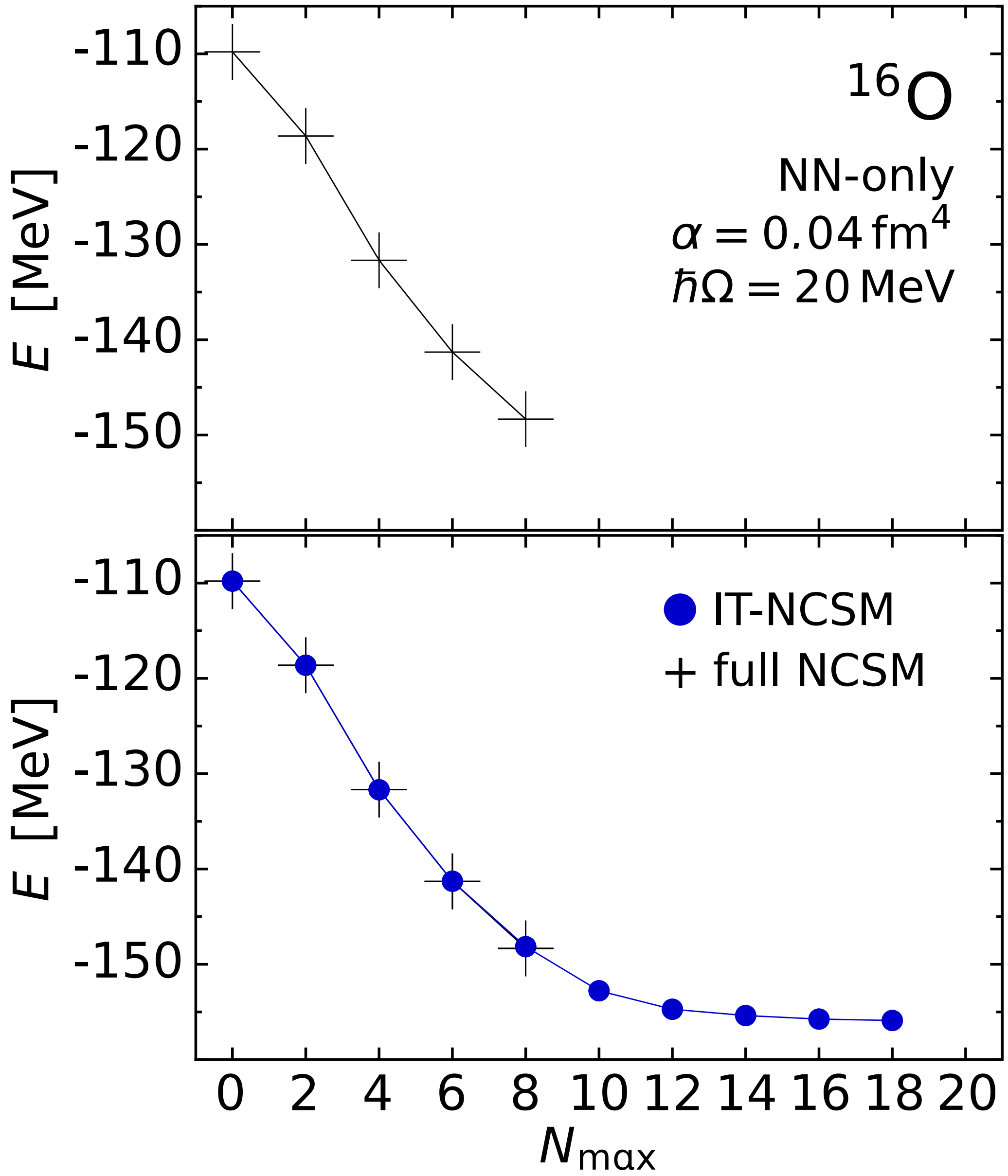
Importance Truncated NCSM

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

- 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})

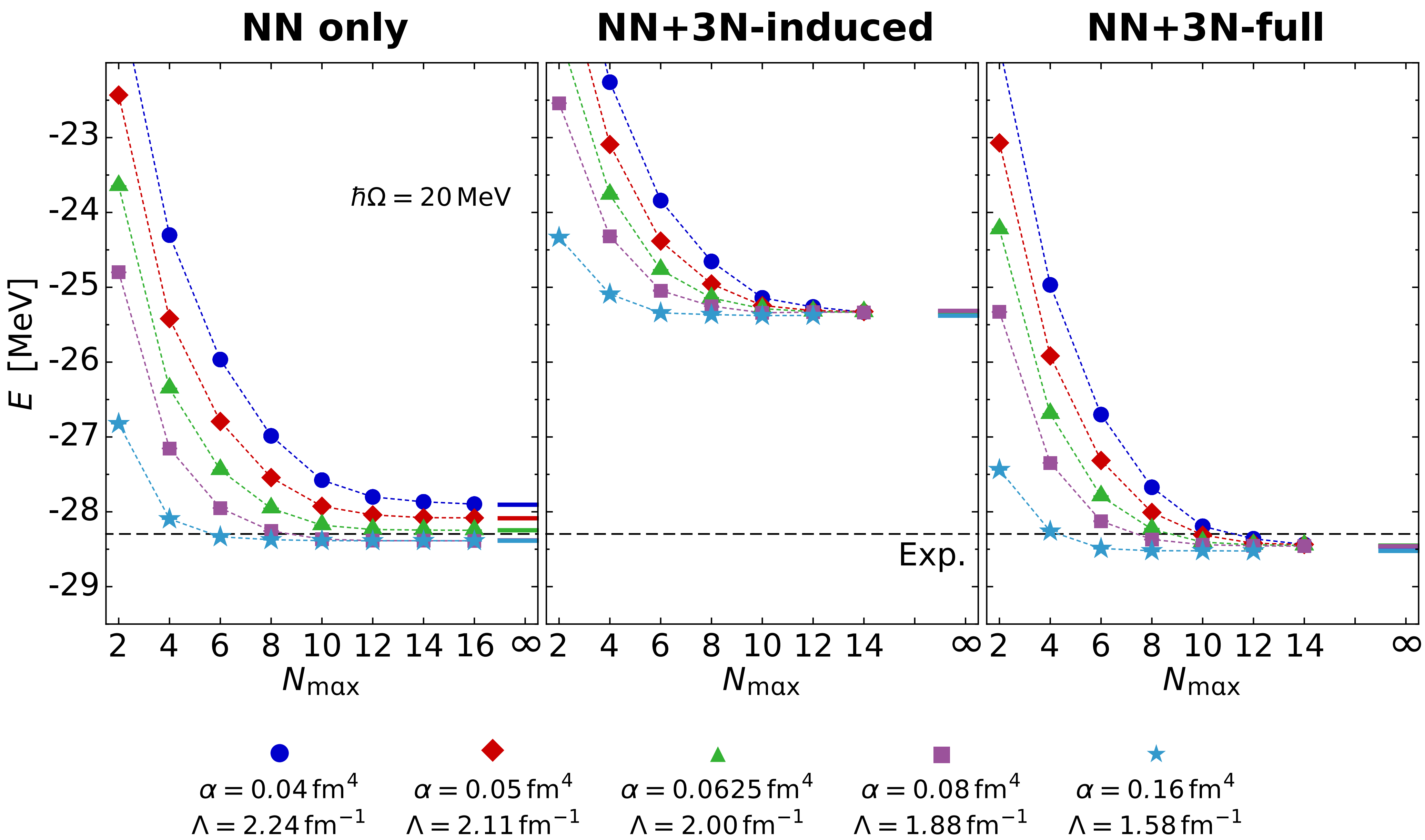
Importance Truncation

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



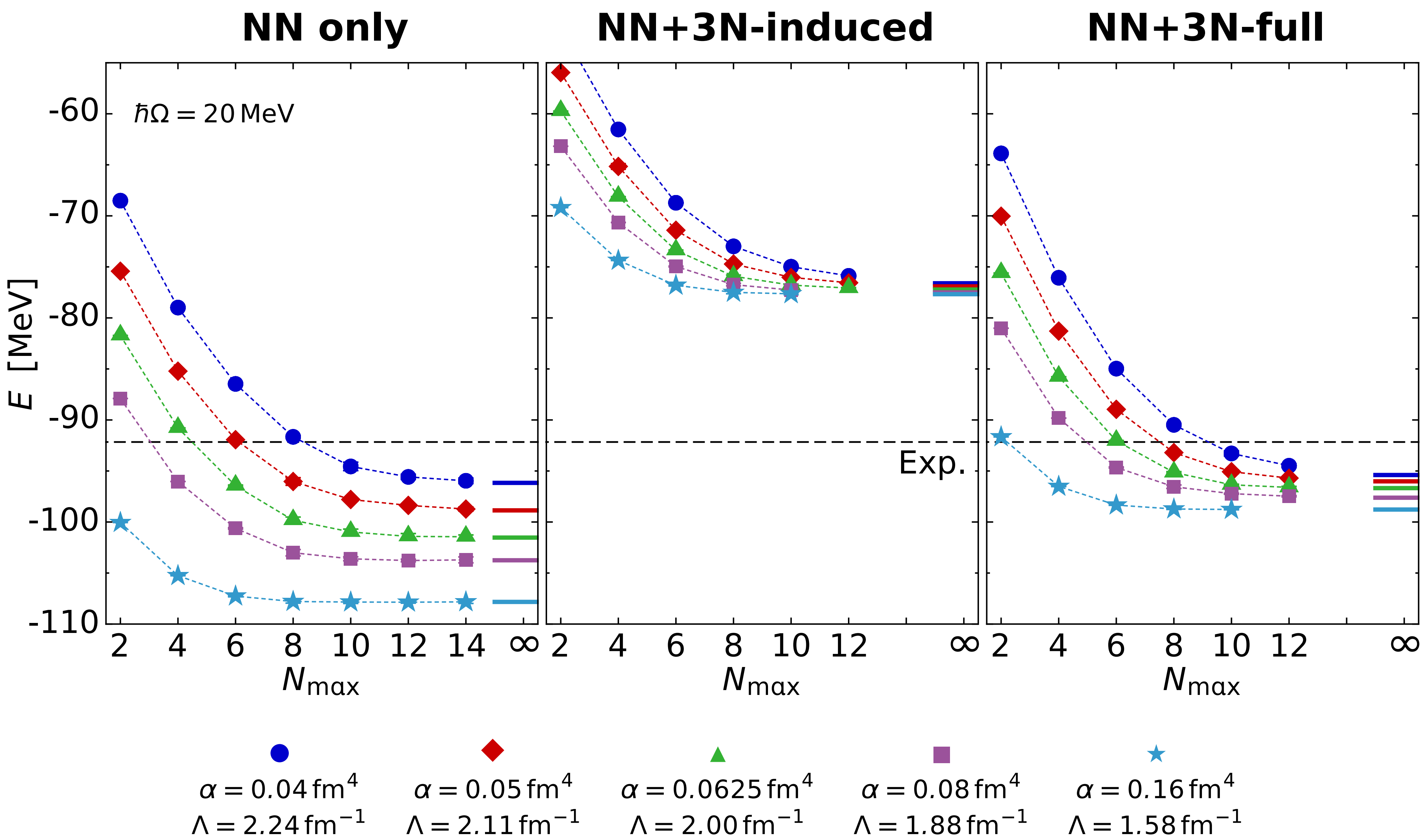
^{4}He: Ground-State Energies

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



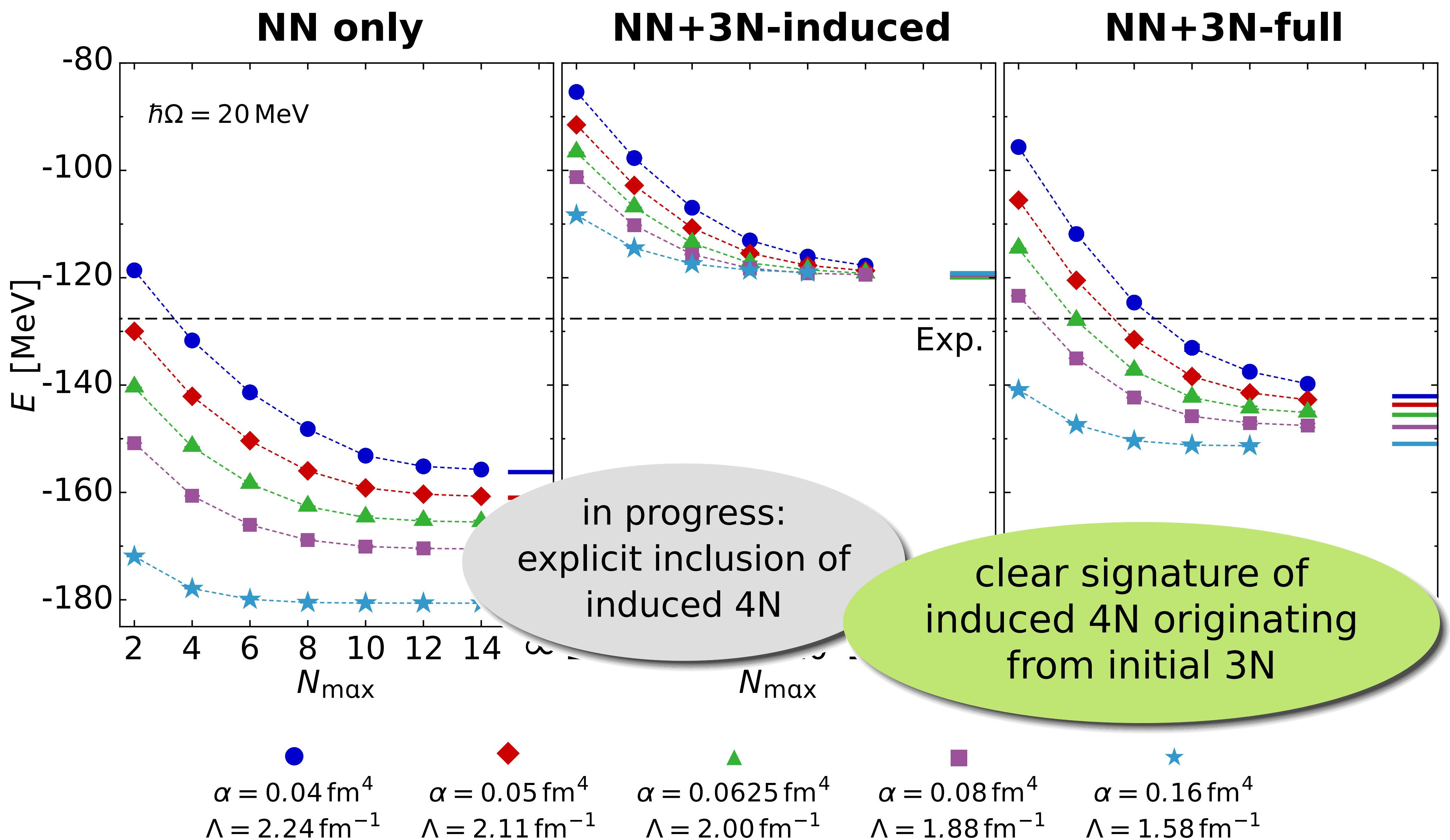
^{12}C: Ground-State Energies

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

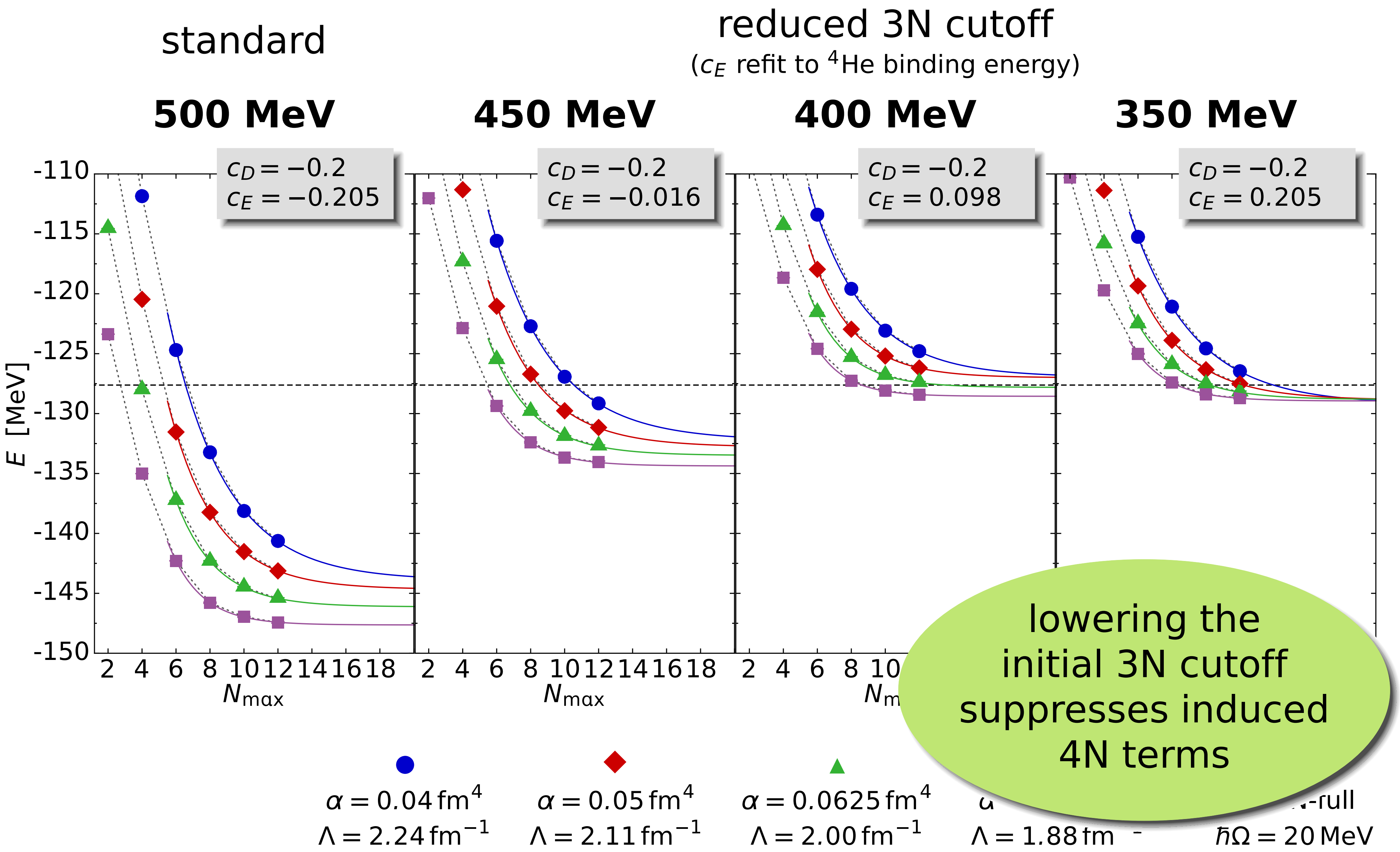


^{16}O: Ground-State Energies

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

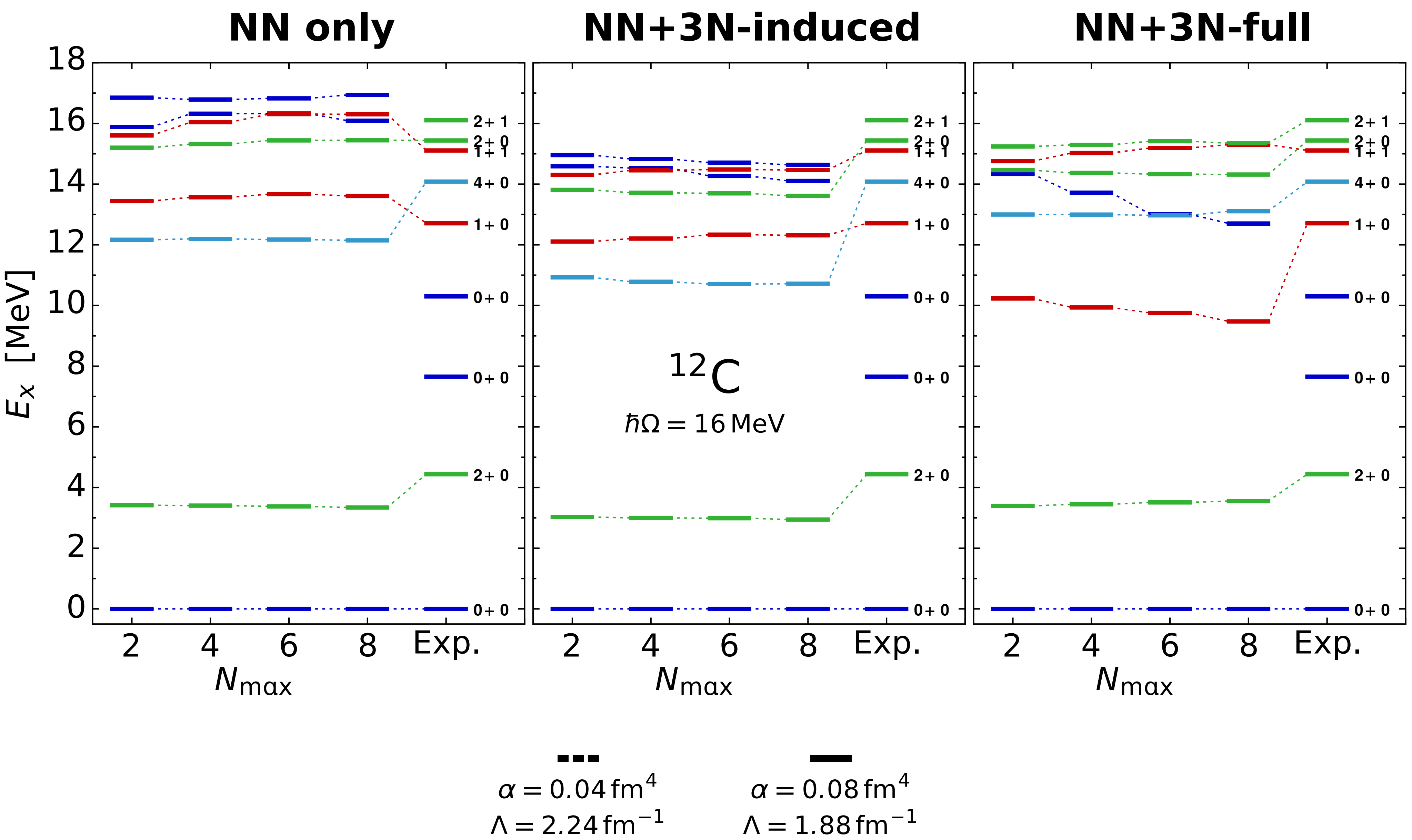


^{16}O: Lowering the Initial 3N Cutoff



Spectroscopy of ^{12}C

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



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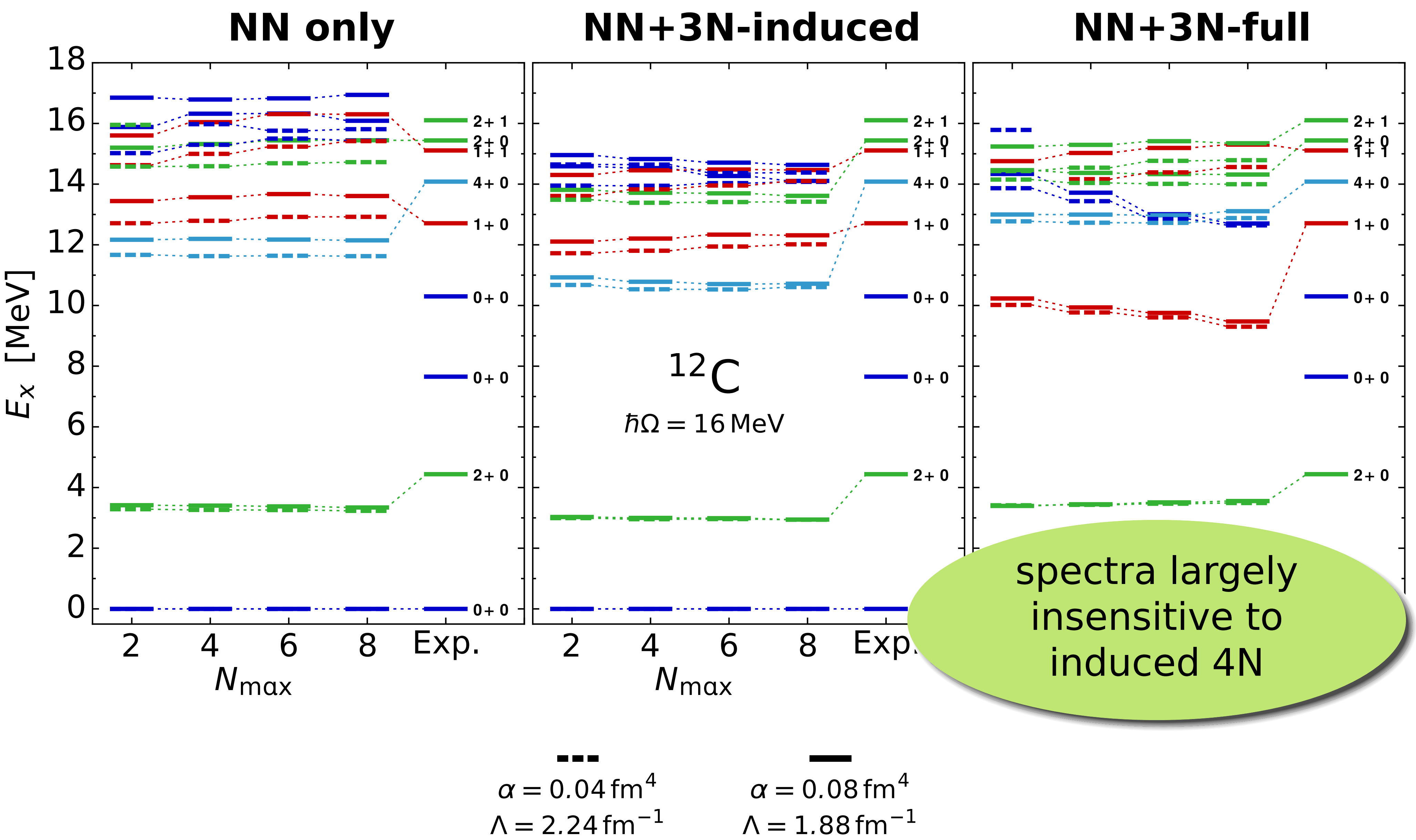


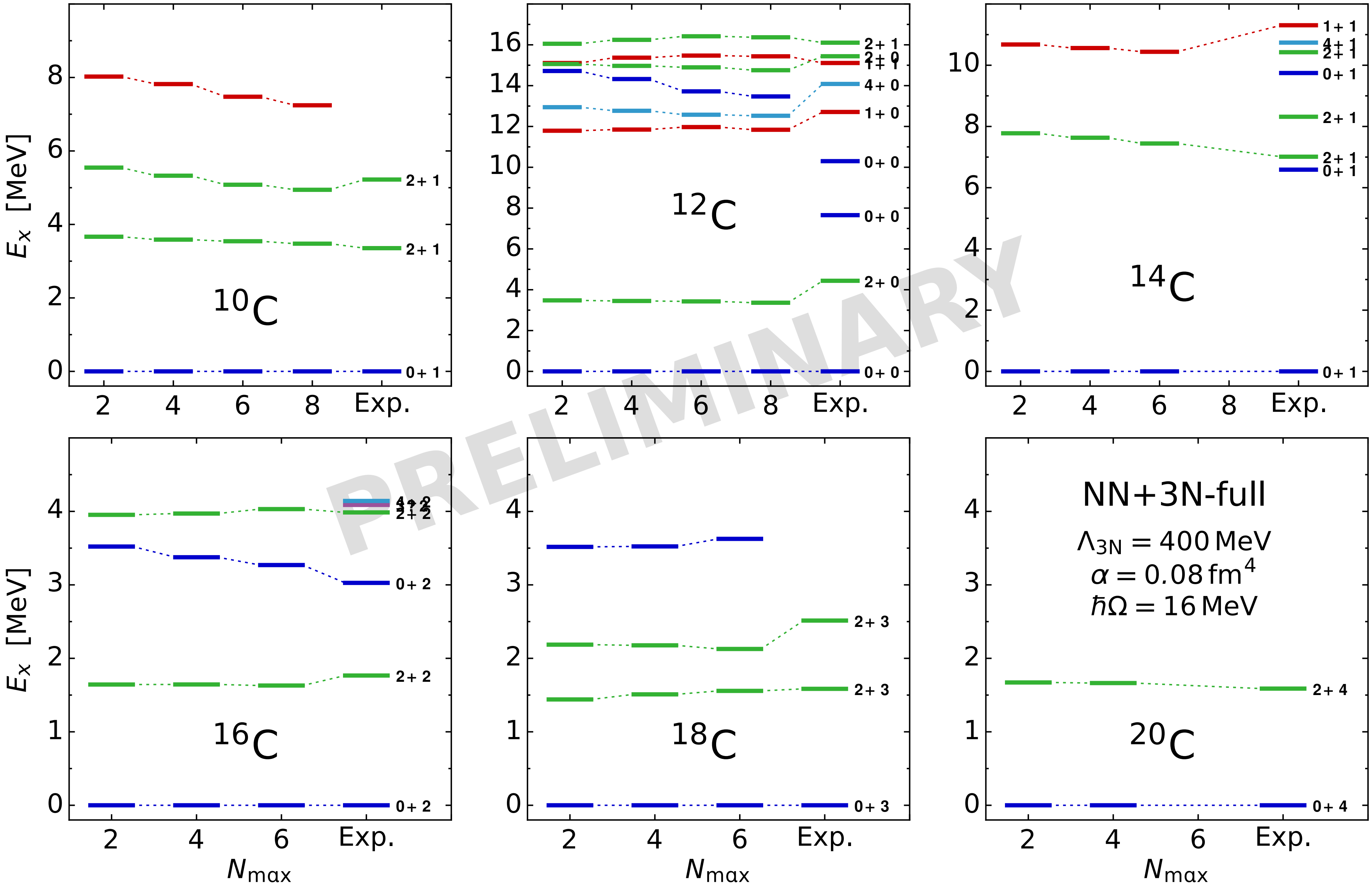
The Bottom Line...

- 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

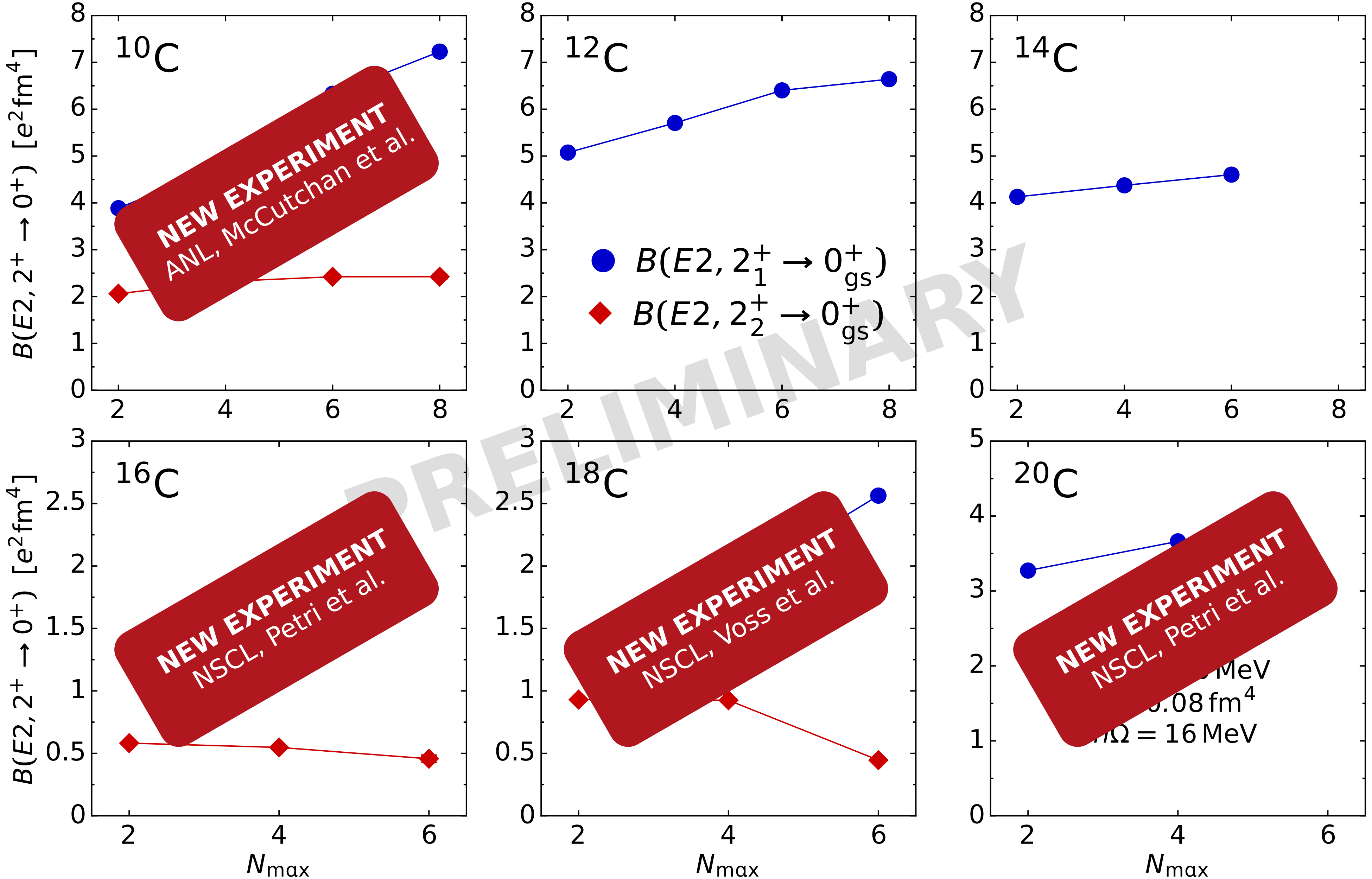
- **applications**: spectroscopy of p- and sd-shell nuclei and ground states with reduced initial 3N cutoff
- **next-generation SRG**: include induced 4N contributions or suppress many-body terms with modified SRG-generators
- **next-generation chiral 3N**: use consistent chiral Hamiltonians and propagate uncertainties to many-body observables

Ab Initio Calculations for p- and sd-Shell Nuclei

Spectroscopy of Carbon Isotopes

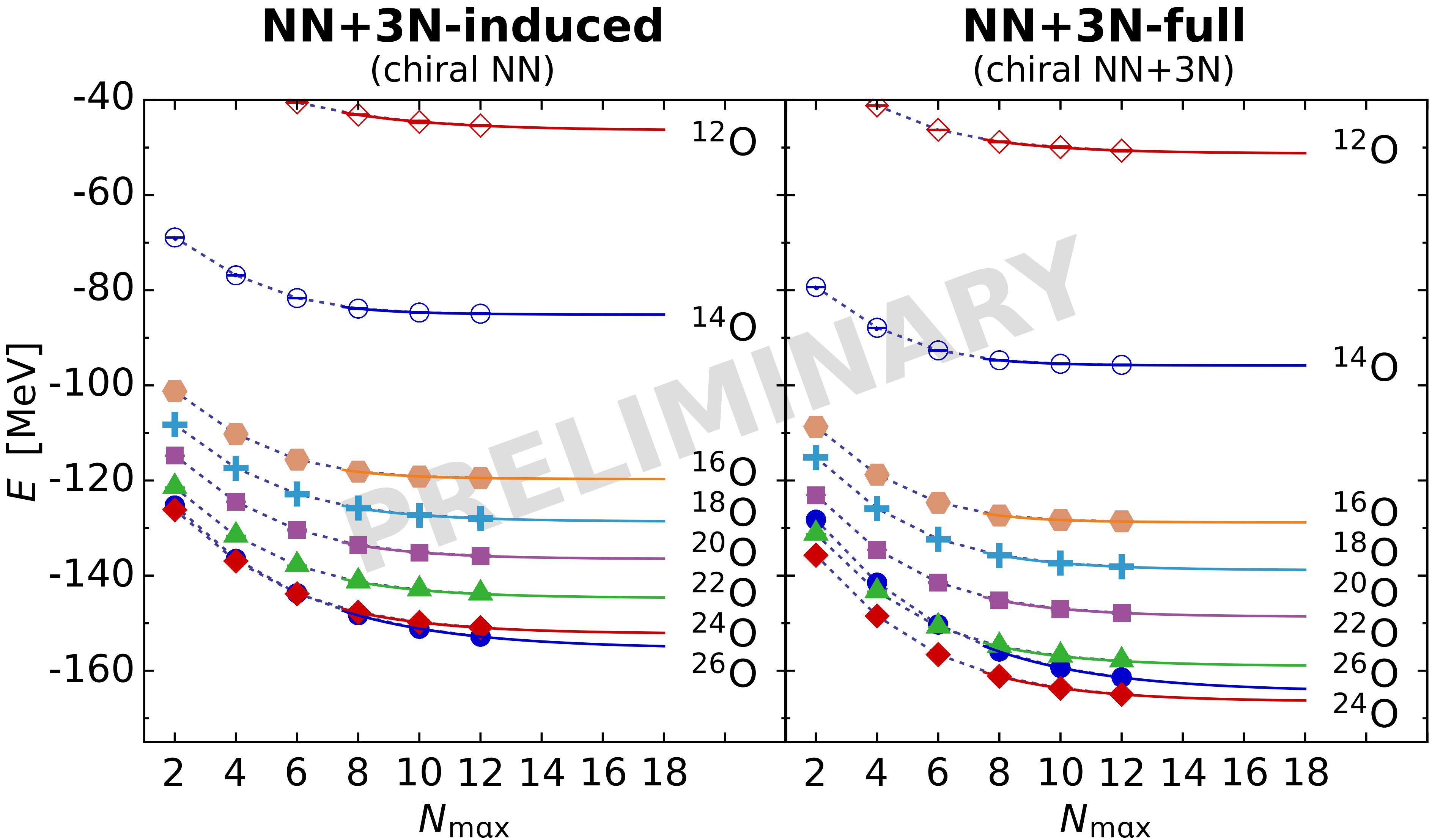


Spectroscopy of Carbon Isotopes



Ground States of Oxygen Isotopes

Hergert, Binder, Calci, Langhammer, Roth; in prep.



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

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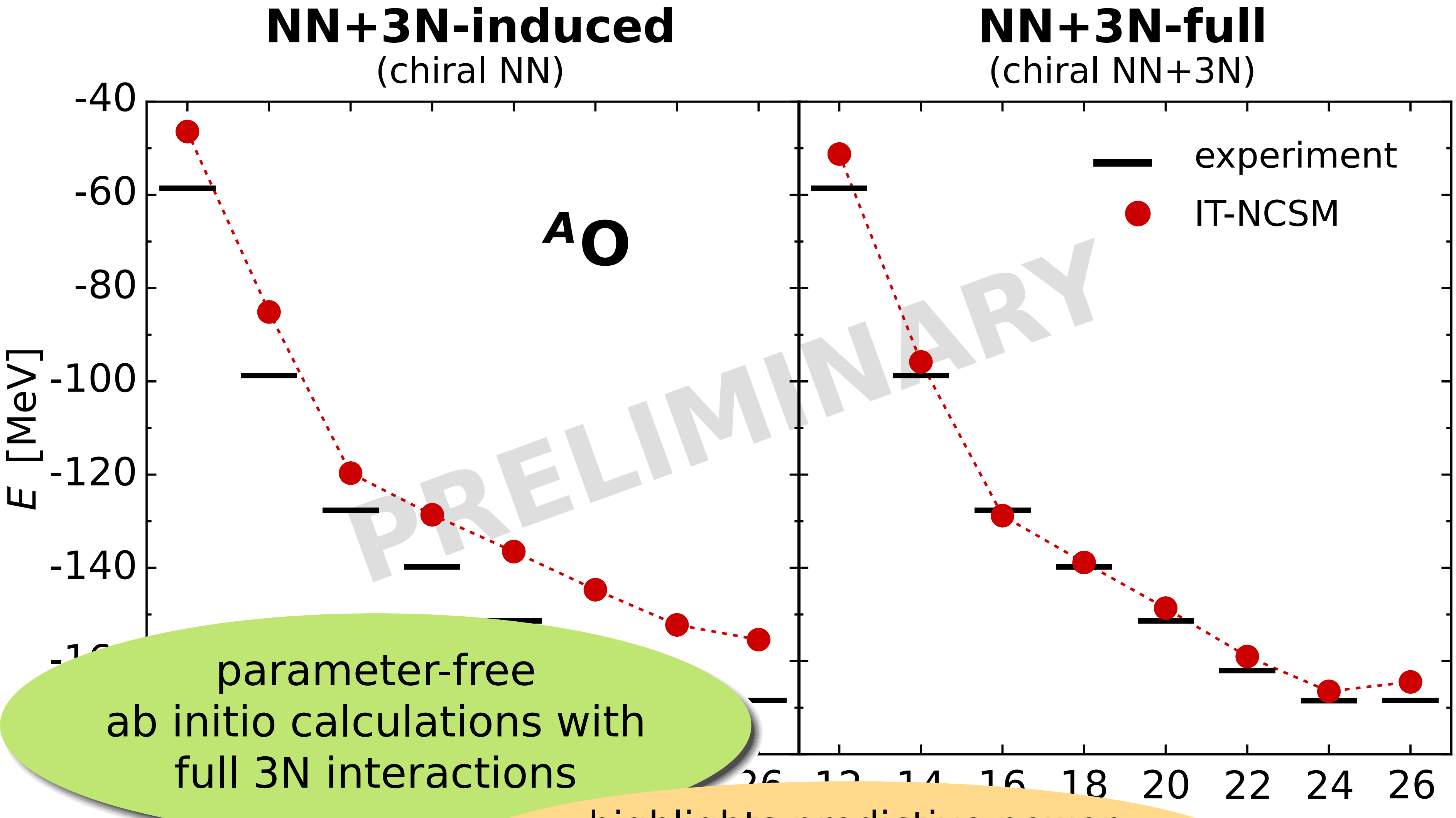

parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

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

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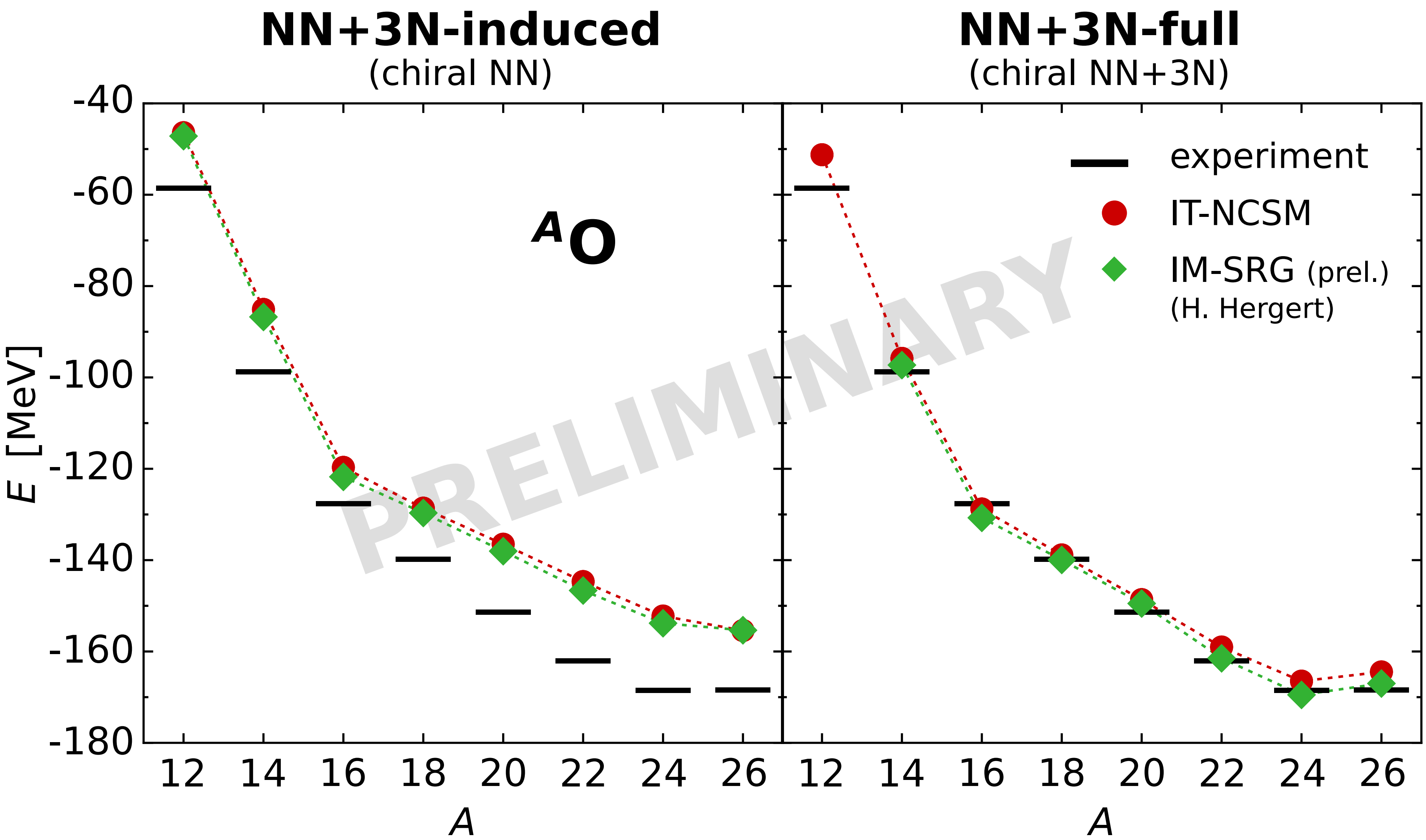

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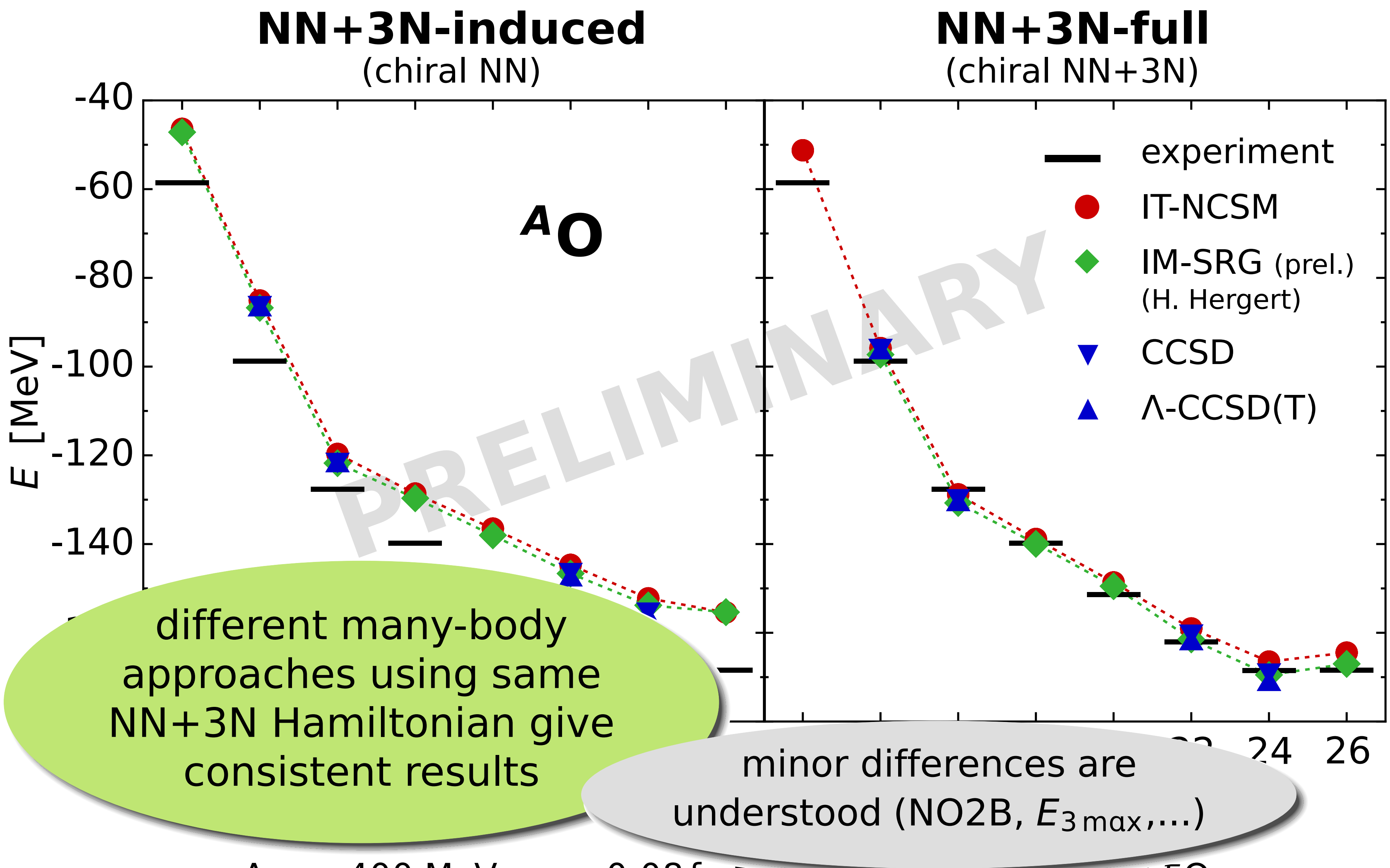

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Ab Initio Calculations for Heavy Nuclei

Roth, Binder, Vobig et al. — Phys. Rev. Lett. 109, 052501 (2012)
Binder, Langhammer, Calci et al. — arXiv:1211.4748
Hergert, Bogner, Binder et al. — arXiv:1212.1190

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

- **premium option: explicit 3N**
  - extend coupled-cluster equations for explicit 3N interactions
  - CCSD-3B, Λ-CCSD(T)-3B are feasible, but much more expensive

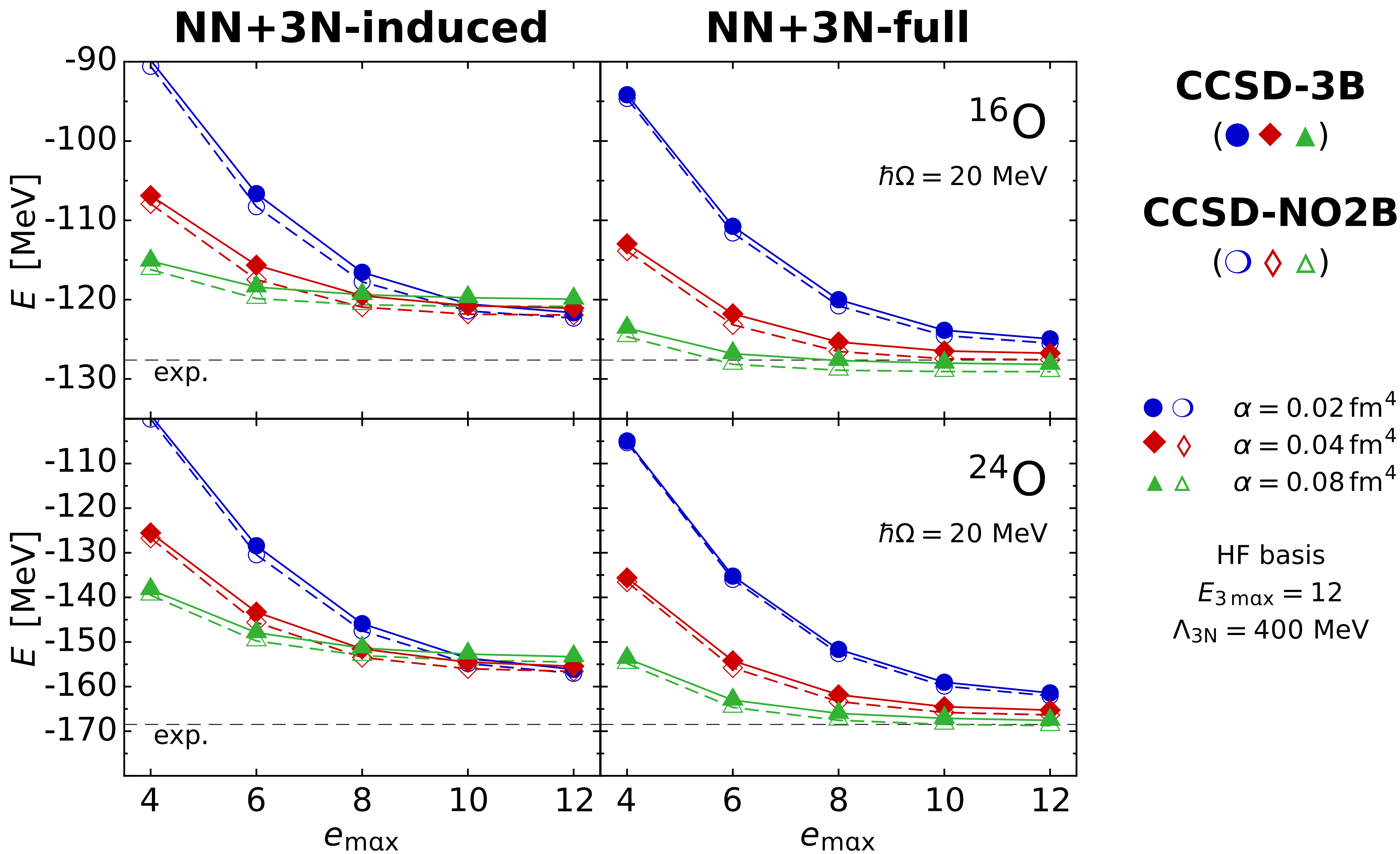
- **low-cost option: normal-ordered two-body approximation**
  - write 3N interaction in normal-ordered form with respect to the actual *A*-body reference determinant (HF state)

$$
\begin{aligned}
\mathrm{V}_{3N} &= \sum V^{3N}_{\circ\circ\circ\circ\circ\circ}\, a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ a_\circ \\
&= W^{0B} + \sum W^{1B}_{\circ\circ}\, \{a^\dagger_\circ\, a_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ\} \\
&\quad + \sum W^{3B}_{\circ\circ\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ a_\circ\}
\end{aligned}
$$

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

CCSD with Explicit 3N Interactions

Binder et al.; arXiv:1211.4748



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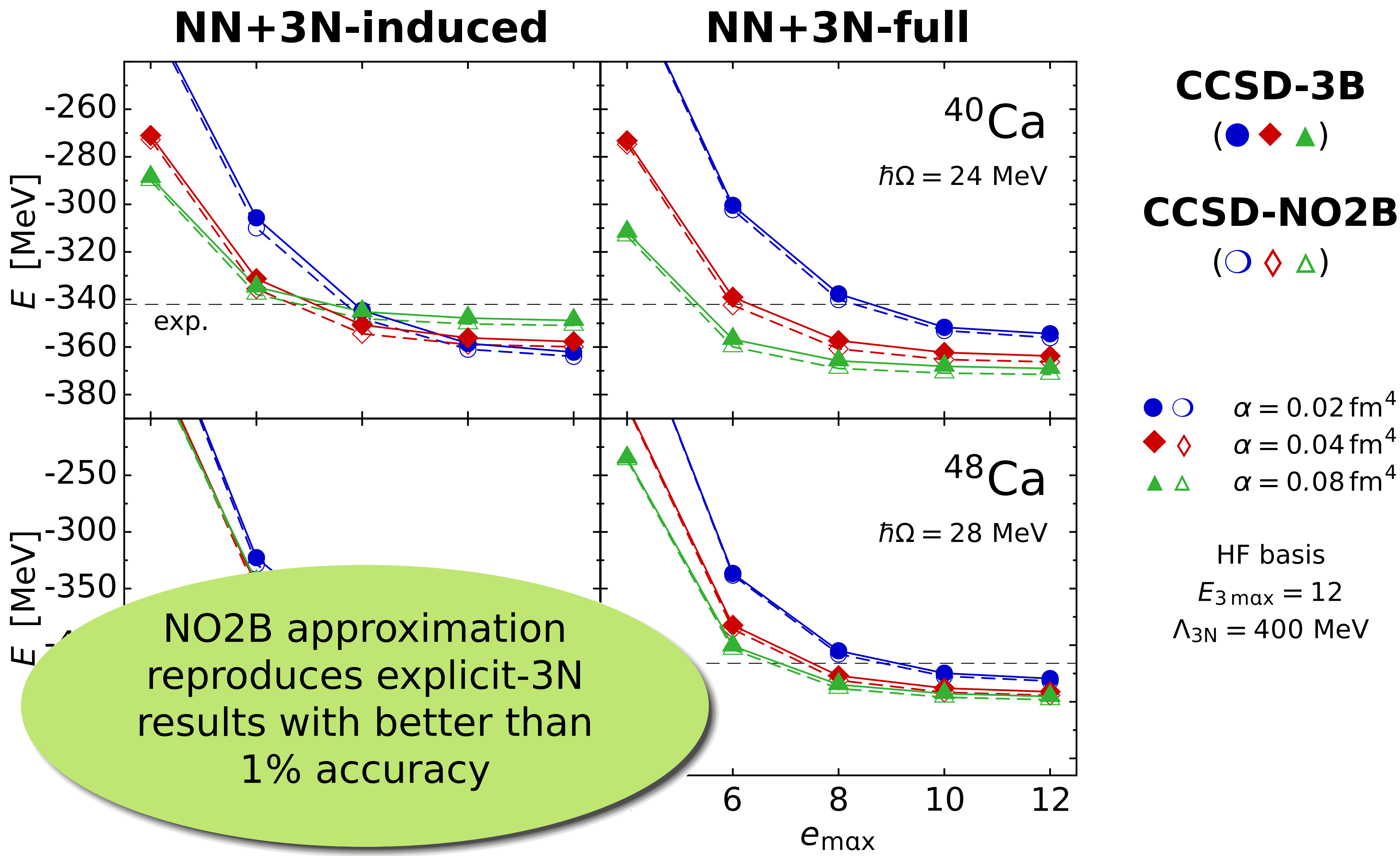
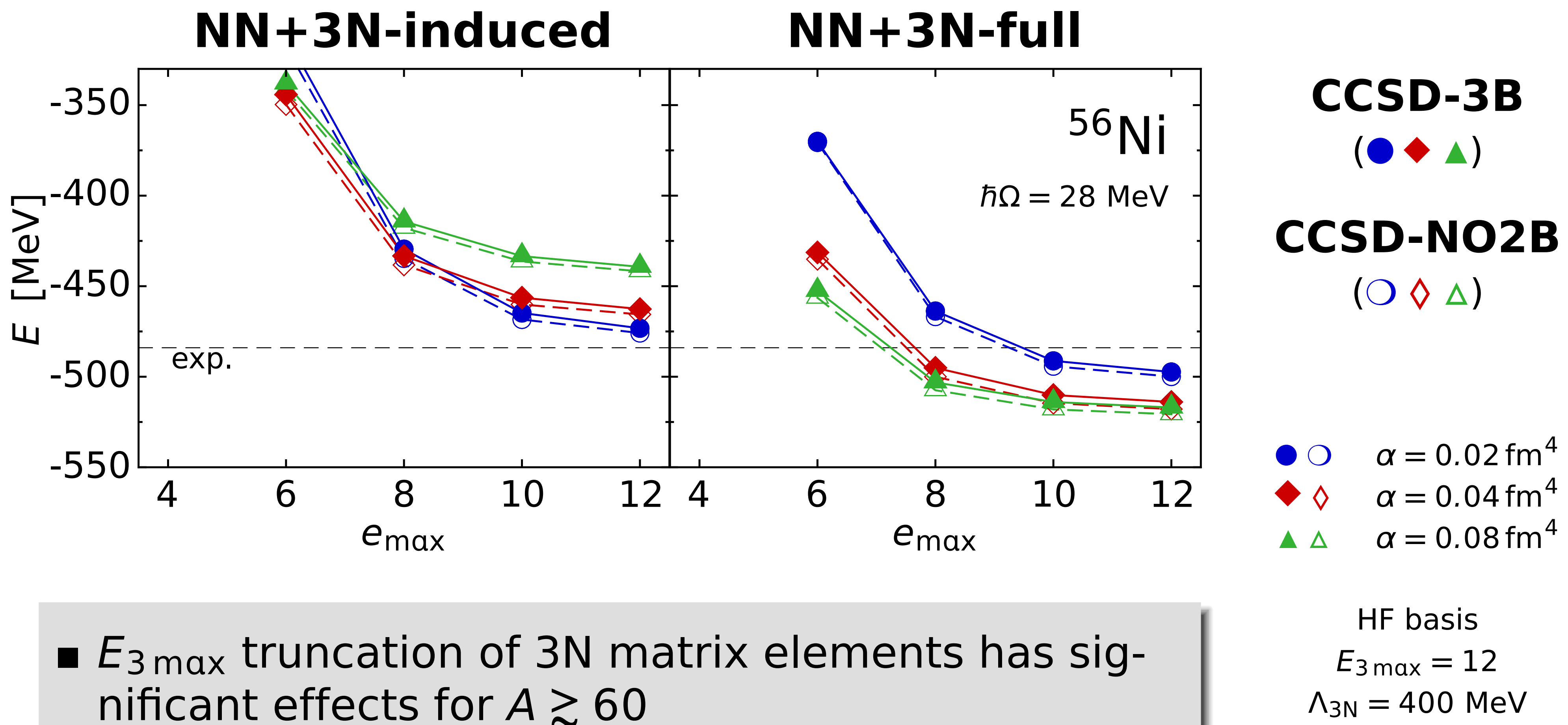


NO2B approximation reproduces explicit-3N results with better than 1% accuracy

CCSD with Explicit 3N Interactions

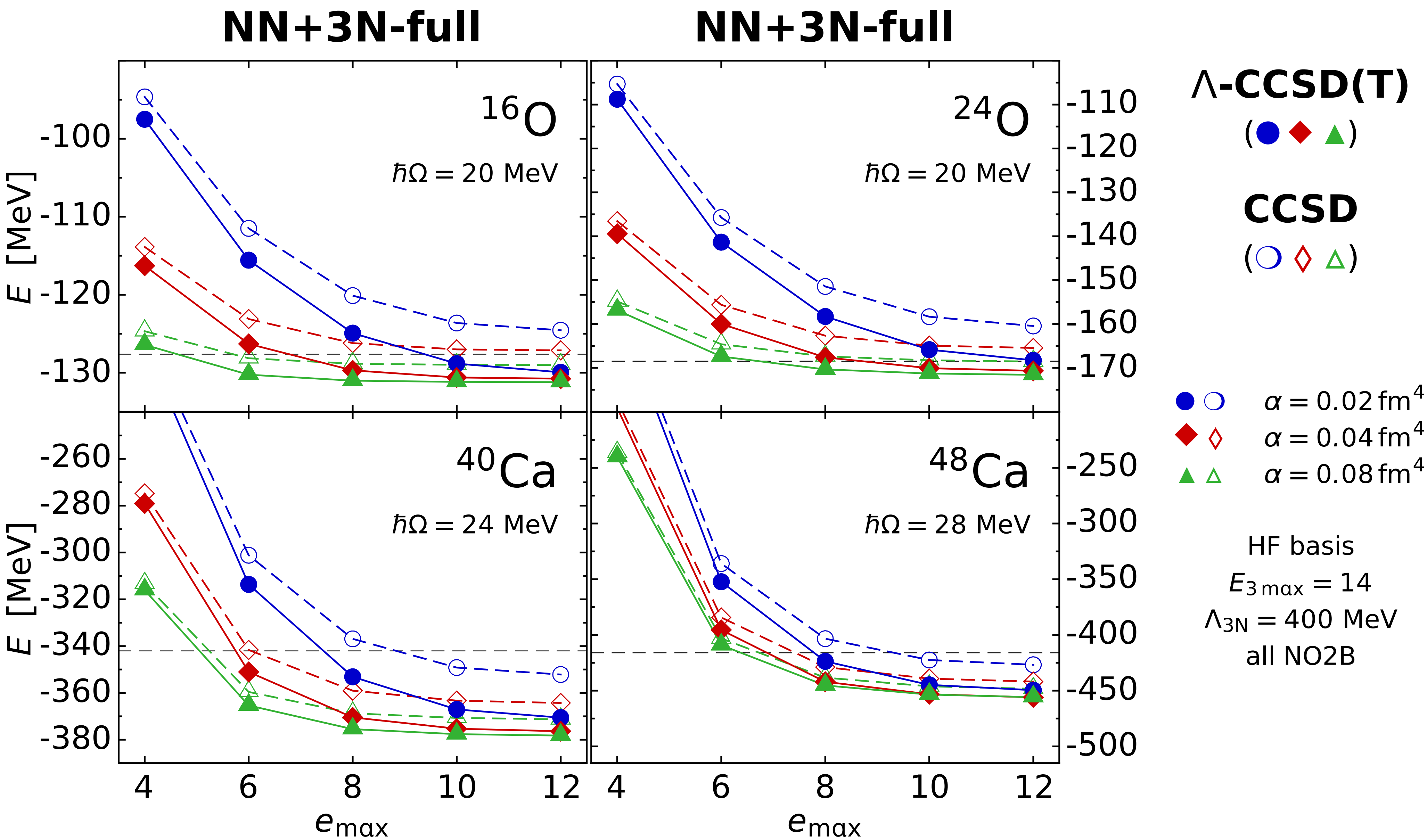
Binder et al.; arXiv:1211.4748



- $E_{3\,\mathrm{max}}$ truncation of 3N matrix elements has significant effects for $A \gtrsim 60$
- many-body framework is ready to go to heavier nuclei... still cheap with NO2B approximation

Λ-CCSD(T) with NO2B Approximation

Binder et al.; arXiv:1211.4748



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 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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COMPUTING TIME