Ab Initio Nuclear Structure Theory with Chiral NN+3N Interactions

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

NN+3N Interaction from Chiral EFT

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

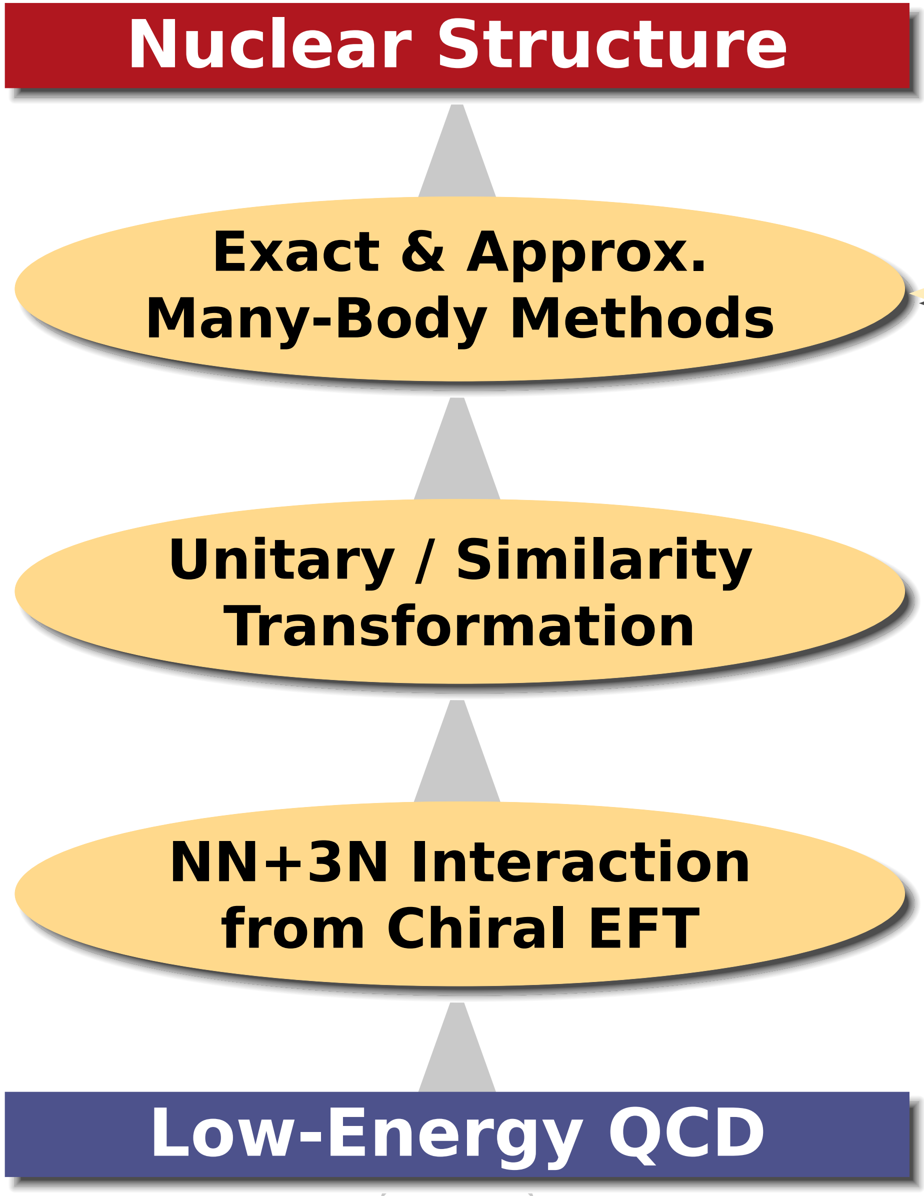
Unitary / Similarity Transformation

- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently

NN+3N Interaction from Chiral EFT

Low-Energy QCD

From QCD to Nuclear Structure



- accurate solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (MBPT,...)
- all rely on truncated model spaces & benefit from unitary transformation

From QCD to Nuclear Structure

Nuclear Structure

Exact & Approx. Many-Body Methods

Importance Truncated NCSM & Coupled-Cluster with NN+3N

Unitary / Similarity Transformation

Similarity Renormalization Group with NN+3N

NN+3N Interaction from Chiral EFT

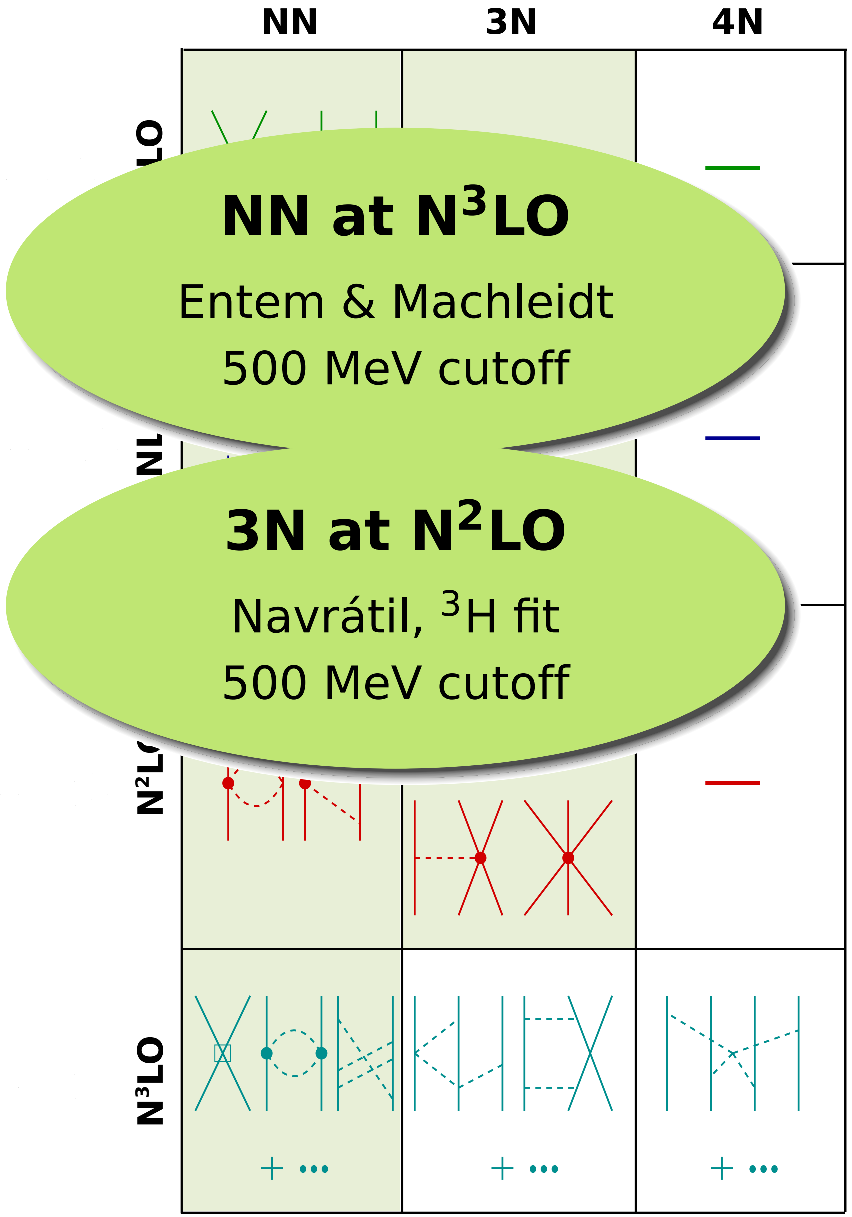
focus on consistent inclusion of chiral 3N interaction

Low-Energy QCD

Nuclear Interactions from Chiral EFT

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



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

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

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

solve SRG evolution equations using two- & three-body Jacobi HO representation

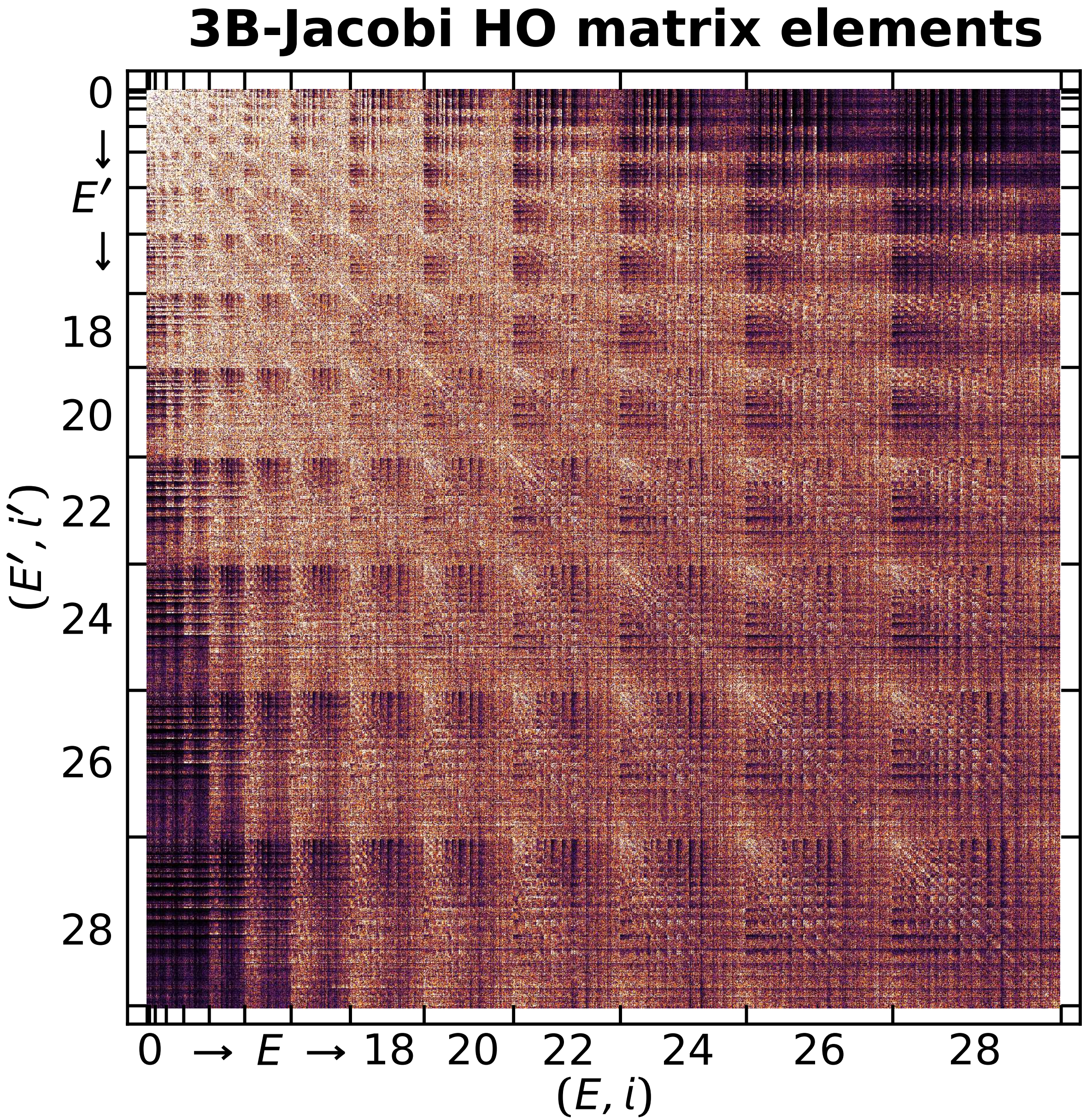
- **evolution equations** for $\tilde{H}_\alpha$ and U

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

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

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

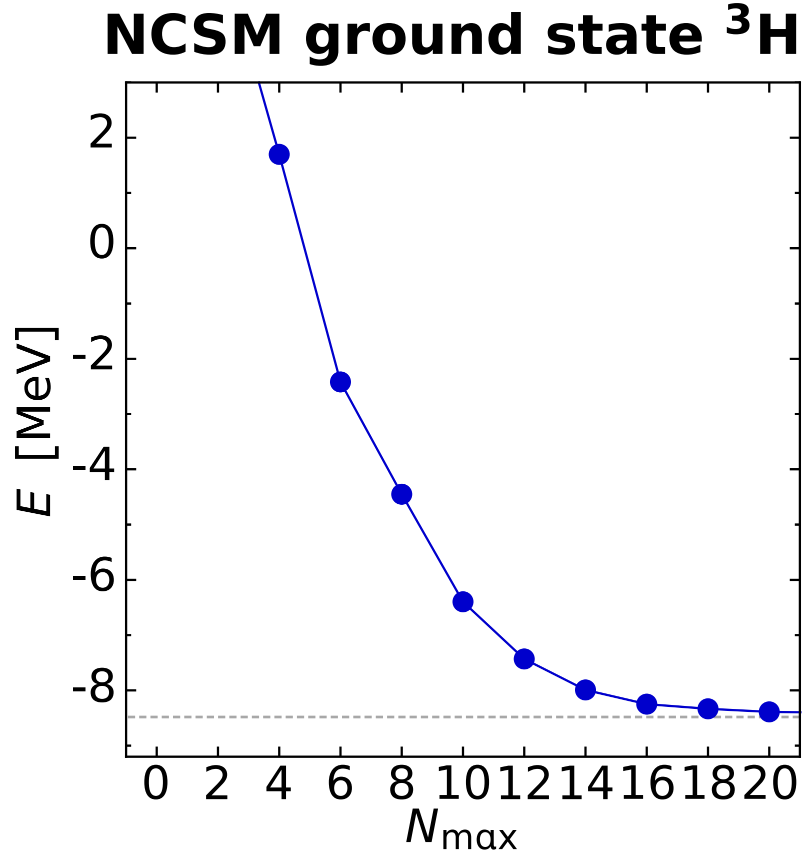
SRG Evolution in Three-Body Space



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

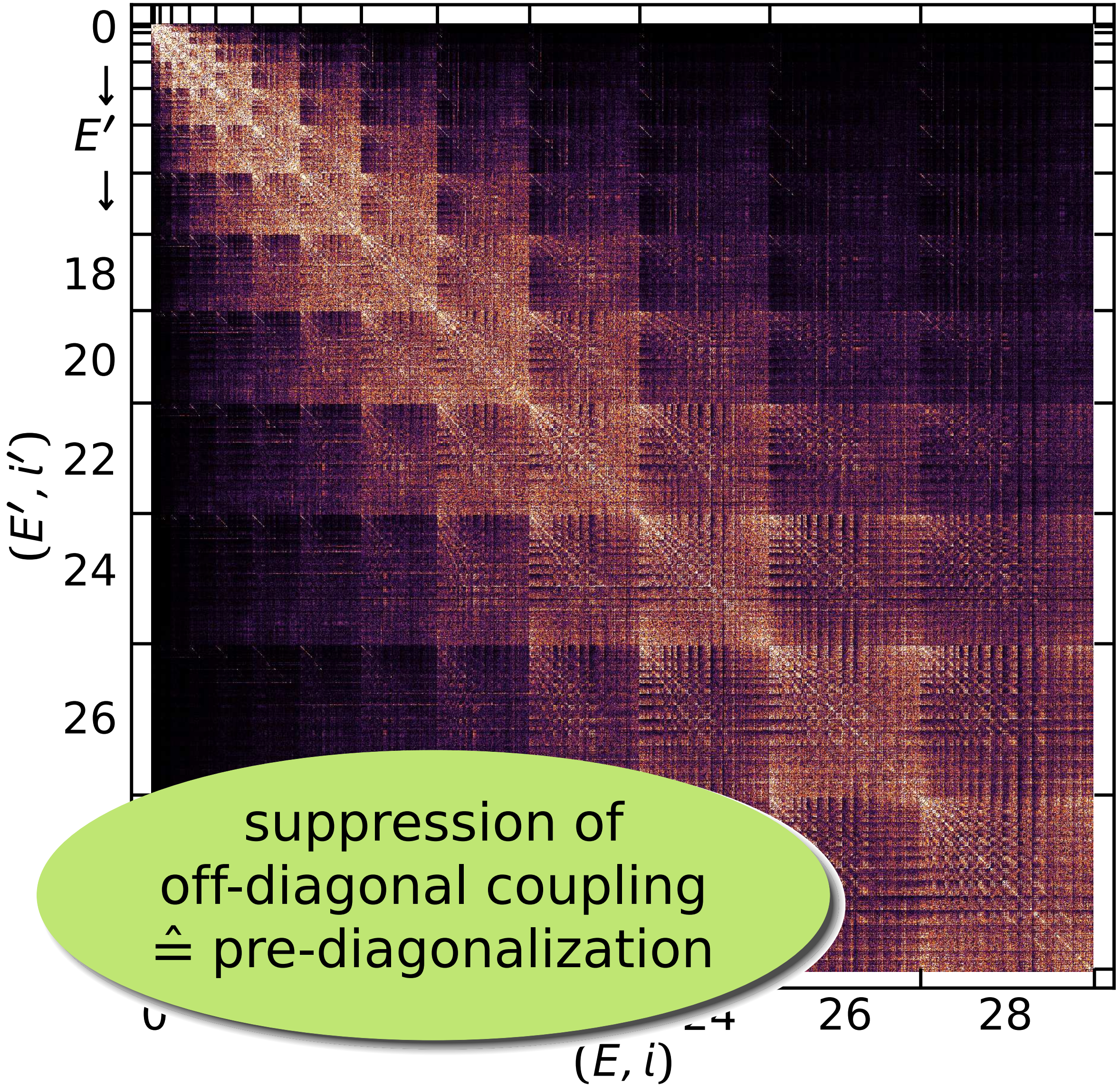
$\Lambda = \infty\,\text{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



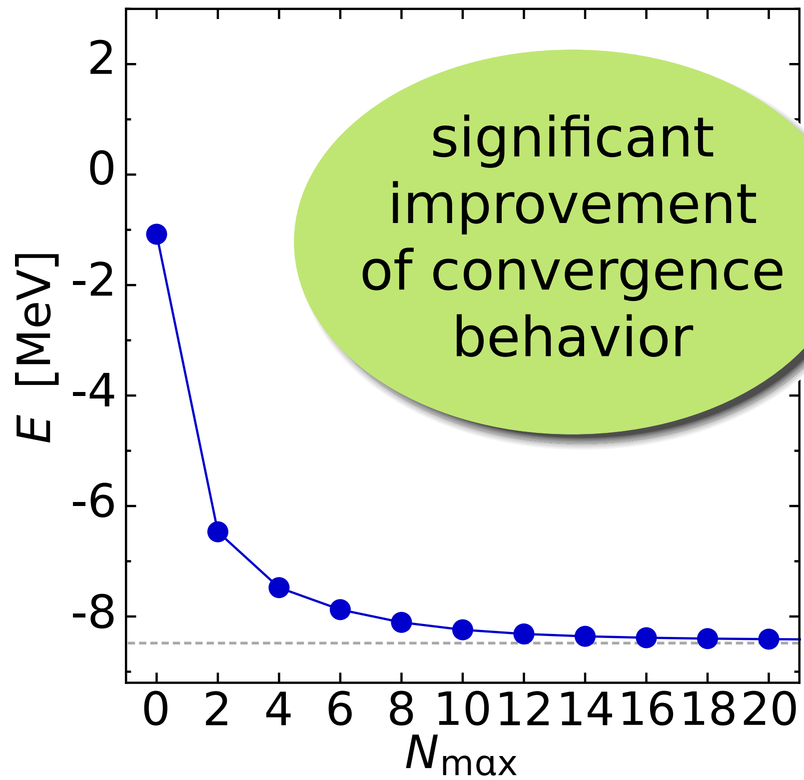
suppression of
off-diagonal coupling
≙ pre-diagonalization

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

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

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

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

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 Hamilt… …d keep two- and three-body terms
- **NN+3N-full**: start with NN+3… and three-body terms

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

Sounds easy, but...

❶ computation of initial 2B/3B-Jacobi HO matrix elements of chiral NN+3N interactions

- we use Petr Navratil's ManyEff code for computing 3B-Jacobi matrix elements and corresponding CFPs

❷ SRG evolution in 2B/3B space and cluster decomposition

- efficient implementation using adaptive ODE solver & BLAS; largest block takes a few hours on single node

❸ transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation

- formulated transformation directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\,max} = 16$ in JT-coupled scheme

❹ data management and on-the-fly decoupling in many-body codes

- invented optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\,max} = 16$ in memory

Importance Truncated NCSM

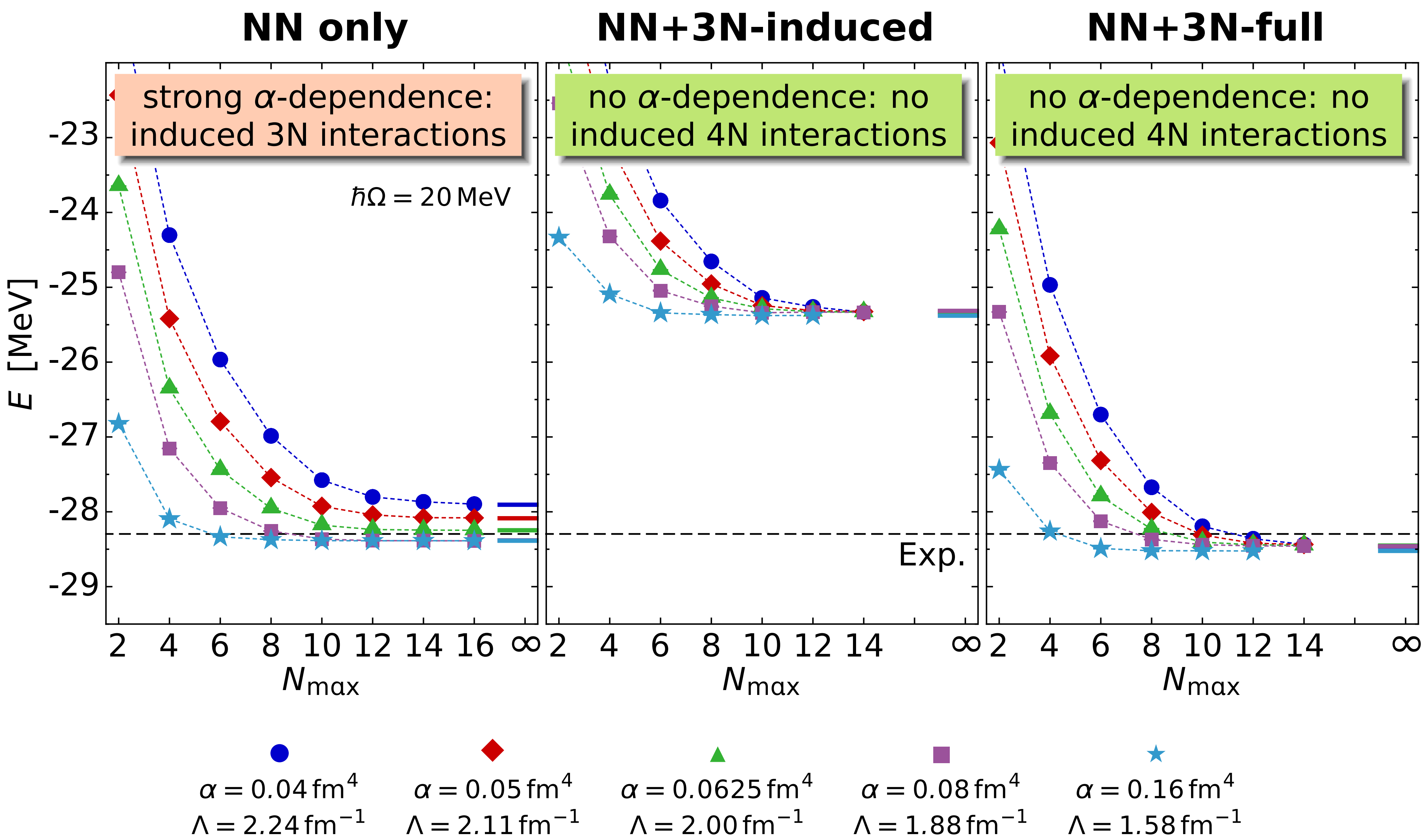
Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Importance Truncated NCSM

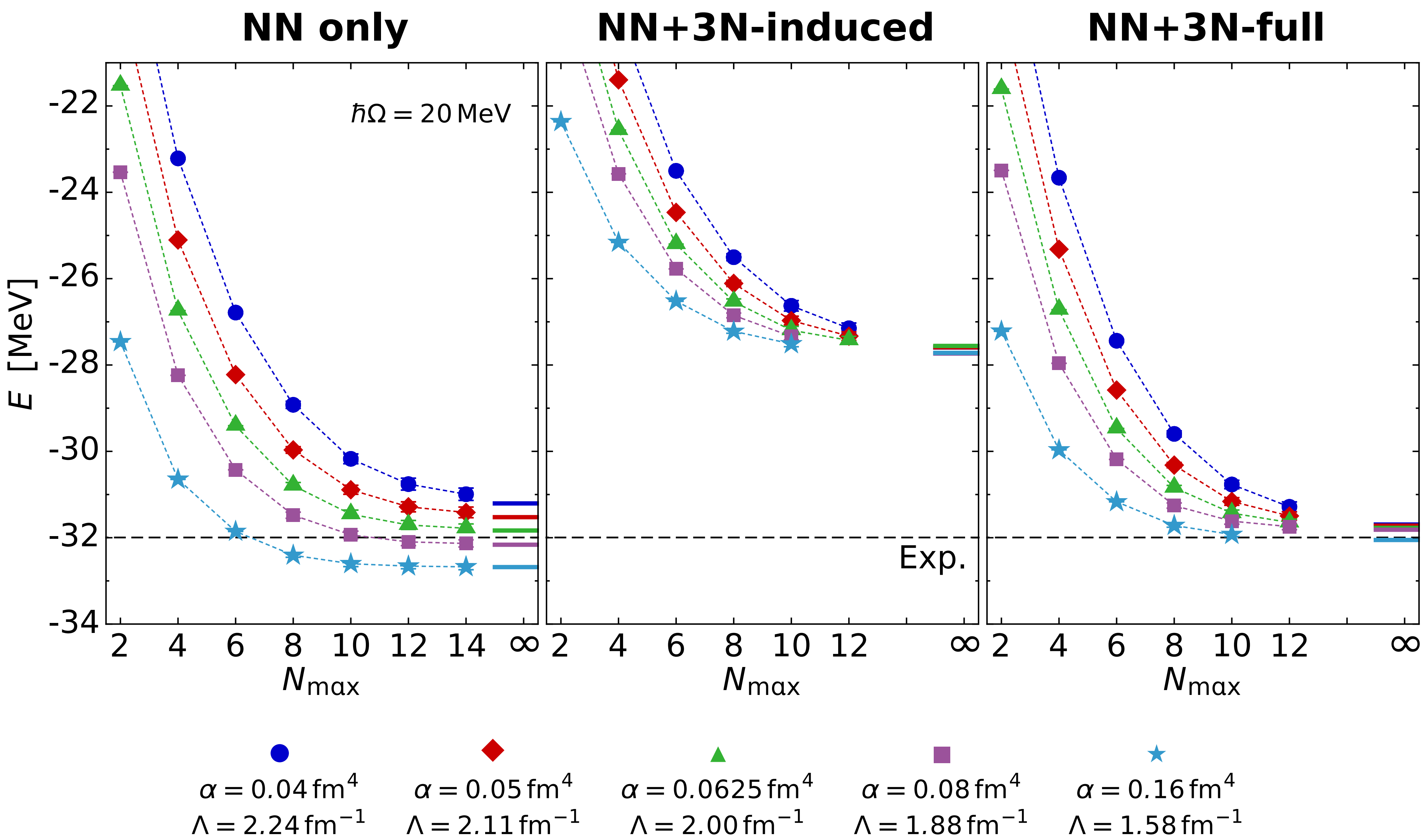
NCSM is one of the most powerful and universal exact ab-initio methods

- 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 $E_{3\max} = 16$

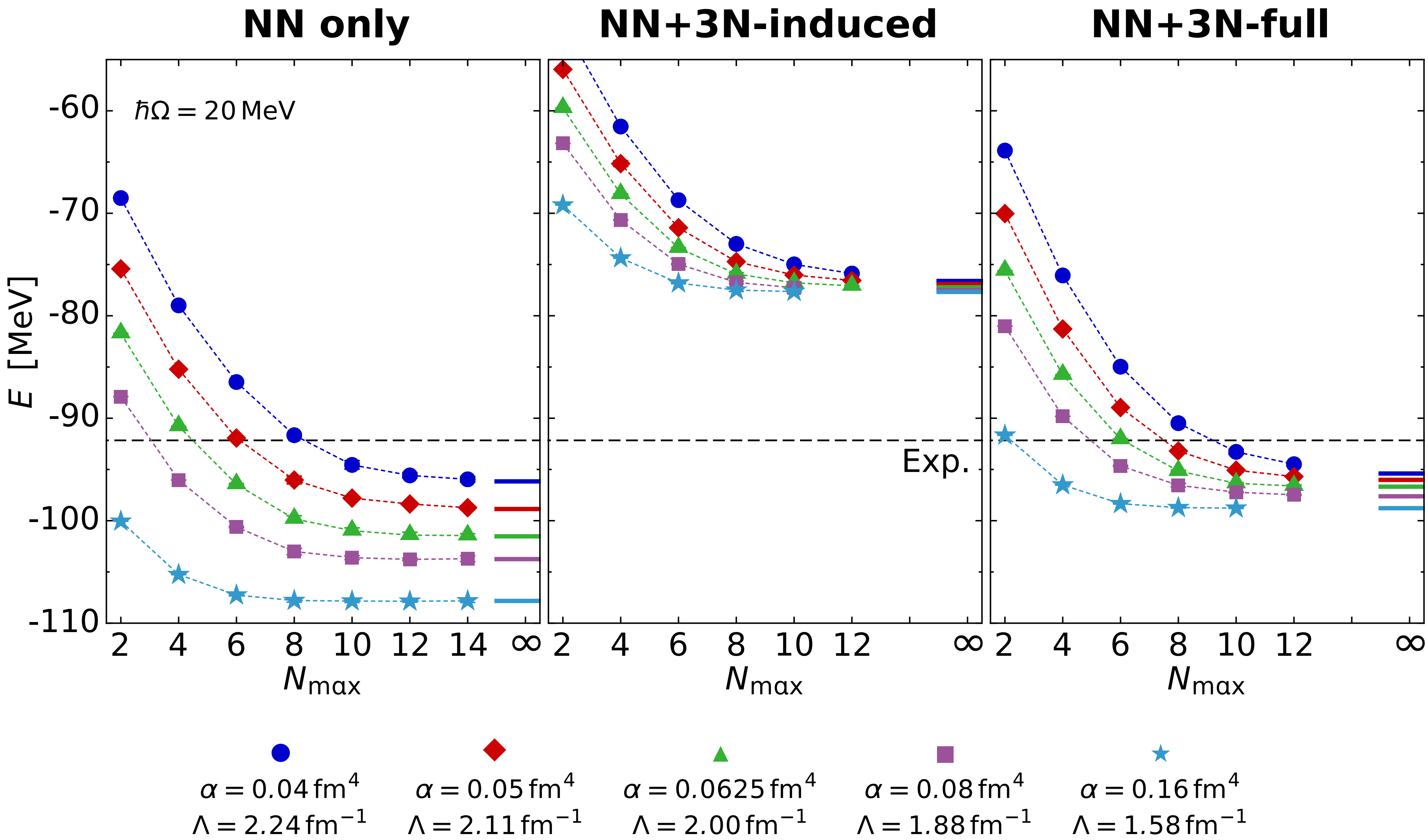
^{4}He: Ground-State Energies



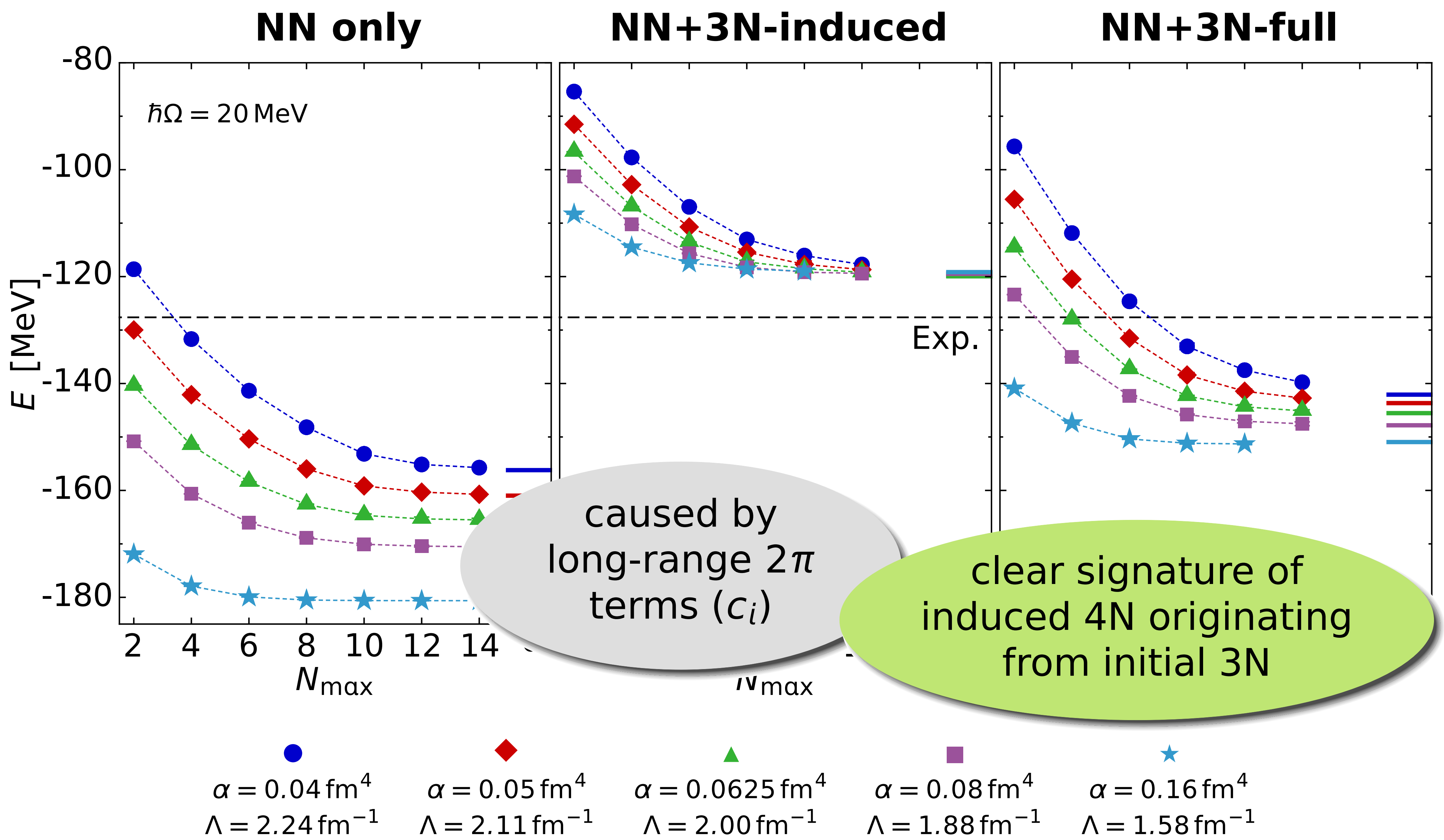
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies



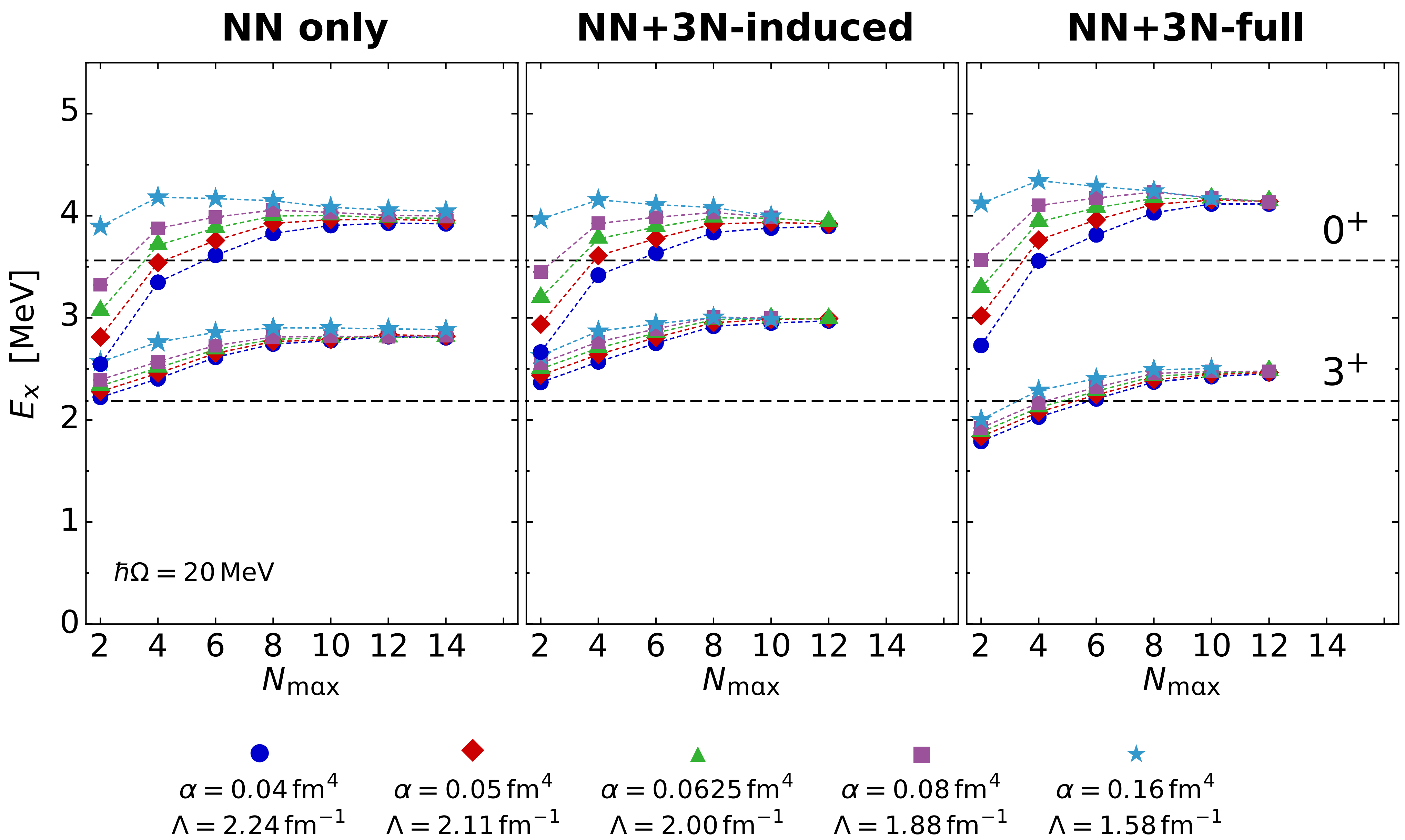
^{16}O: Ground-State Energies



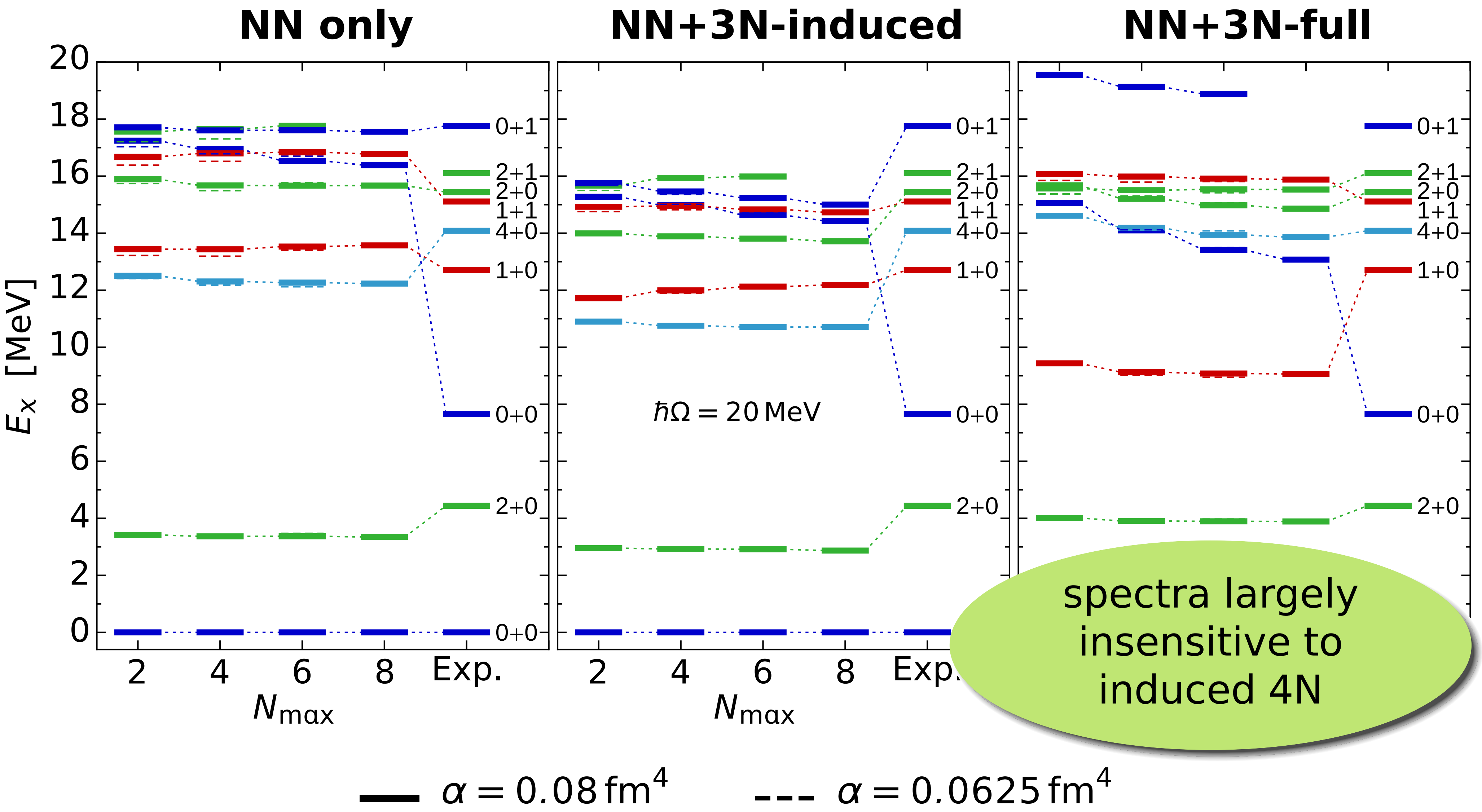
caused by long-range 2π terms (c_i)

clear signature of induced 4N originating from initial 3N

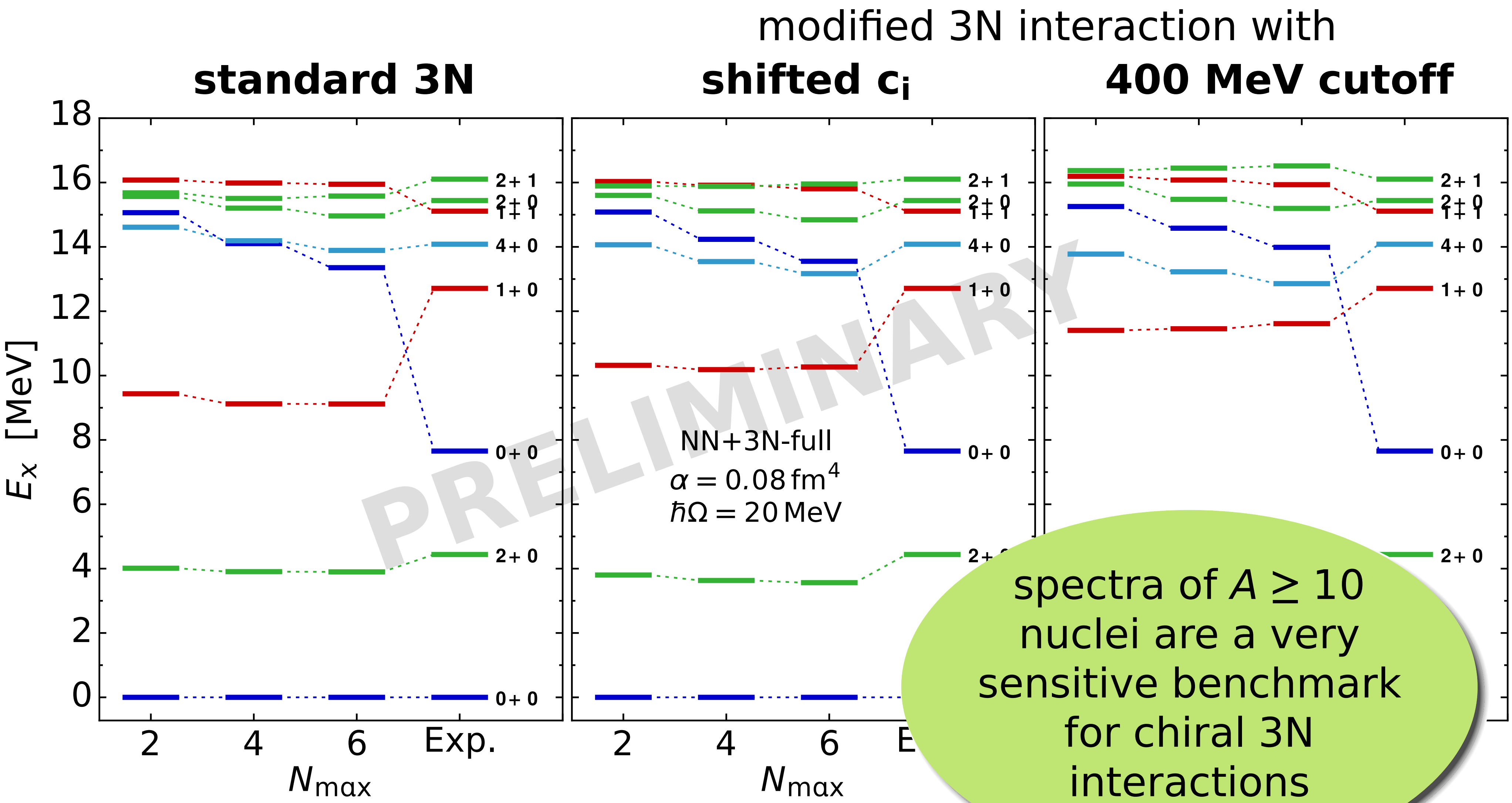
^{6}Li: Excitation Energies



Spectroscopy of ^{12}C

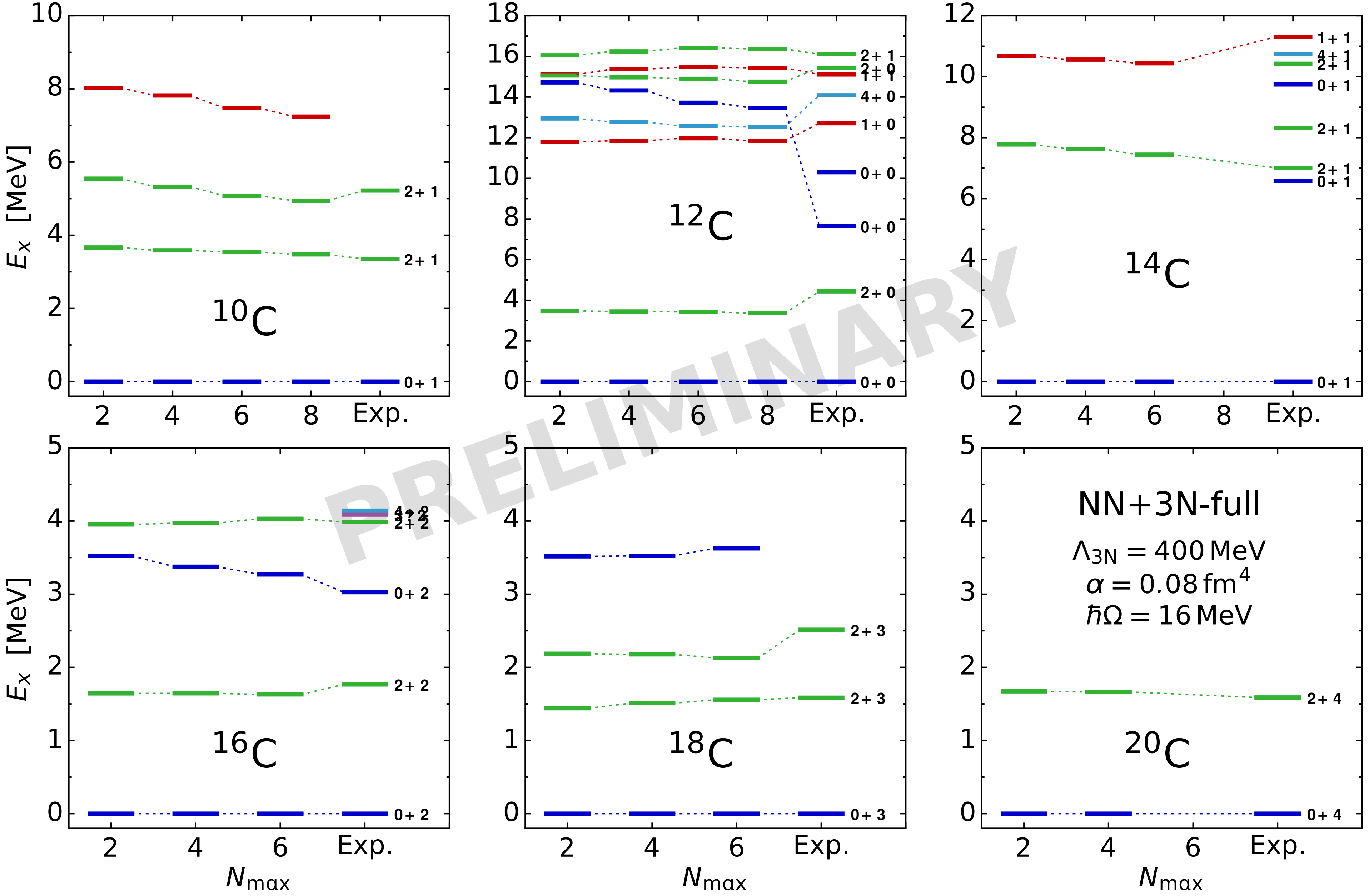


Outlook: Sensitivity on Initial 3N



spectra of $A \geq 10$ nuclei are a very sensitive benchmark for chiral 3N interactions

Outlook: Carbon Isotopic Chain



Normal-Ordered 3N Interaction & Coupled-Cluster Method

Roth, Binder, Vobig et al. — arXiv: 1112.0287 (2011)

Normal-Ordered 3N Interaction

avoid technical challenge of including explicit 3N interactions in many-body calculation

- **idea**: write 3N interaction in normal-ordered form with respect to an A-body reference Slater-determinant ($0\hbar\Omega$ state)

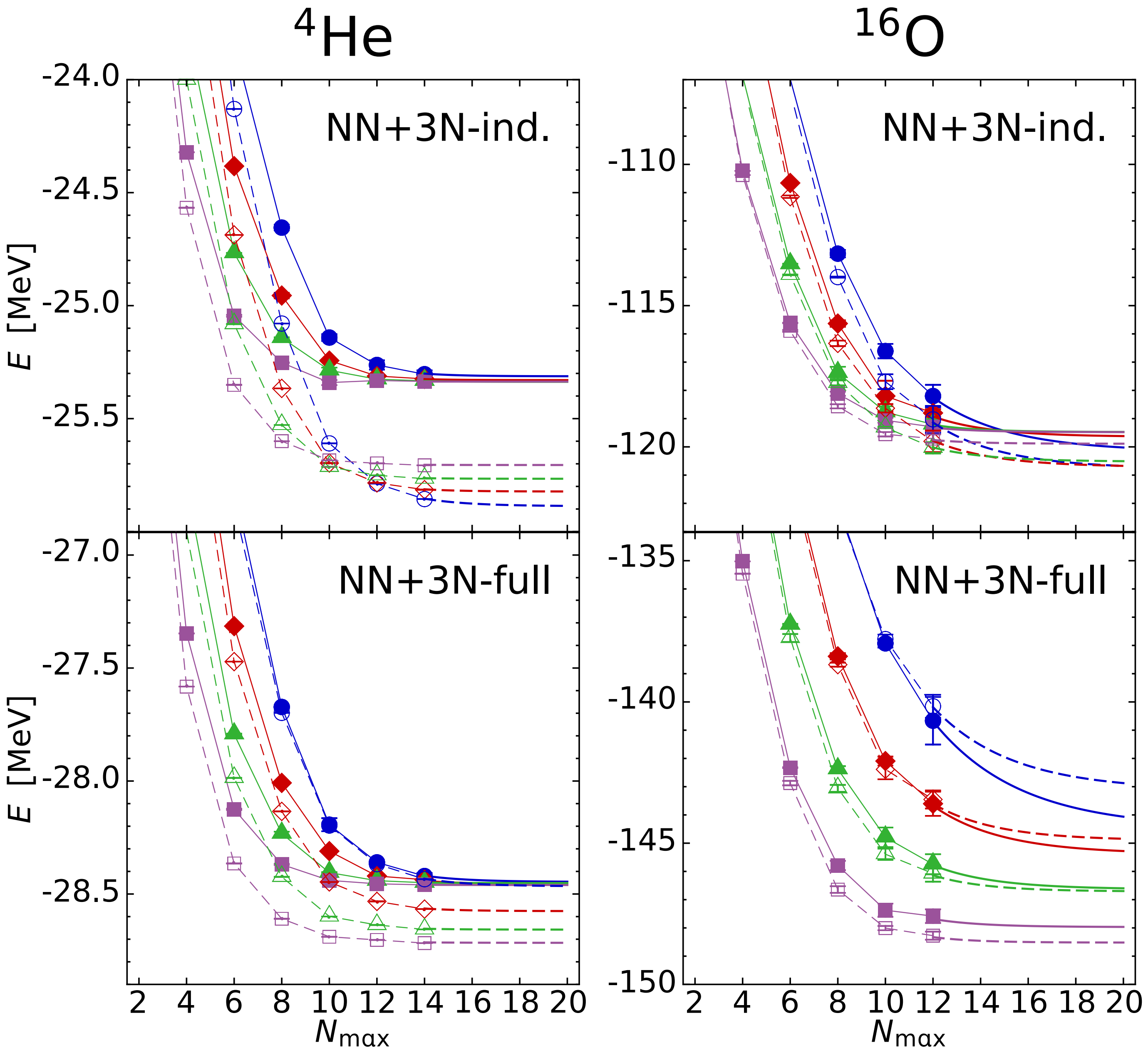
$$V_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ}\, a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ a_\circ$$

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

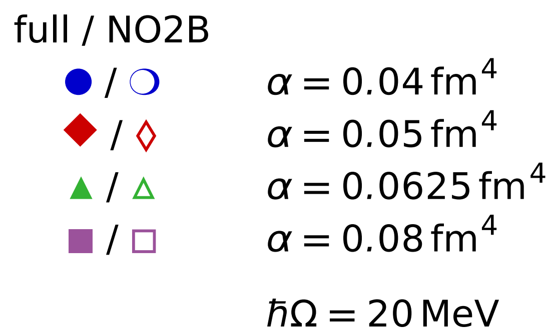
$$+ \sum W^{3B}_{\circ\circ\circ\circ\circ\circ}\, \{a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ\, a_\circ a_\circ a_\circ\}$$

- **question**: if we neglect the normal-ordered 3B term, how well does this approximation work ?

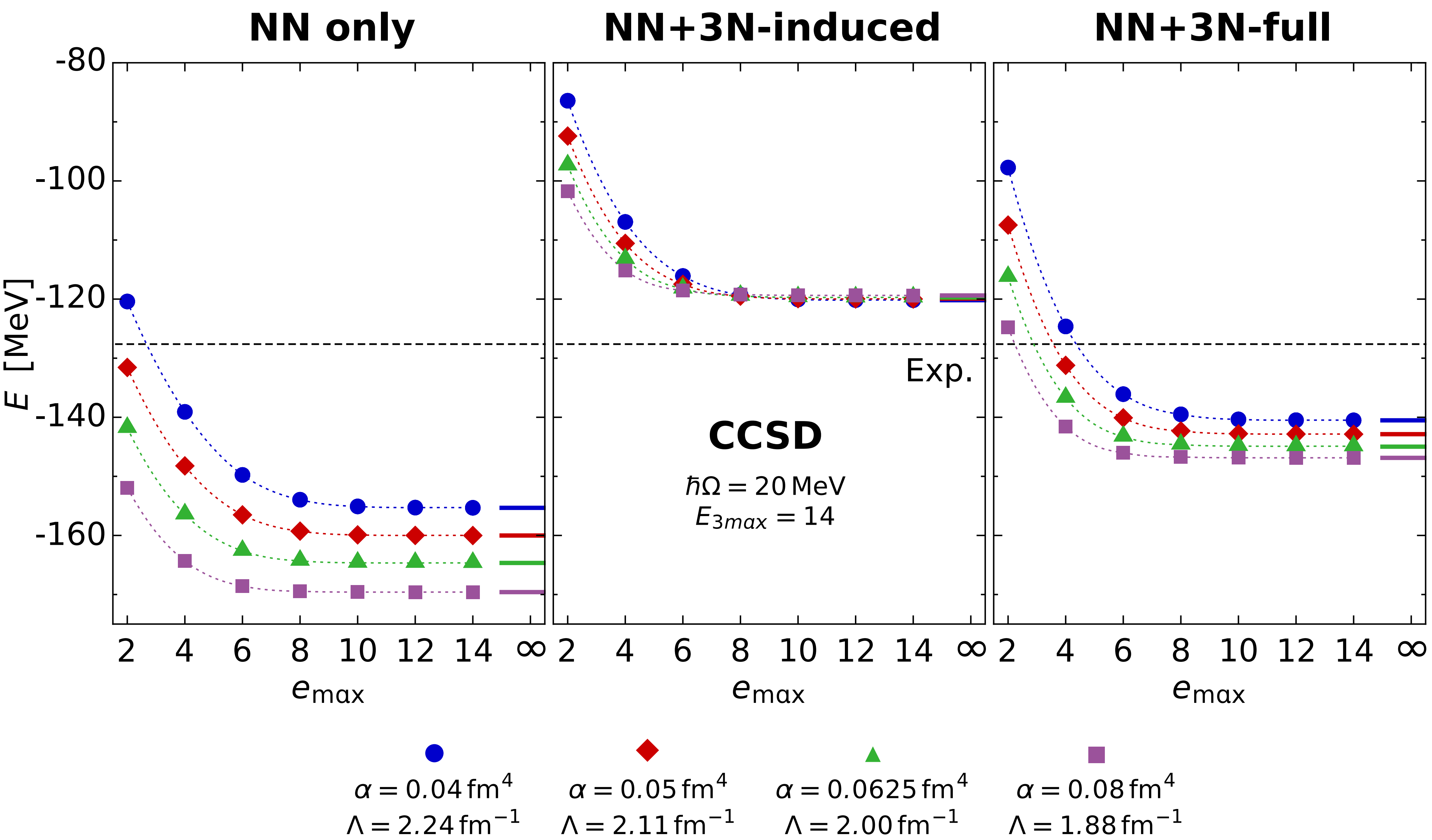
Benchmark of Normal-Ordered 3N



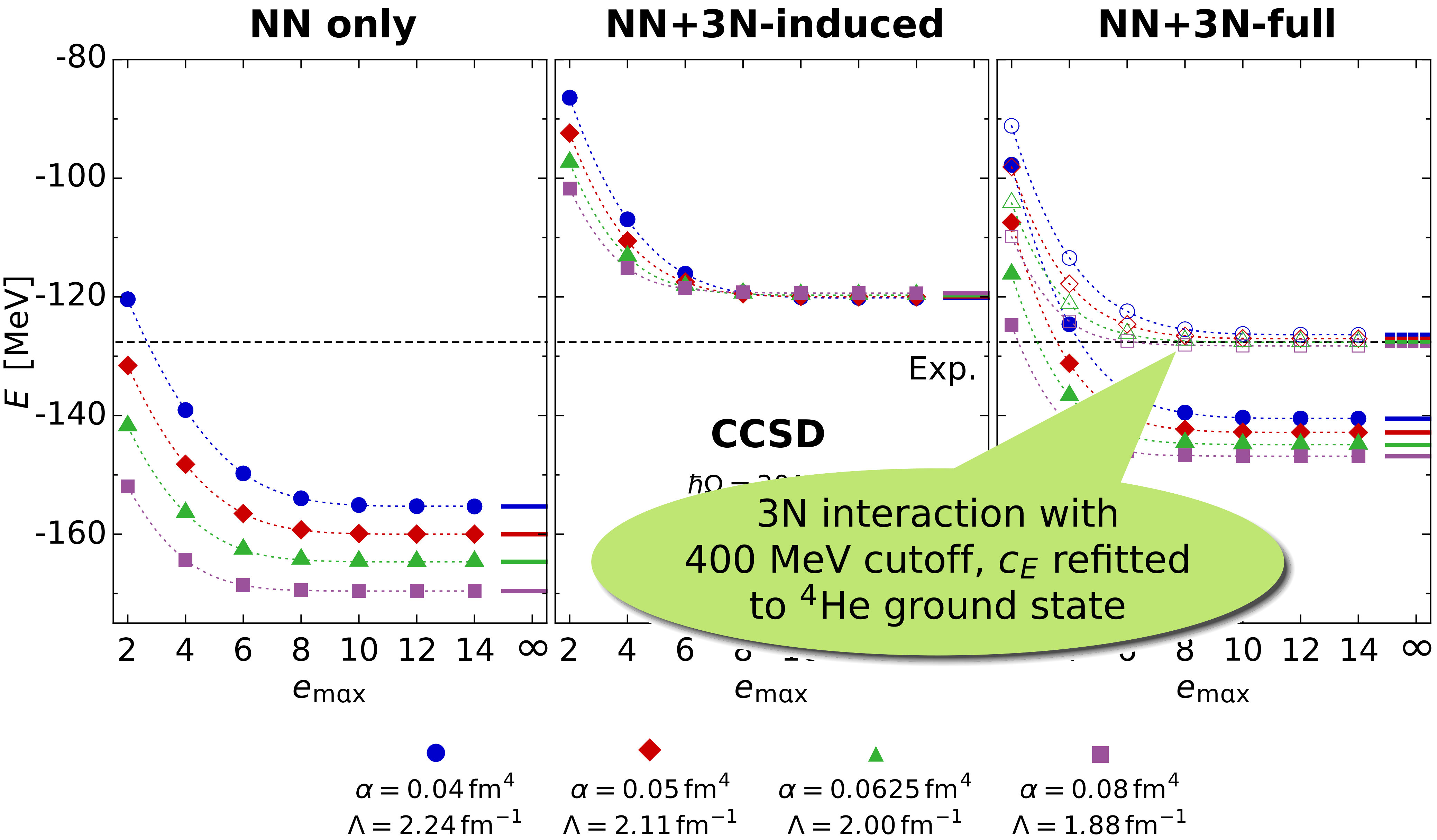
- compare IT-NCSM results with full 3N to normal-ord. 3N truncated at the 2B level
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O



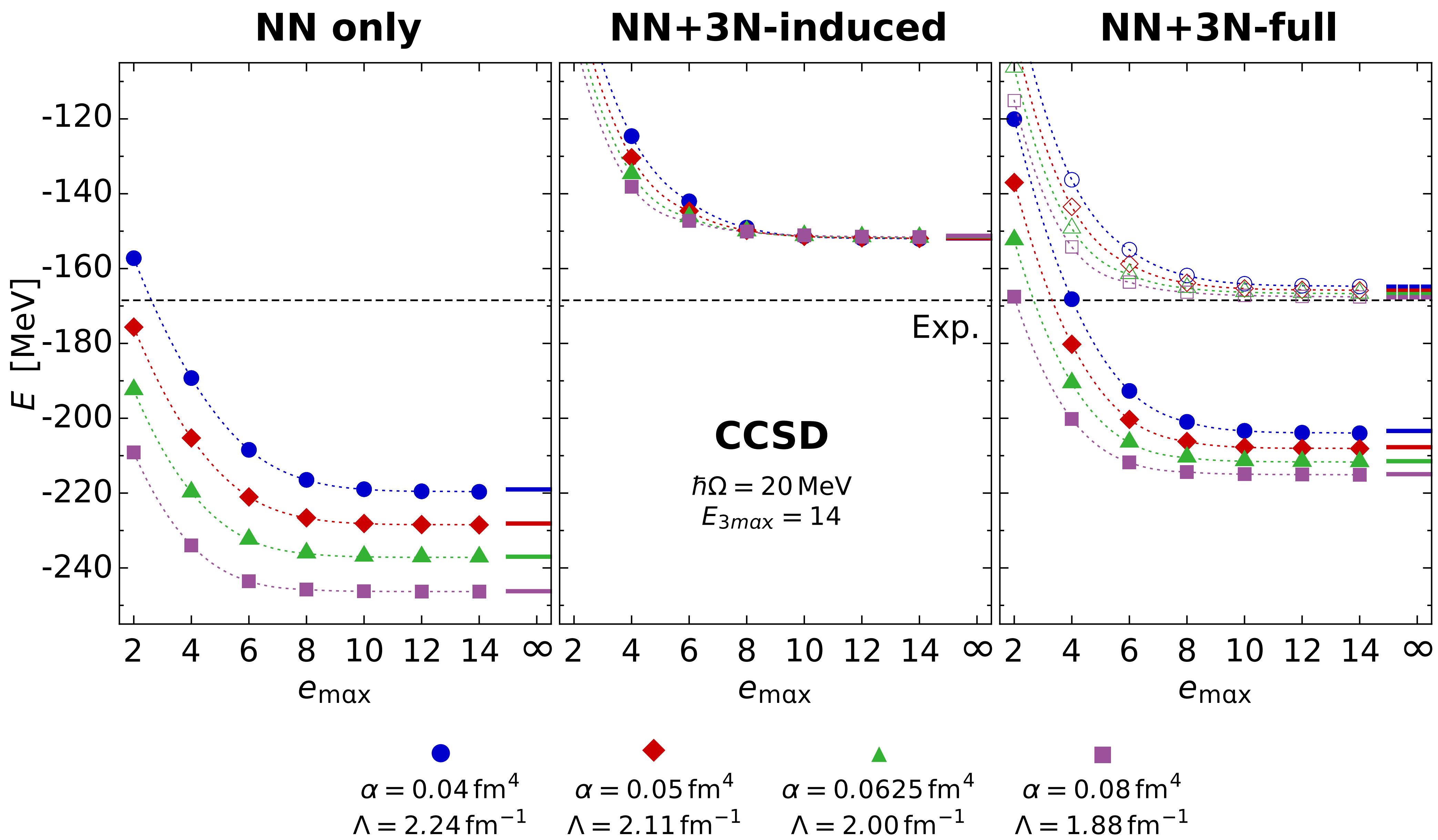
^{16}O: Coupled-Cluster with $3N_{NO2B}$



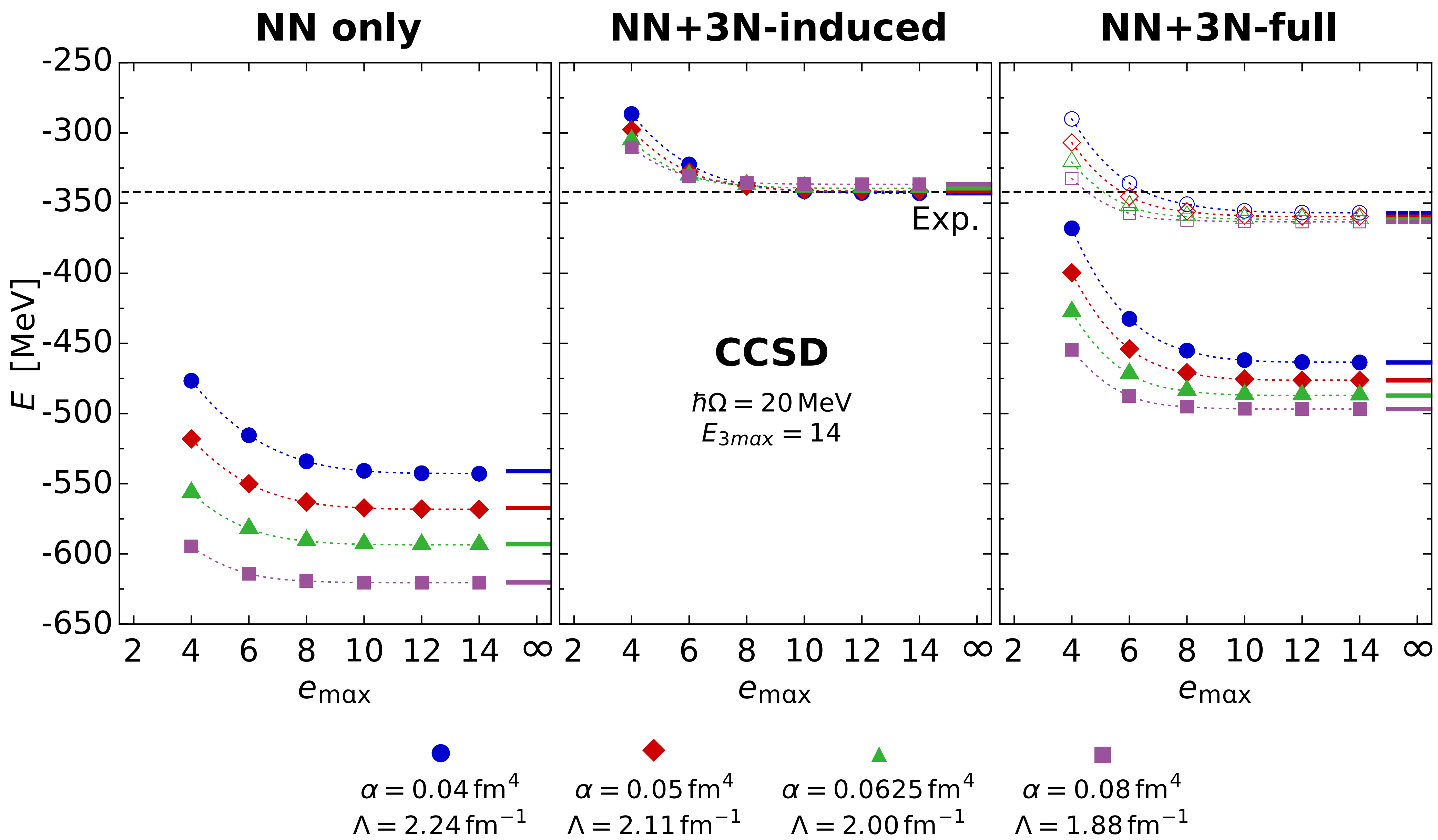
^{16}O: Coupled-Cluster with $3N_{NO2B}$



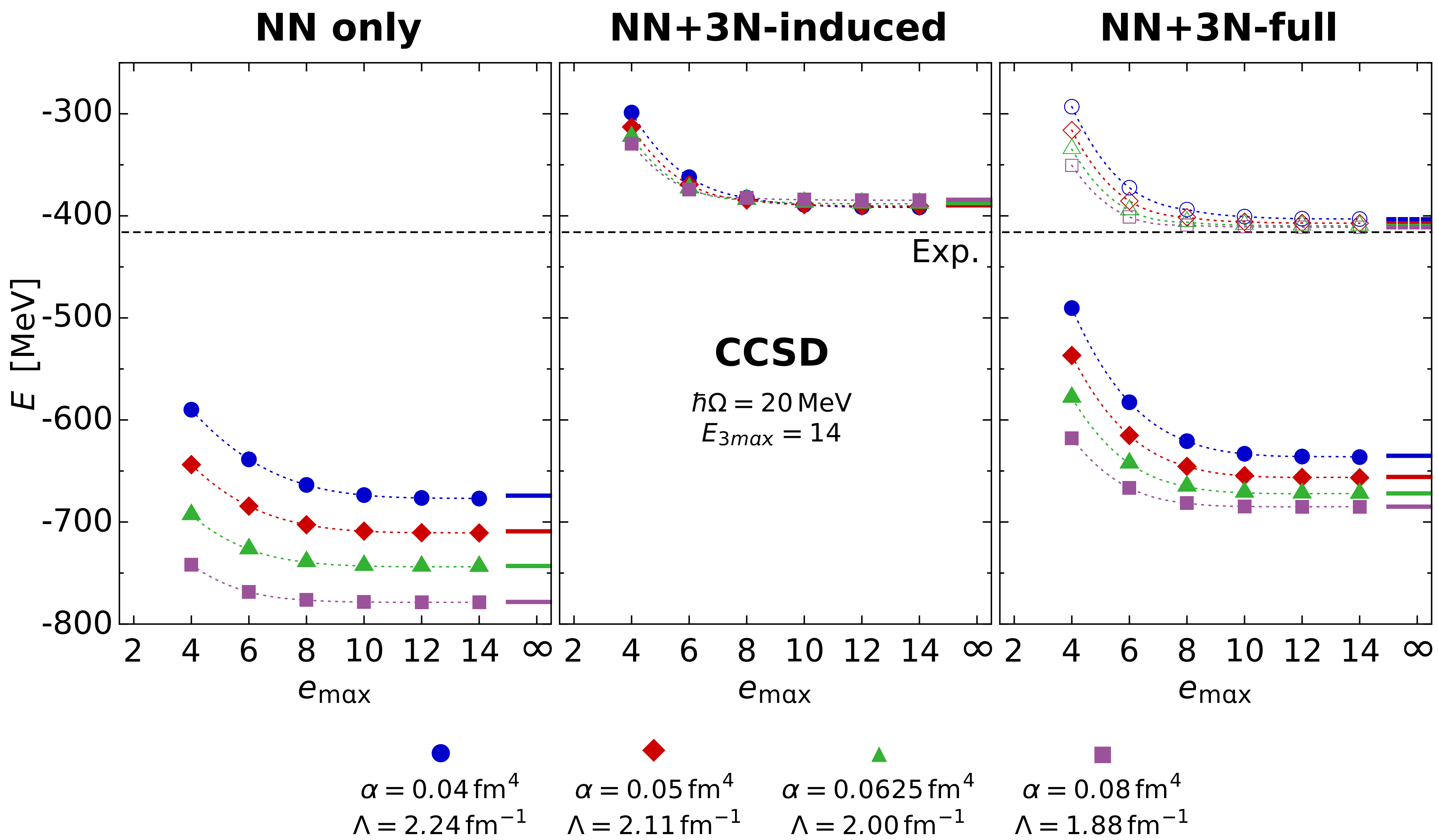
^{24}O: Coupled-Cluster with $3N_{NO2B}$



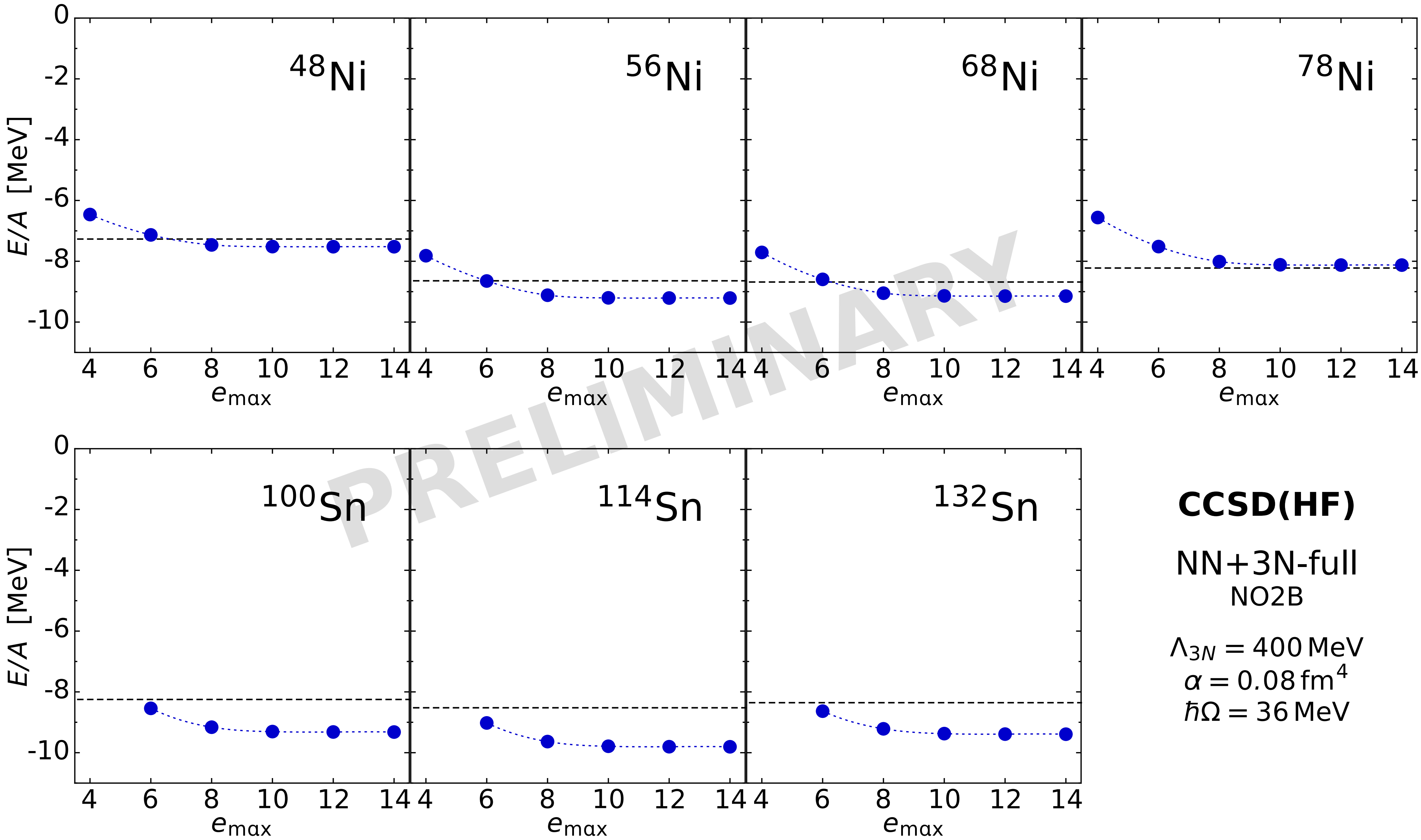
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



^{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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    IPN Orsay, F

COMPUTING TIME

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