Coupled-Cluster Calculations of Medium-Mass Nuclei

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

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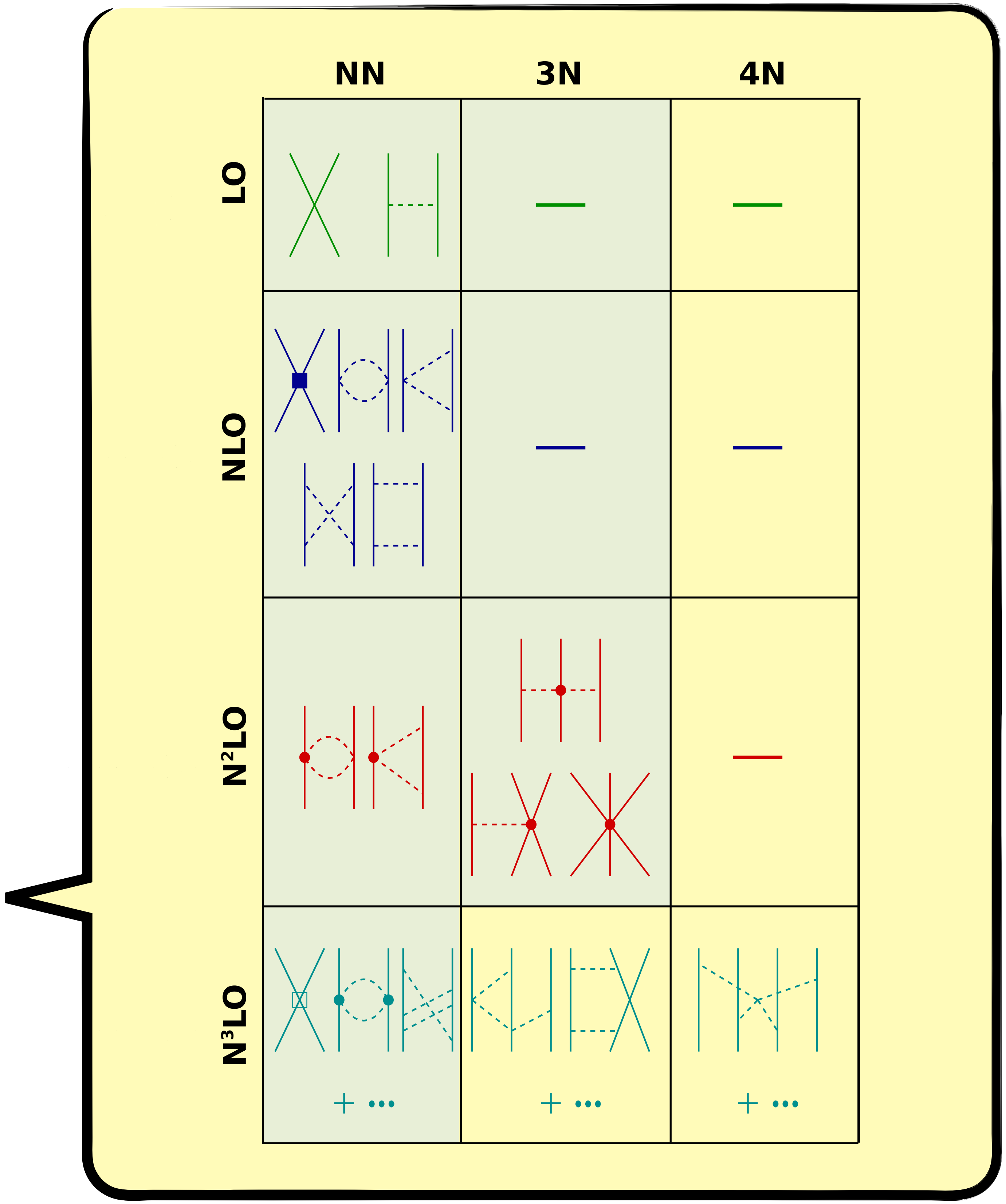
Nuclear Structure

NN+3N interaction
from Chiral EFT

Low-Energy QCD



From QCD to Nuclear Structure

Nuclear Structure

Unitary Transformed Hamiltonian

adapt Hamiltonian to truncated low-energy model spaces

NN+3N interaction from Chiral EFT

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

Exact & Approx. Many-Body Methods

Unitary Transformed Hamiltonian

NN+3N interaction from Chiral EFT

Low-Energy QCD

- ab initio solution of the manybody problem for light & medium-mass nuclei (NCSM, CC)
- controlled approximations for heavier nuclei (HF & MBPT)
- all rely on restricted model spaces & benefit from unitary transformations

Uncertainty Summary

Similarity Renormalization Group

E. Jurgenson et al. --- Phys. Rev. Lett. 103, 082501 (2009)

R. Roth et al. --- Phys. Rev. Lett. 107, 072501 (2011)

Similarity Renormalization Group

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

- **unitary transformation** of Hamiltonian (and other observables)

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

- **evolution equations** for $\tilde{H}_\alpha$ and U_α depending on generator η_α

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\tilde{H}_\alpha = \left[\eta_\alpha, \tilde{H}_\alpha\right] \qquad \frac{\mathrm{d}}{\mathrm{d}\alpha}U_\alpha = -U_\alpha \; \eta_\alpha$$

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

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

Calculations in A-Body Space

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

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

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

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

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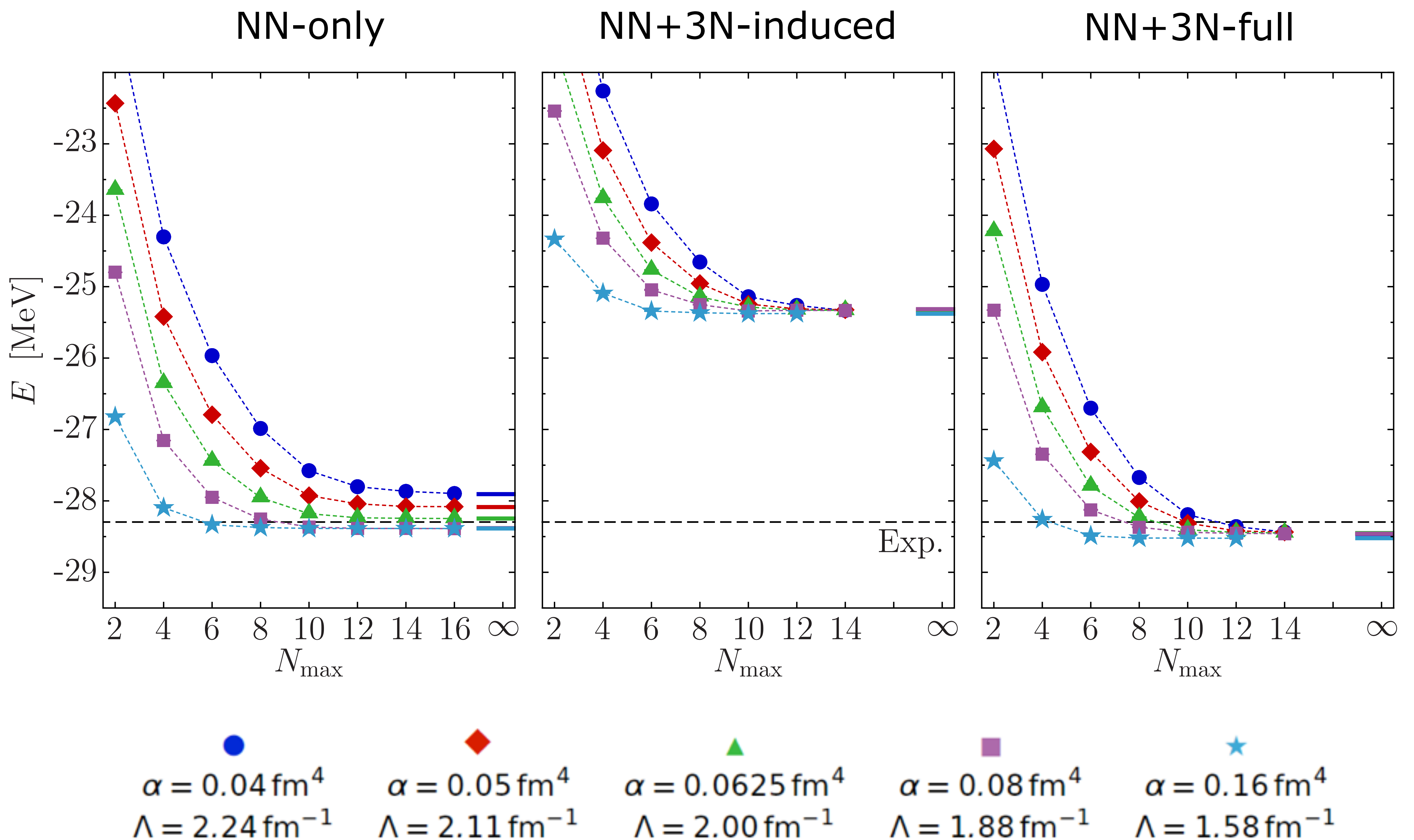
^{4}He: IT-NCSM Ground-State Energies



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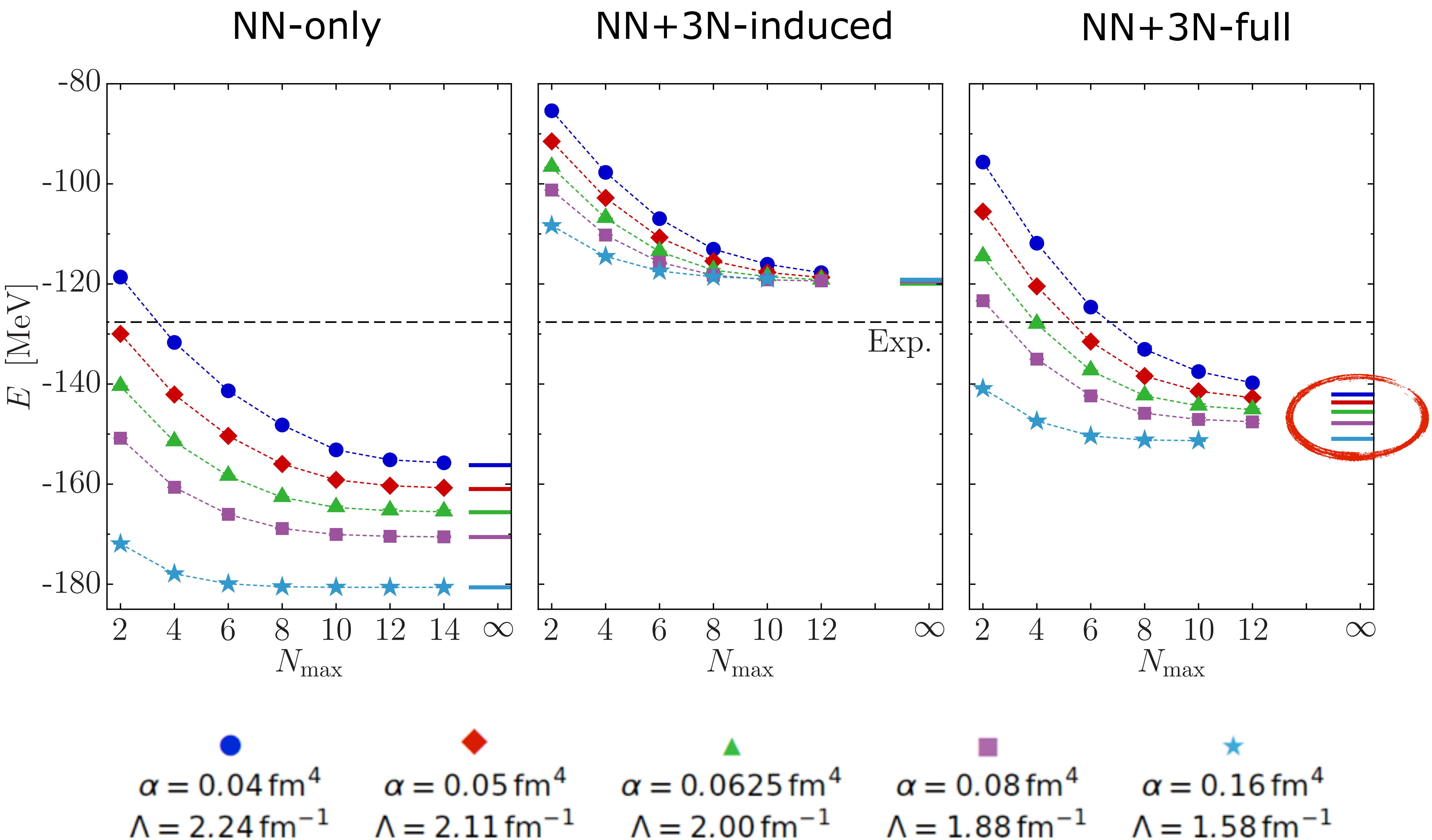

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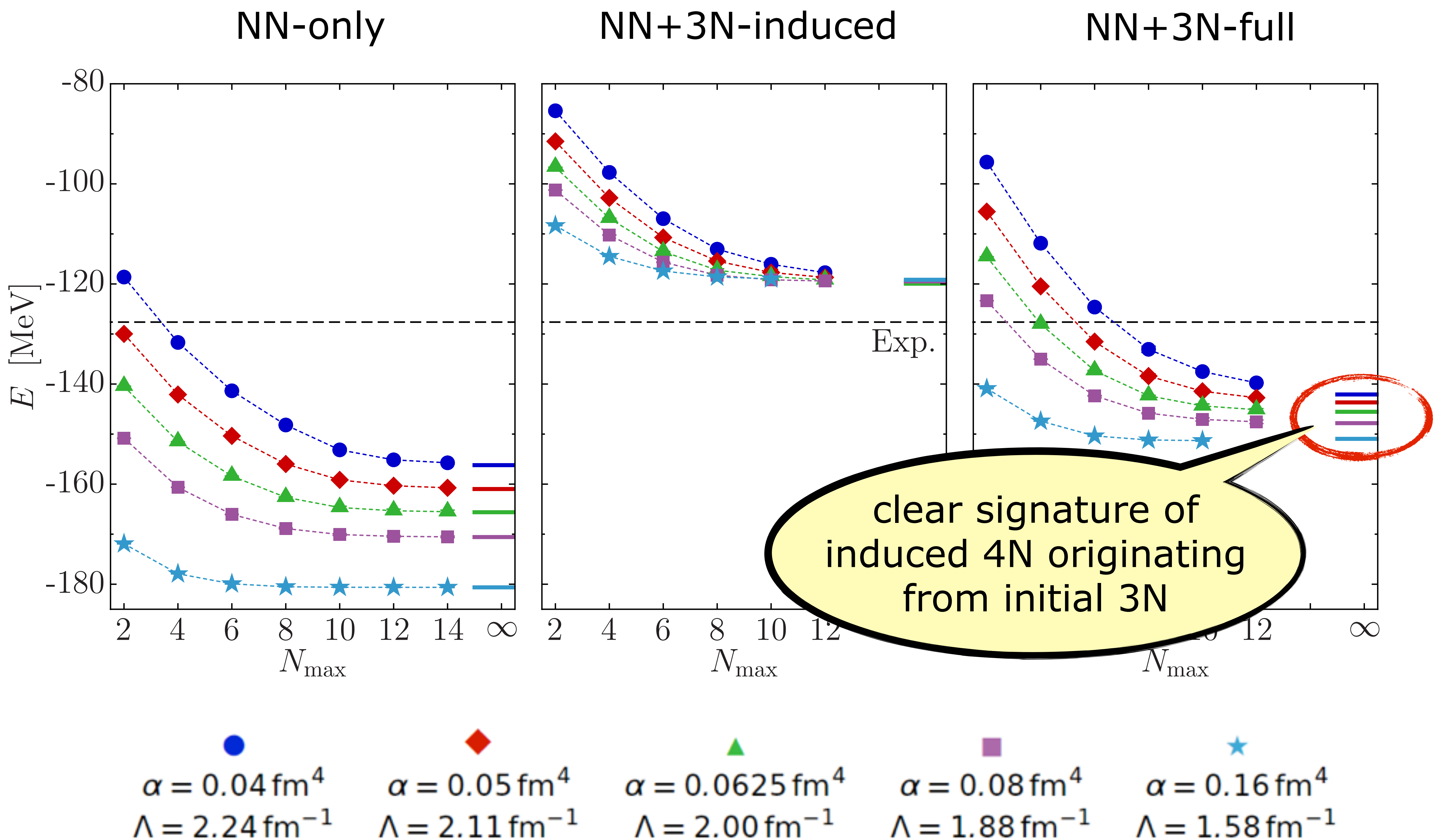

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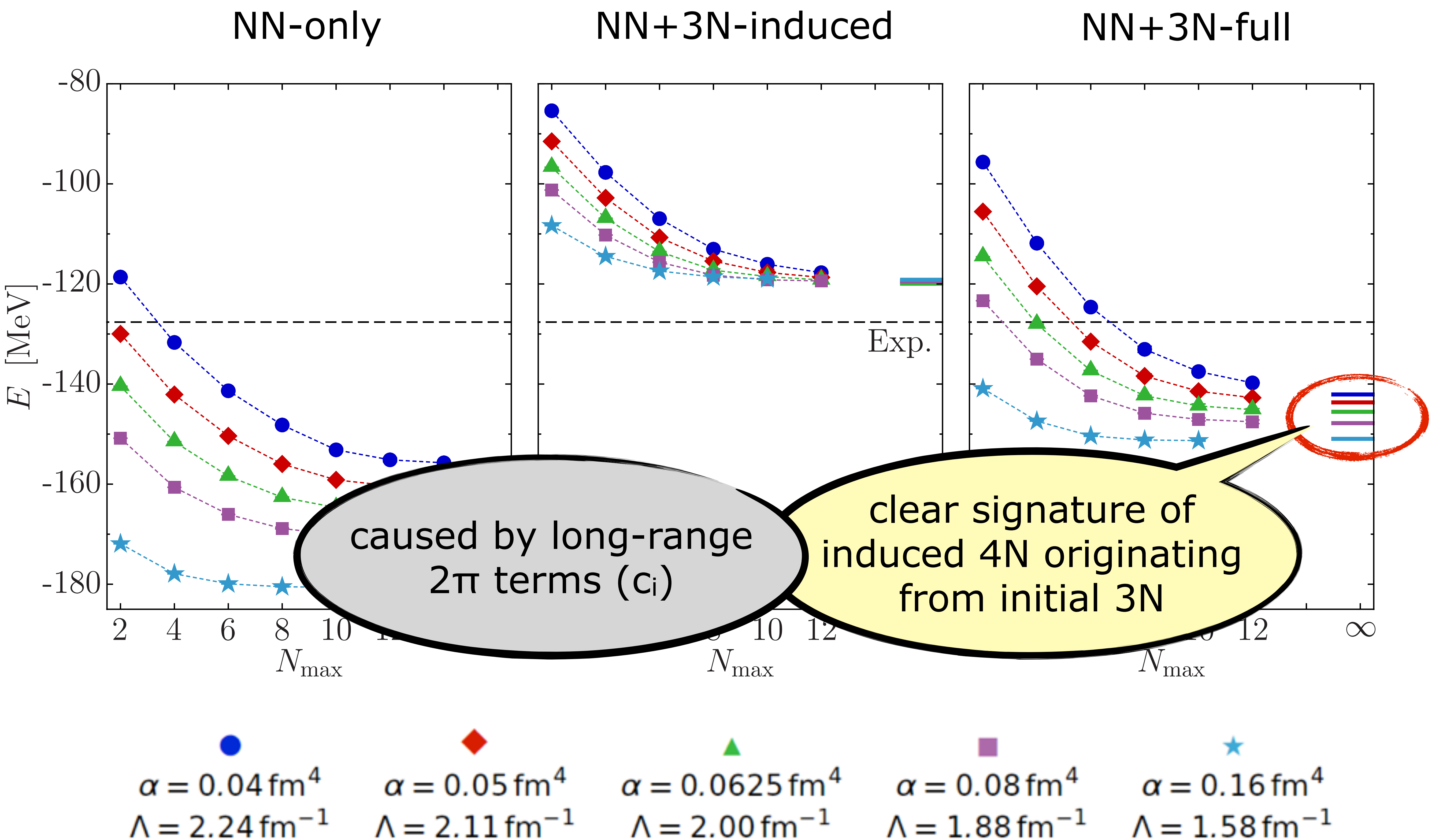

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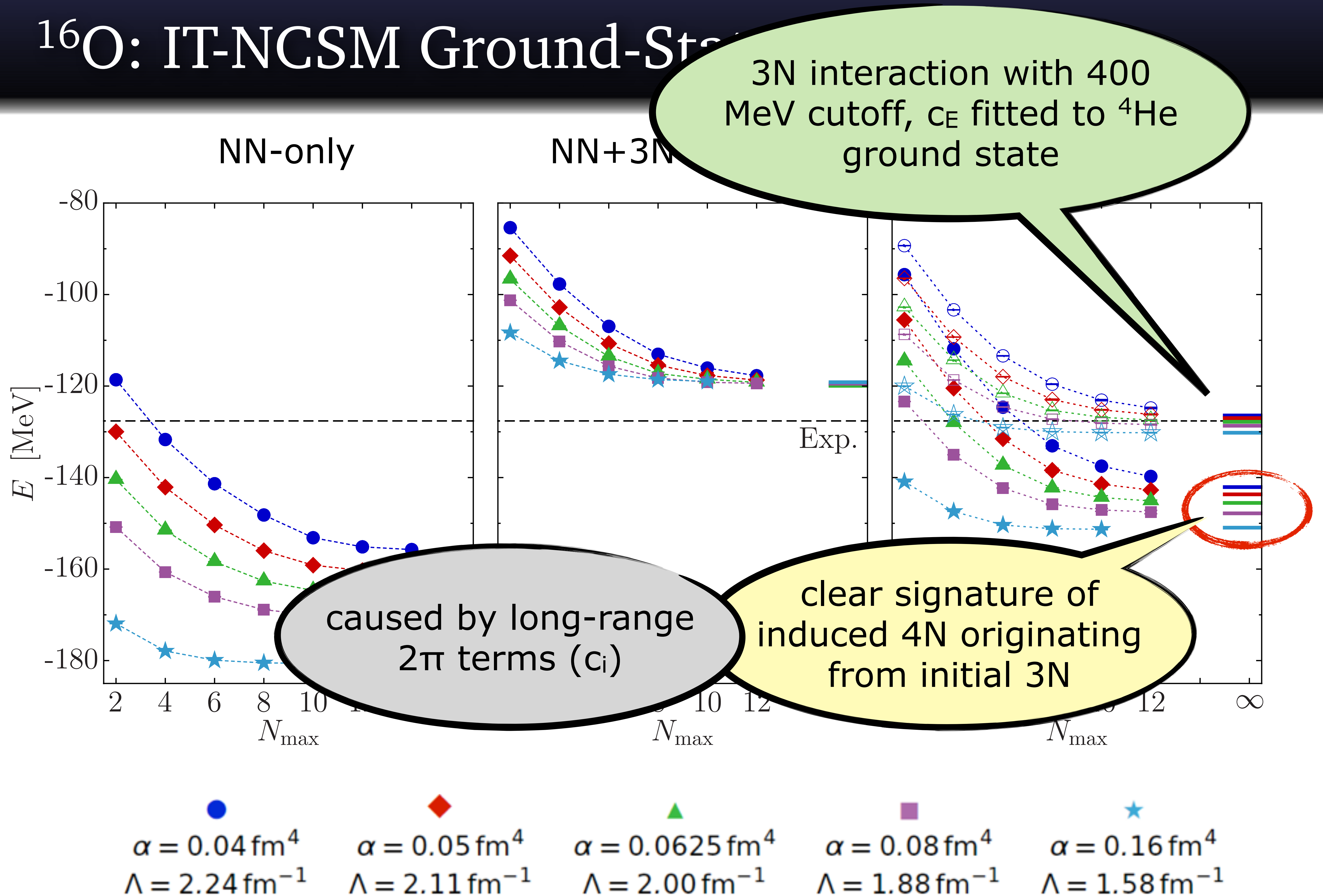

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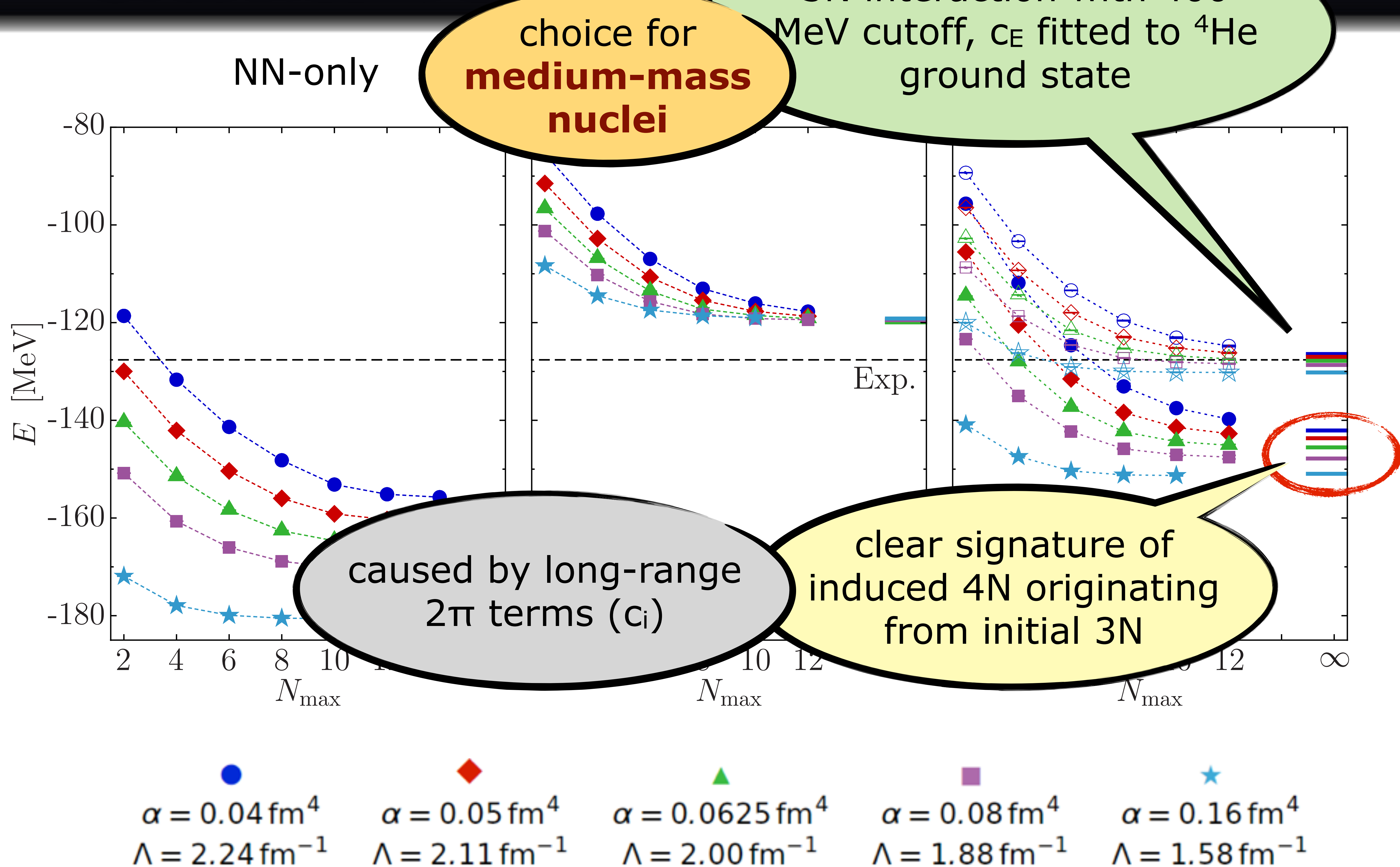

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- **Similarity Renormalization Group**
  - ☑ α-dependence: low-cutoff 3N interaction

Normal-Ordering Two-Body Approximation

G. Hagen, T. Papenbrock, D.J. Dean et al. --- Phys. Rev. C 76, 034302 (2007)

R. Roth, S. Binder, K. Vobig et al. --- Phys. Rev. Lett. 109, 052501(R) (2012)

S. Binder, J. Langhammer, A. Calci et al. --- Phys. Rev. C 82, 021303 (2013)

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)

$$\hat{V}_{3\mathrm{N}} = \sum V^{3\mathrm{N}}_{\circ\circ\circ\circ\circ\circ} \, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$
$$= W^{0\mathrm{B}} + \sum W^{1\mathrm{B}}_{\circ\circ} \, \hat{a}^\dagger_\circ \hat{a}_\circ + \sum W^{2\mathrm{B}}_{\circ\circ\circ\circ} \, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ$$
$$+ \sum W^{3\mathrm{B}}_{\circ\circ\circ\circ\circ\circ} \, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

- **Normal-Ordering Two-Body Approximation (NO2B)**: discard residual normal-ordered 3B part $W^{3\mathrm{B}}$

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$$
\begin{aligned}
\hat{V}_{3\mathrm{N}} &= \sum V^{3\mathrm{N}}_{\circ\circ\circ\circ\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ \\
&= W^{0\mathrm{B}} + \sum W^{1\mathrm{B}}_{\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}_\circ + \sum W^{2\mathrm{B}}_{\circ\circ\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \\
&\quad + \sum W^{3\mathrm{B}}_{\circ\circ\circ\circ\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ
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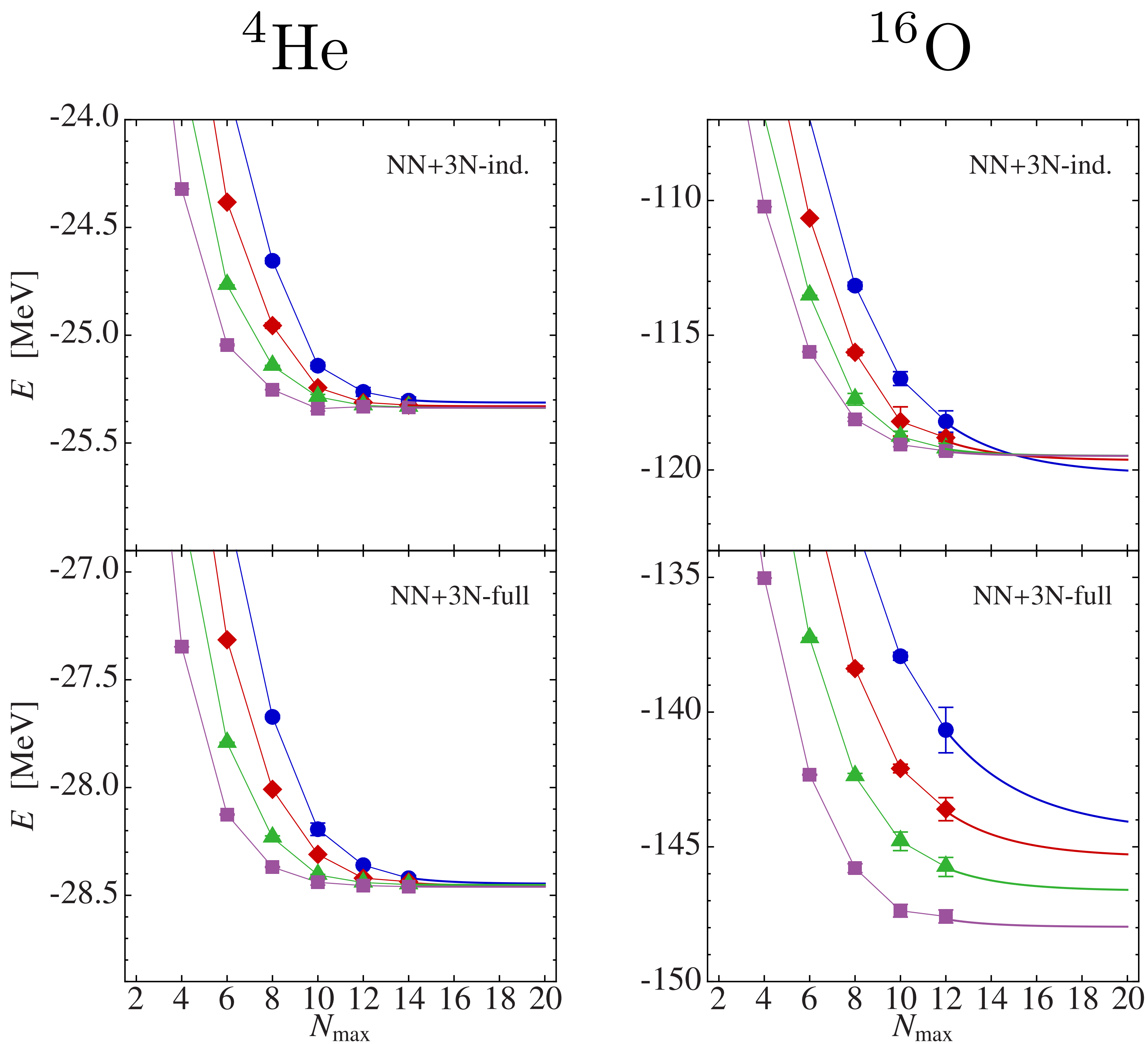
Benchmark of Normal-Ordered 3N



- compare IT-NCSM results with explicit 3N to normal-ordered 3N truncated at the 2B level (NO2B)
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O

● / ○ $\alpha = 0.04\ \mathrm{fm}^4$
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▲ / △ $\alpha = 0.0625\ \mathrm{fm}^4$
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$\hbar\Omega = 20\ \mathrm{MeV}$

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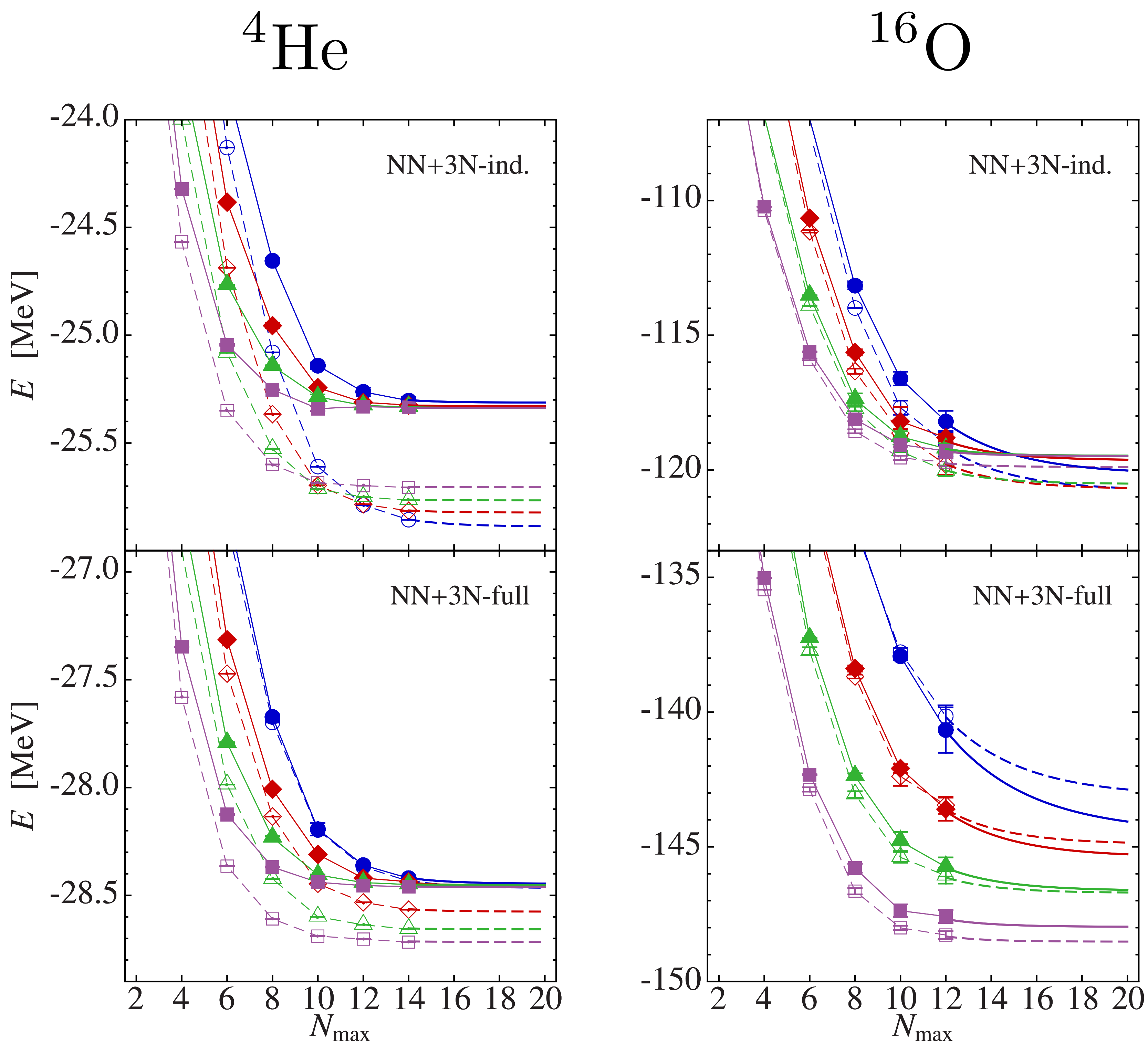

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- **Normal-Ordering 2B Approximation**
  - ☑ error in light nuclei: 1-2%

Coupled Cluster Method

G. Hagen, T. Papenbrock, D.J. Dean, M. Hjorth-Jensen --- Phys. Rev. C 82, 034330 (2010)

G. Hagen, T. Papenbrock, D.J. Dean et al. --- Phys. Rev. C 76, 034302 (2007)

Coupled Cluster Approach

- **exponential Ansatz** for wave operator

$$|\Psi\rangle = \hat{\Omega}|\Phi_0\rangle = e^{\hat{T}_1+\hat{T}_2+\cdots+\hat{T}_A}|\Phi_0\rangle$$

- $\hat{T}_n$: ***npnh* excitation** (cluster) operators

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk\ldots \\ abc\ldots}} t^{abc\ldots}_{ijk\ldots} \{\hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}^\dagger_c \ldots \hat{a}_k \hat{a}_j \hat{a}_i\}$$

- **similarity-transformed** Schroedinger equation

$$\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle \ , \quad \hat{\mathcal{H}} = e^{-\hat{T}} \ \hat{H}_N \ e^{\hat{T}}$$

- $\hat{\mathcal{H}}$: non-Hermitian **effective Hamiltonian**

CCSD

- **CCSD**: truncate $\hat{T}$ at the **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

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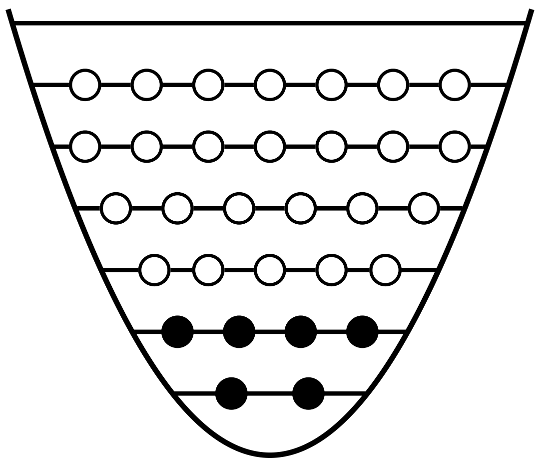

$|\Phi_0\rangle$

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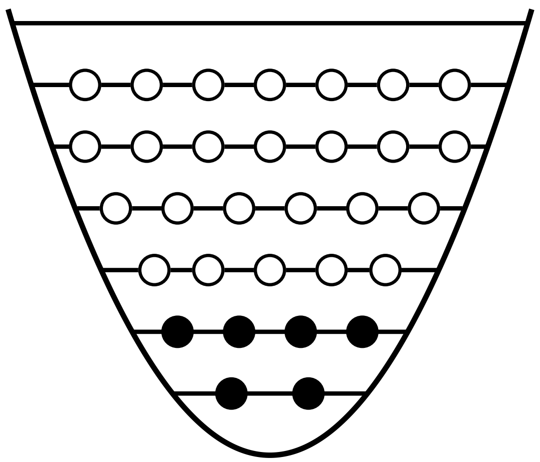

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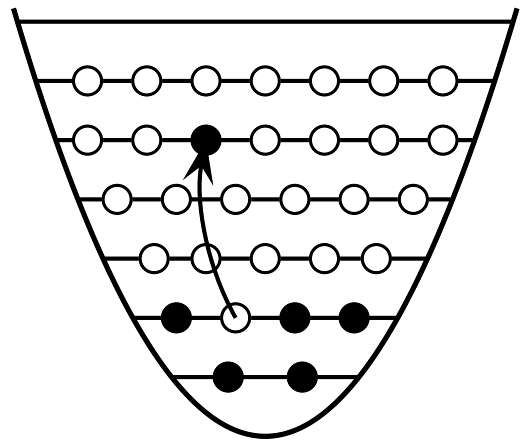

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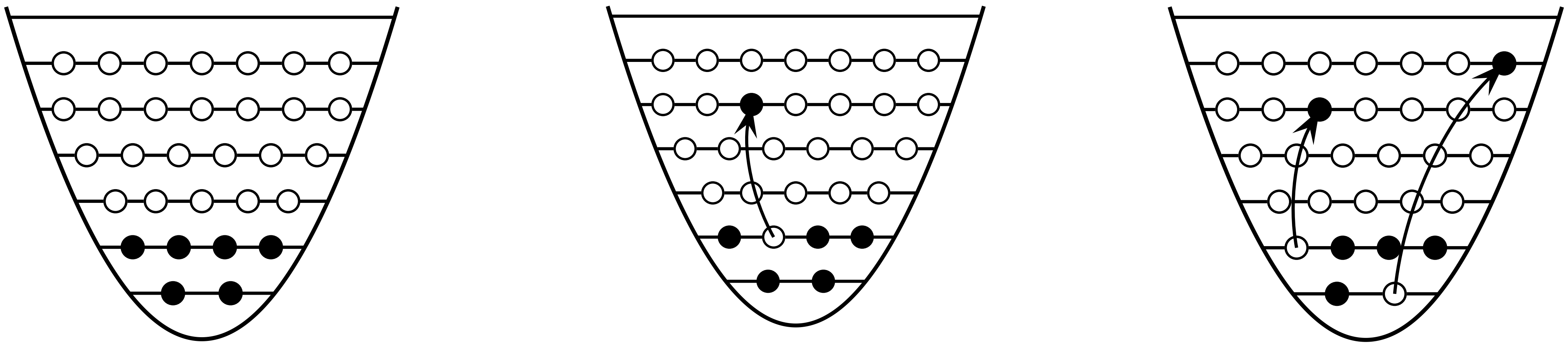

$|\Phi_0\rangle$ $\quad$ $\hat{T}_1 \, |\Phi_0\rangle$ $\quad$ $\hat{T}_2 \, |\Phi_0\rangle$

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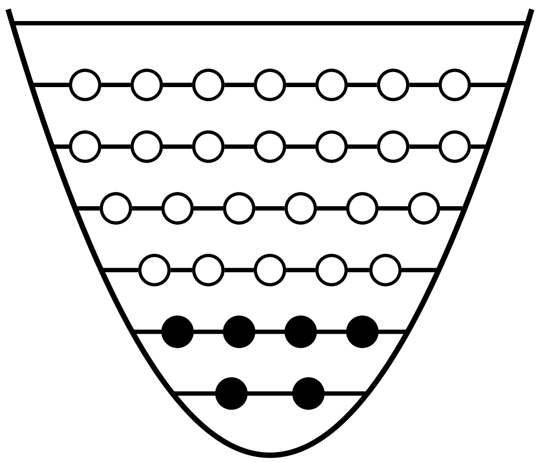

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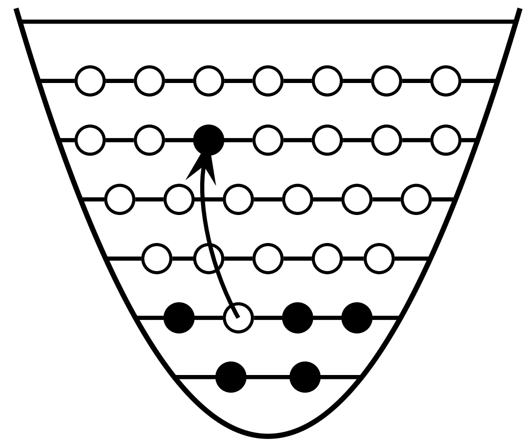
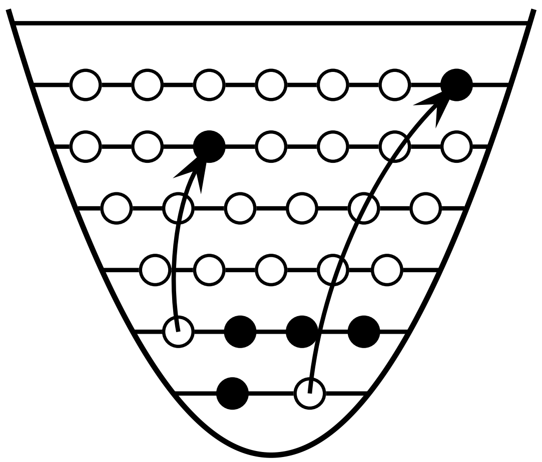
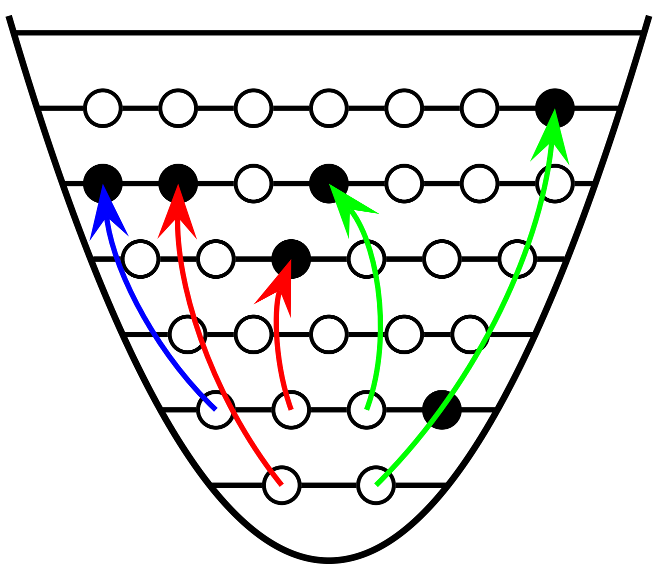


$\hat{T}_1 \, |\Phi_0\rangle$



$\hat{T}_2 \, |\Phi_0\rangle$



$\hat{T}_1 \, \hat{T}_2 \, \hat{T}_2 \, |\Phi_0\rangle$

CCSD

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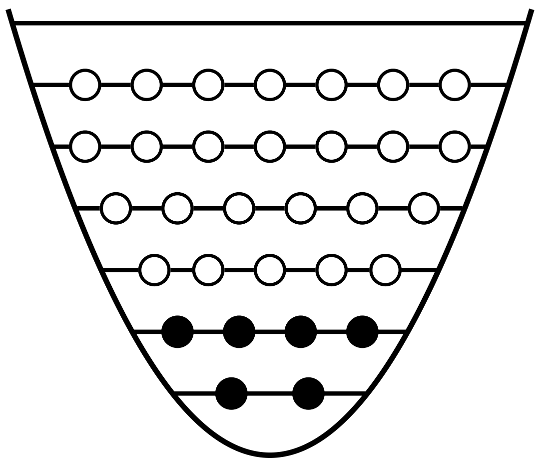
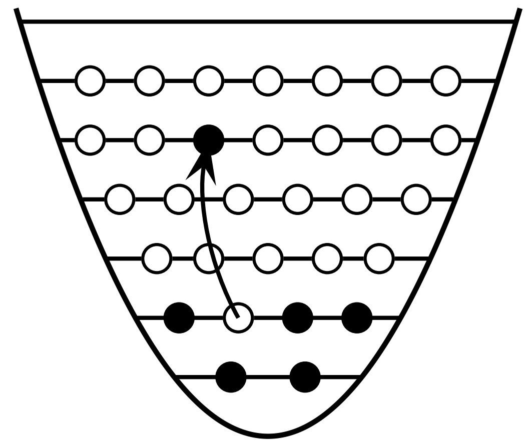
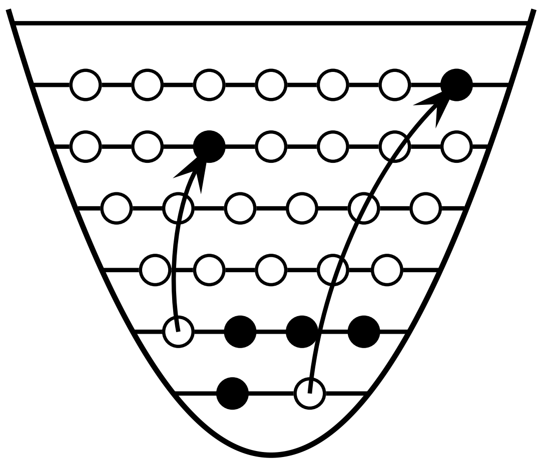


$|\Phi_0\rangle$



$\hat{T}_1\,|\Phi_0\rangle$



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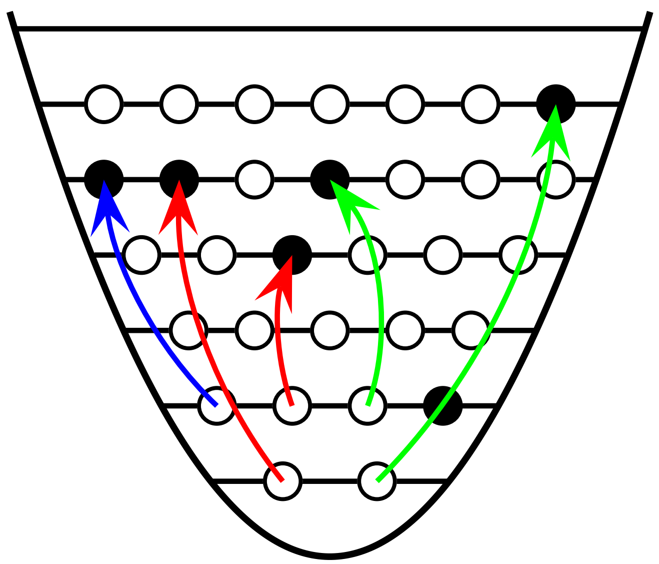


$\hat{T}_1\,\hat{T}_2\,\hat{T}_2\,|\Phi_0\rangle$

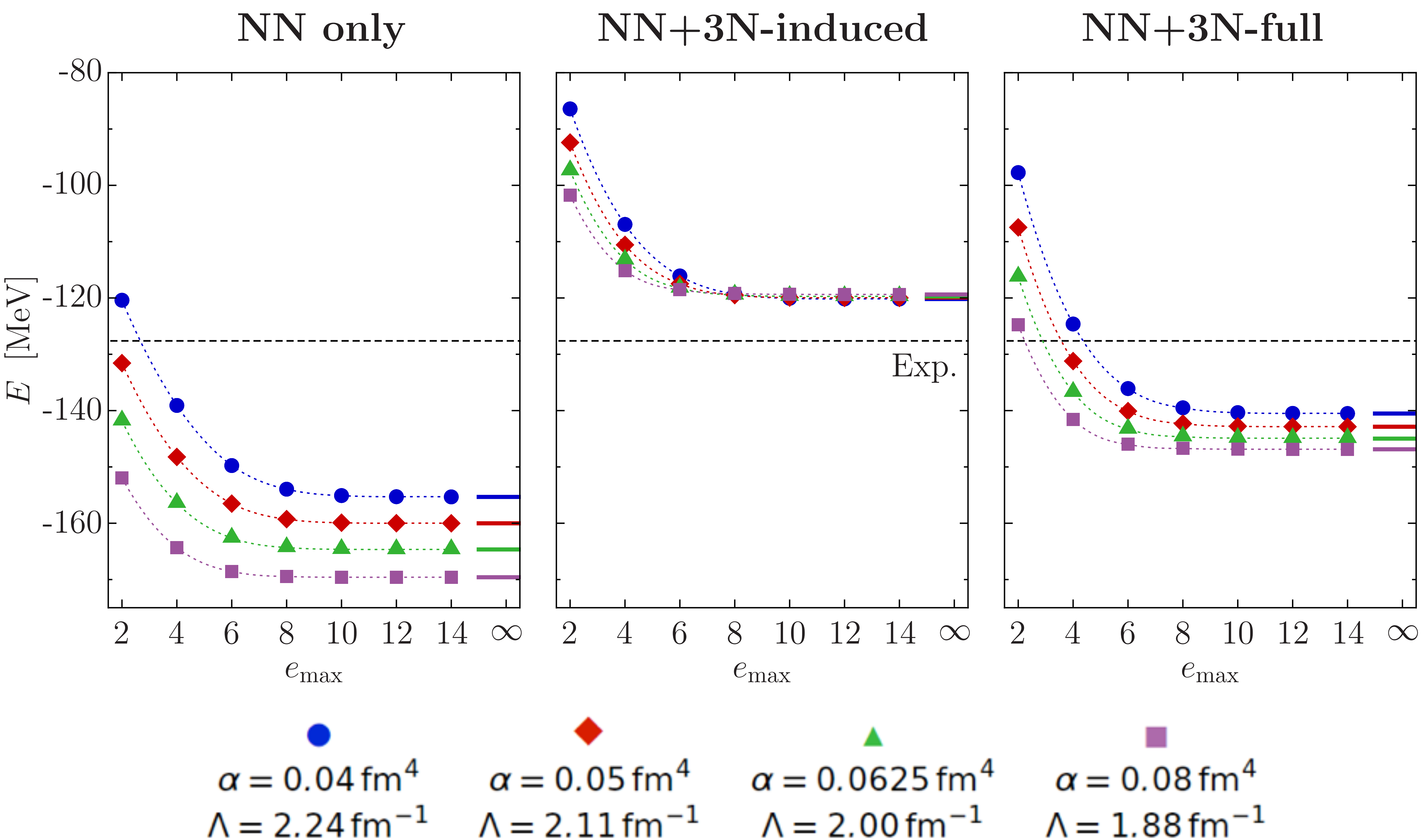
- CCSD equations

$$\Delta E_{\text{CCSD}} = \langle \Phi_0 | \hat{\mathcal{H}} | \Phi_0 \rangle$$

$$0 = \langle \Phi_i^a | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall\ a, i$$

$$0 = \langle \Phi_{ij}^{ab} | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall\ a, b, i, j$$

^{16}O: CCSD with $3N_{NO2B}$



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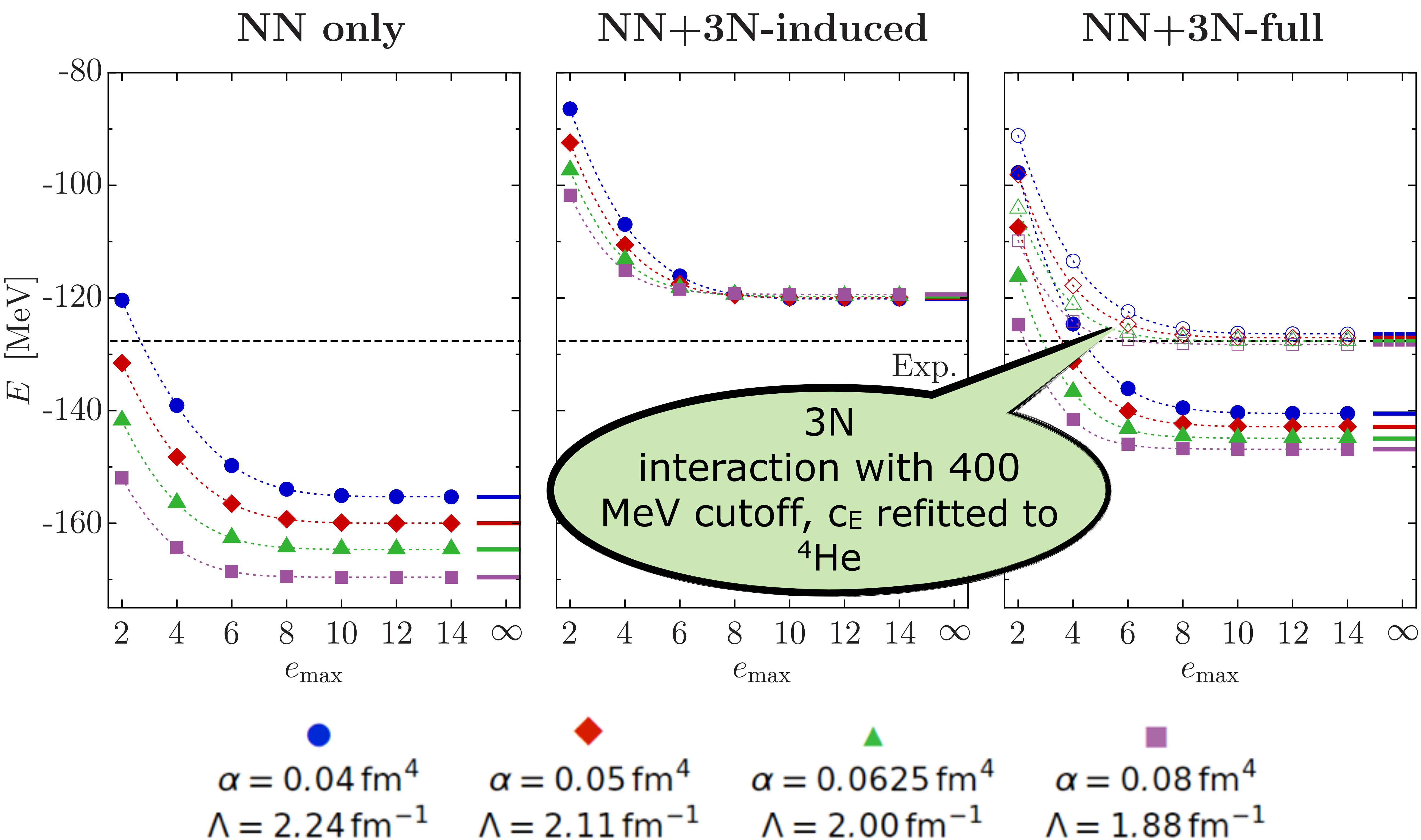
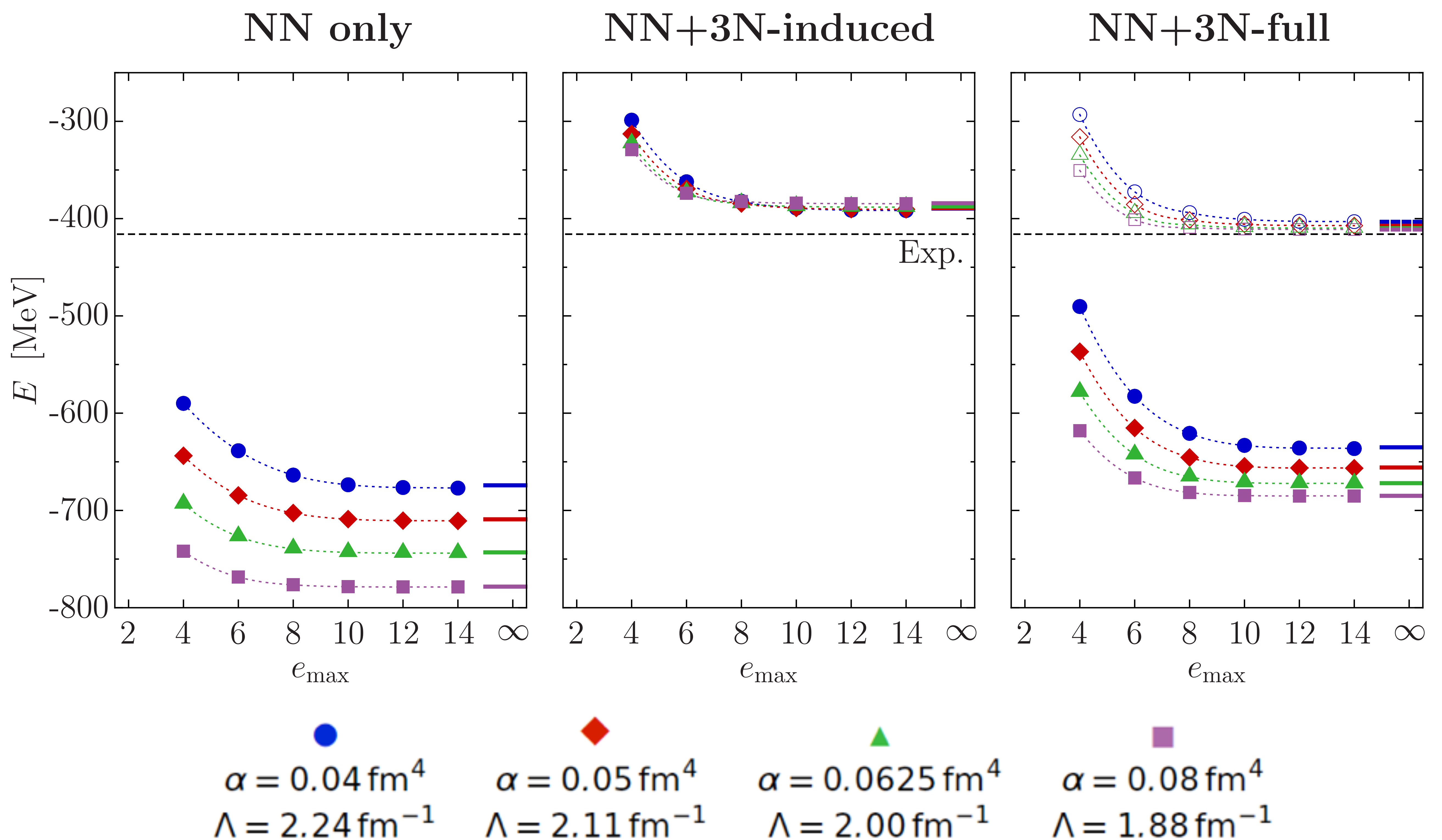


^{48}Ca: CCSD with $3N_{NO2B}$



ΛCCSD(T)

A.G. Taube, R. J. Bartlett, The Journal of Chemical Physics 128, 044110 (2008)

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ΛCCSD(T) - Improving upon CCSD

- **CCSDT**, i.e., $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$, **expensive**

- solution of the Coupled-Cluster Λ equations give **a posteriori fourth-order correction** to CC energy functional

$$\mathcal{E} = \langle \Phi_0 | (1 + \hat{\Lambda}) \hat{\mathcal{H}} | \Phi_0 \rangle_C$$

  due to **triple excitations** (non-iterative)

$$\Delta E_{\Lambda\mathrm{CCSD(T)}} = \frac{1}{(3!)^2} \sum_{\substack{abc \\ ijk}} \tilde{\lambda}^{ijk}_{abc} \frac{1}{\epsilon^{abc}_{ijk}} \tilde{t}^{abc}_{ijk}$$

- **however**: only correction to energy, not **wavefunction**

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due to **triple excitations** (non-iterative)

indicator of **convergence** of cluster expansion

$$\Delta E_{\Lambda \mathrm{CCSD(T)}} = \frac{1}{(3!)^2} \sum_{\substack{abc \\ ijk}} \tilde{\lambda}^{ijk}_{abc} \frac{1}{\epsilon^{abc}_{ijk}} \tilde{t}^{abc}_{ijk}$$

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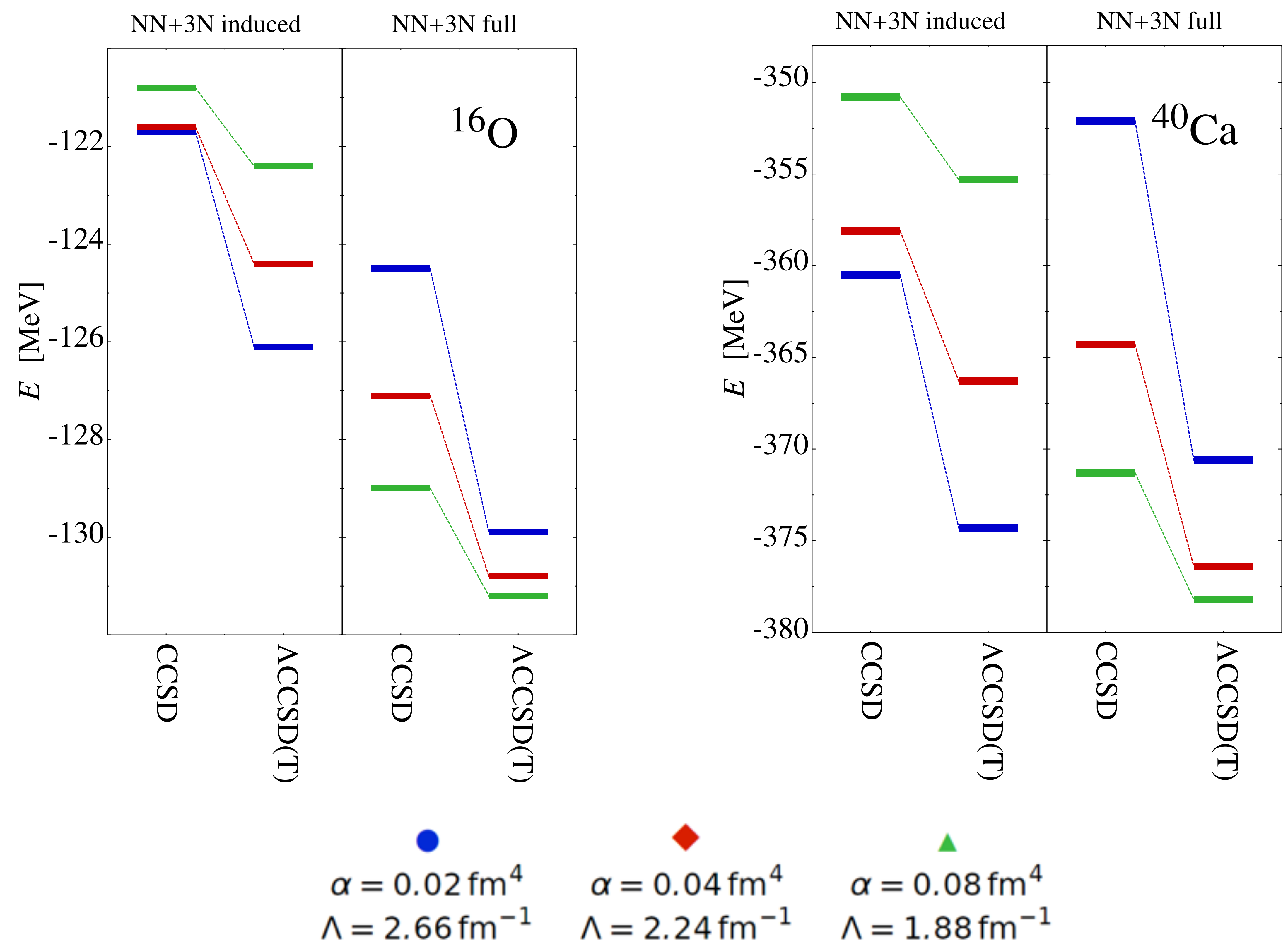
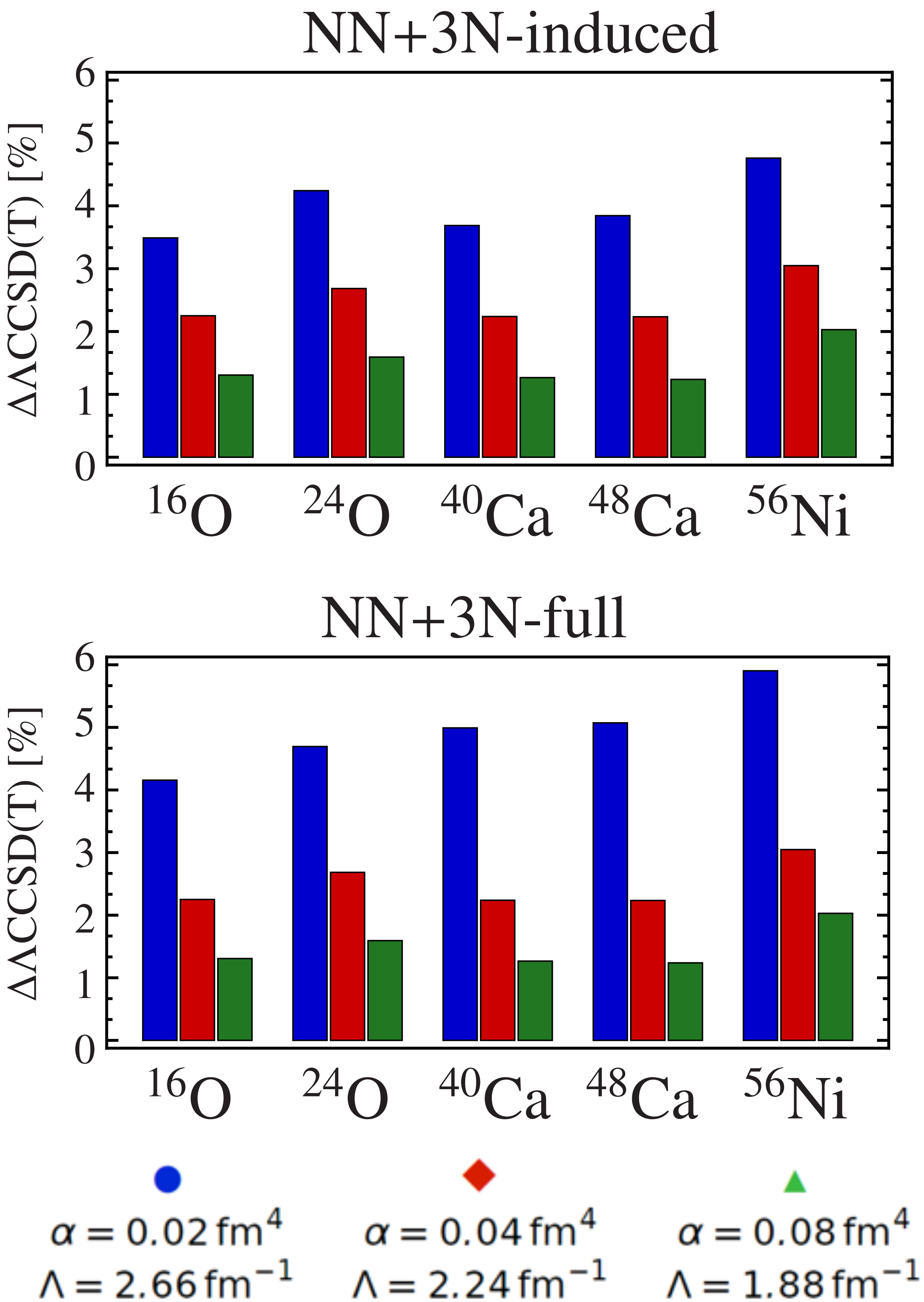
$CCSD_{NO2B}$ vs. $\Lambda CCSD(T)_{NO2B}$



$\text{CCSD}_{\text{NO2B}}$ vs. $\Lambda\text{CCSD(T)}_{\text{NO2B}}$



change in
g.s. energy

- inclusion of **triples excitations mandatory** (up to 6% more binding for heavier nuclei)
- cluster truncation works better for **softer interactions**
- cluster truncation is source of **flow-parameter dependence**
- ΛCCSD(T) is correction for **energy**, not **wavefunction**

$\Rightarrow$ **hard interactions**:

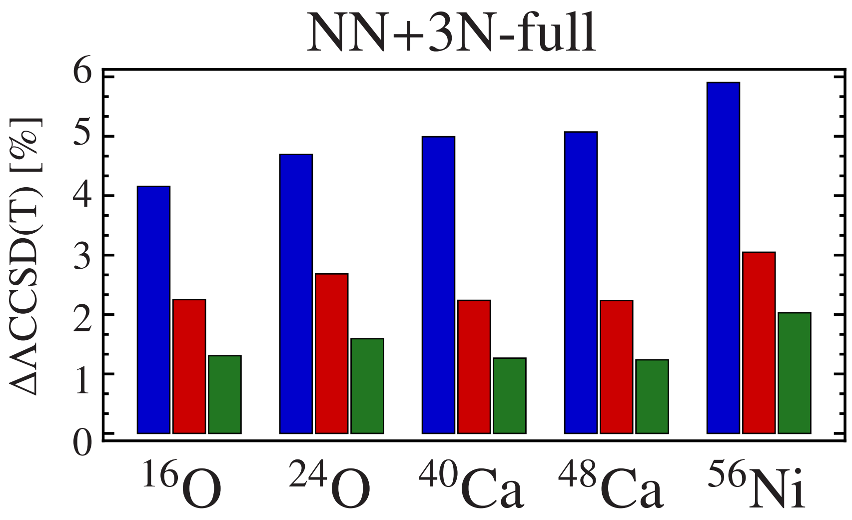
CCSD wavefunction sufficient?

Uncertainty Summary

- **Similarity Renormalization Group**
  - ☑ α-dependence: low-cutoff 3N interaction

- **Normal-Ordering 2B Approximation**
  - ☑ error in light nuclei: 1-2%

- **Cluster Truncation**
  - ☐ up to 6% contributions from ΛCCSD(T)
  - ☑ soft interactions: only 1-2%
  - ☑ no strong increase with mass number



Coupled-Cluster with Explicit 3N Interactions

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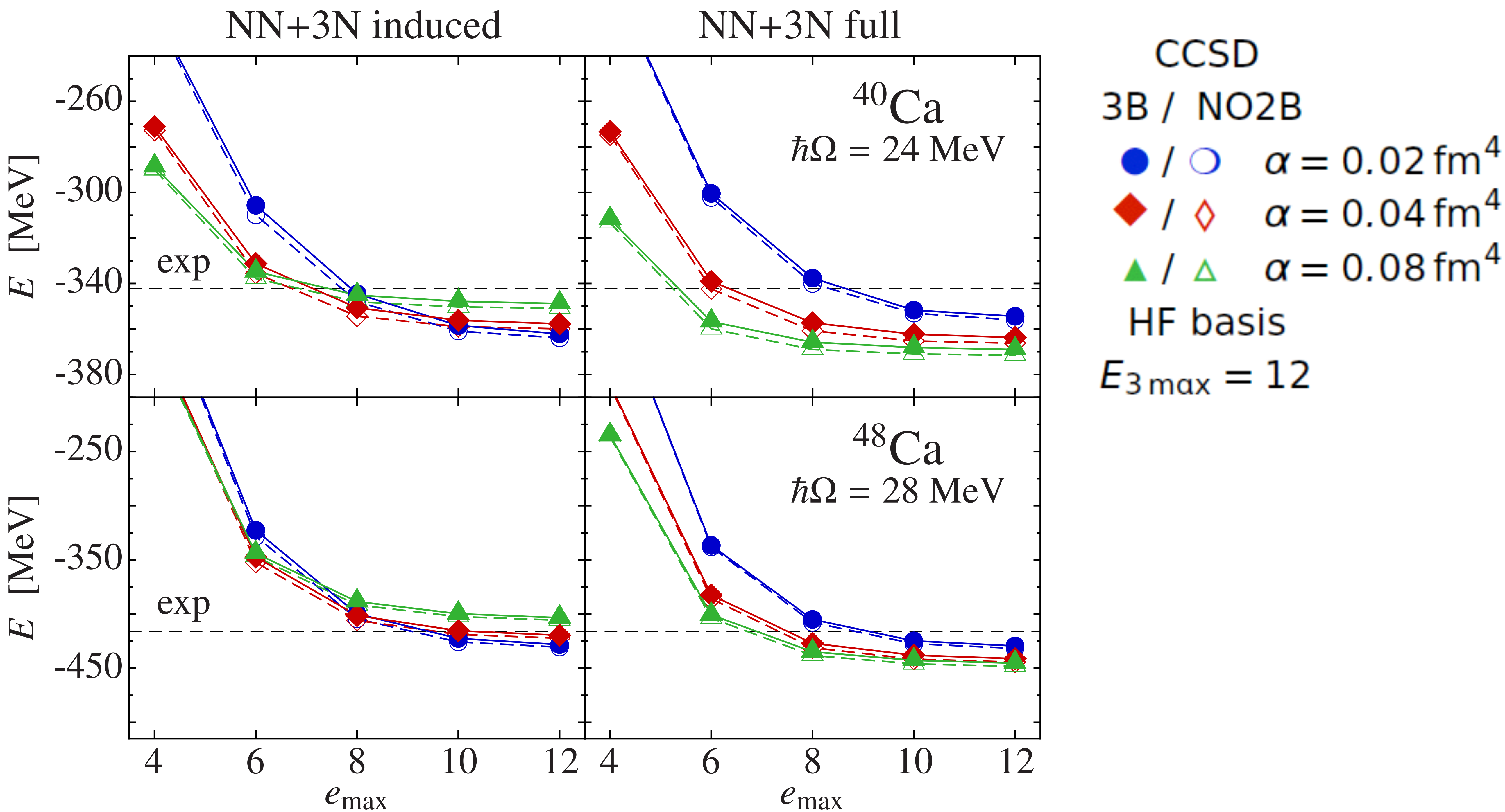
CCSD with Explicit 3N Interaction



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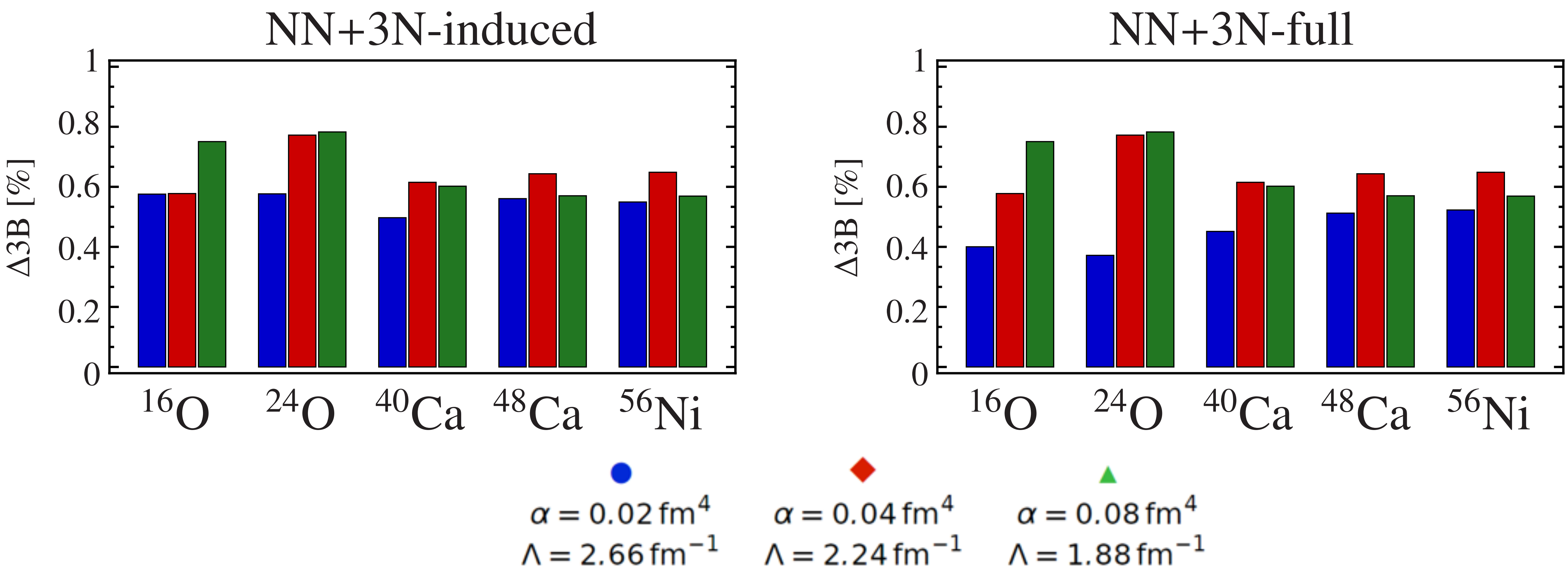
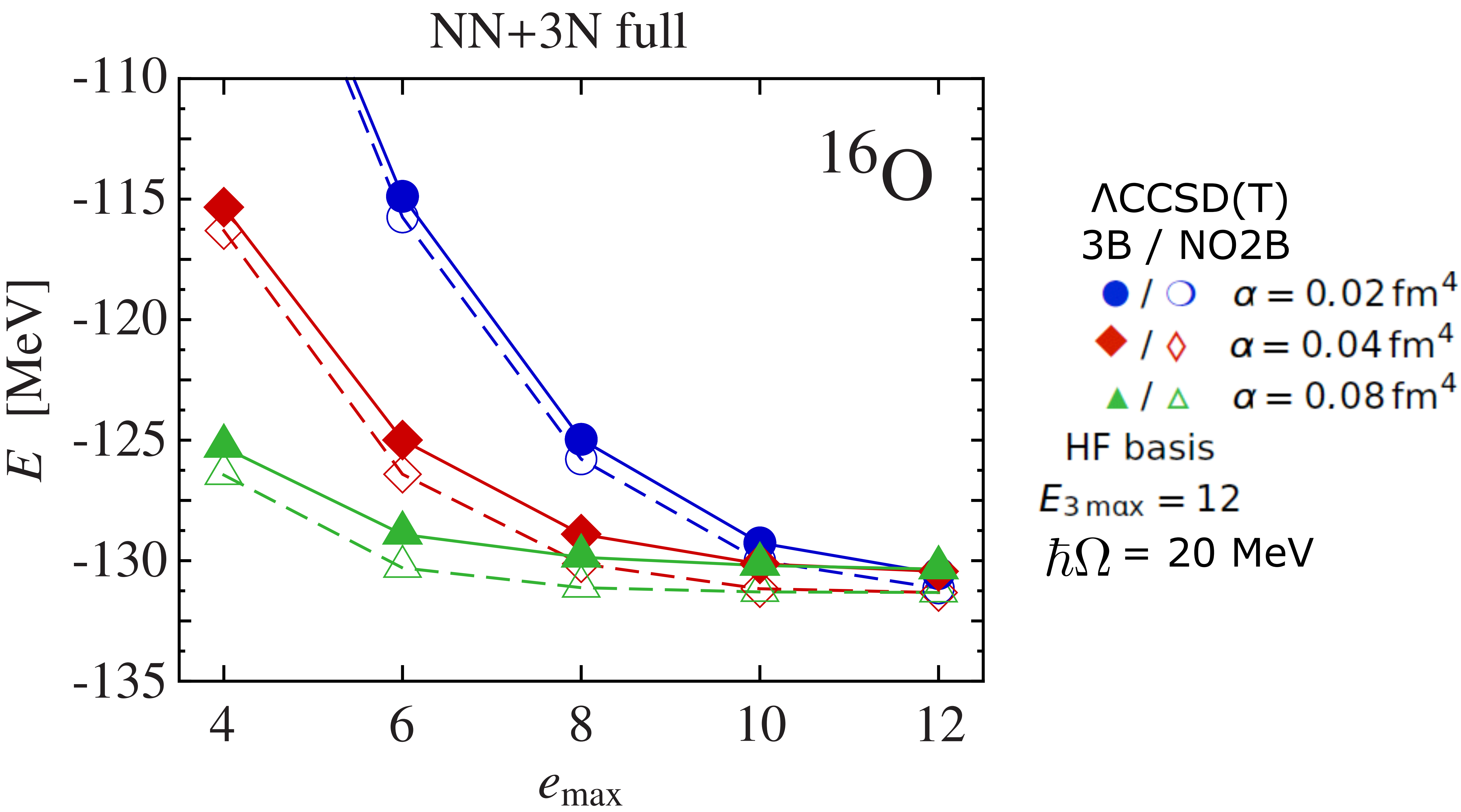


- **excellent agreement** between NO2B and explicit 3N (deviation < 1% for all nuclei considered)
- quality of NO2B **independent** of $e_{\mathrm{max}}, \hbar\Omega, \alpha$
- **efficient and accurate** way to include 3N interactions

ΛCCSD(T) with Explicit 3N Interaction



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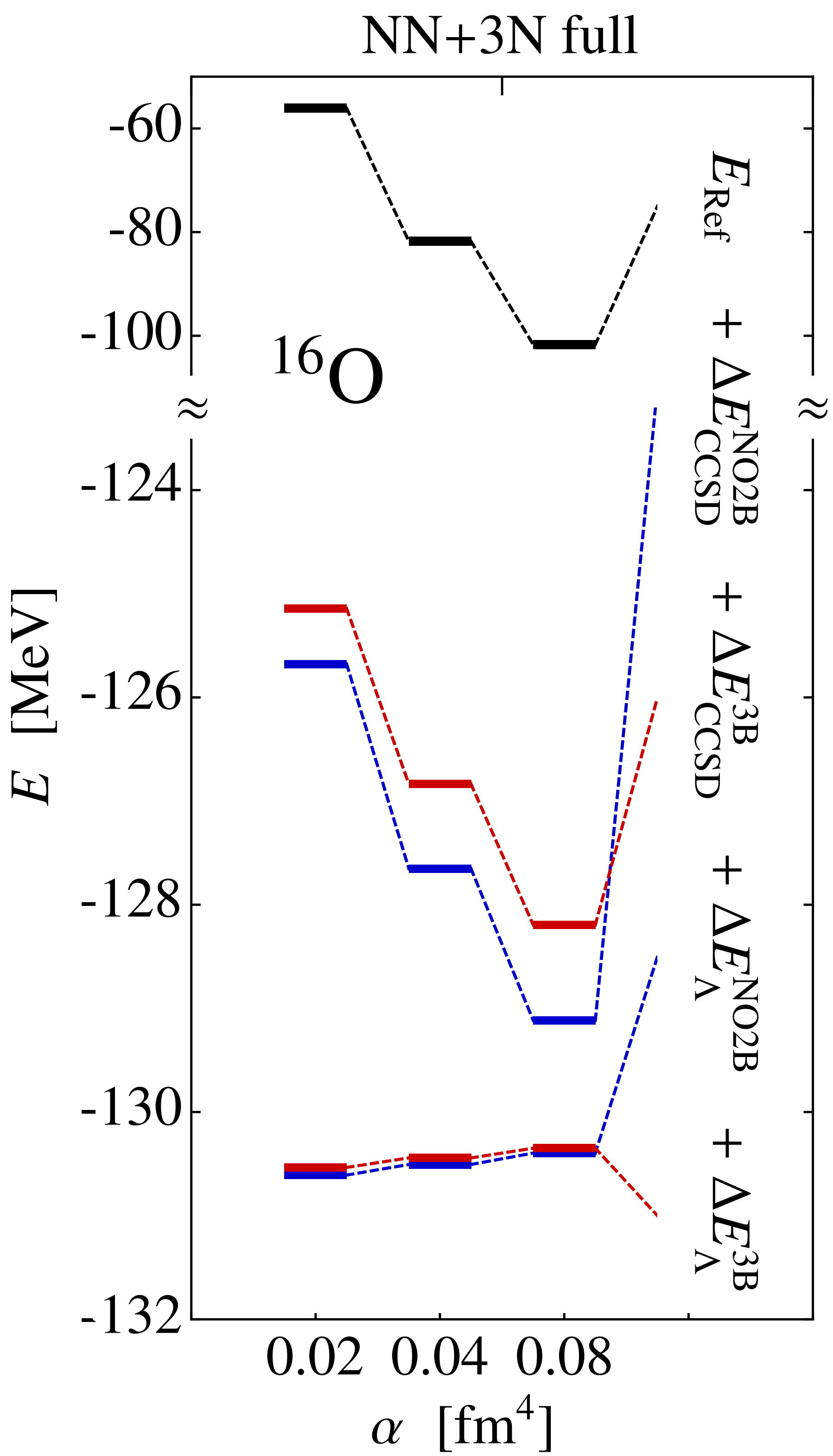
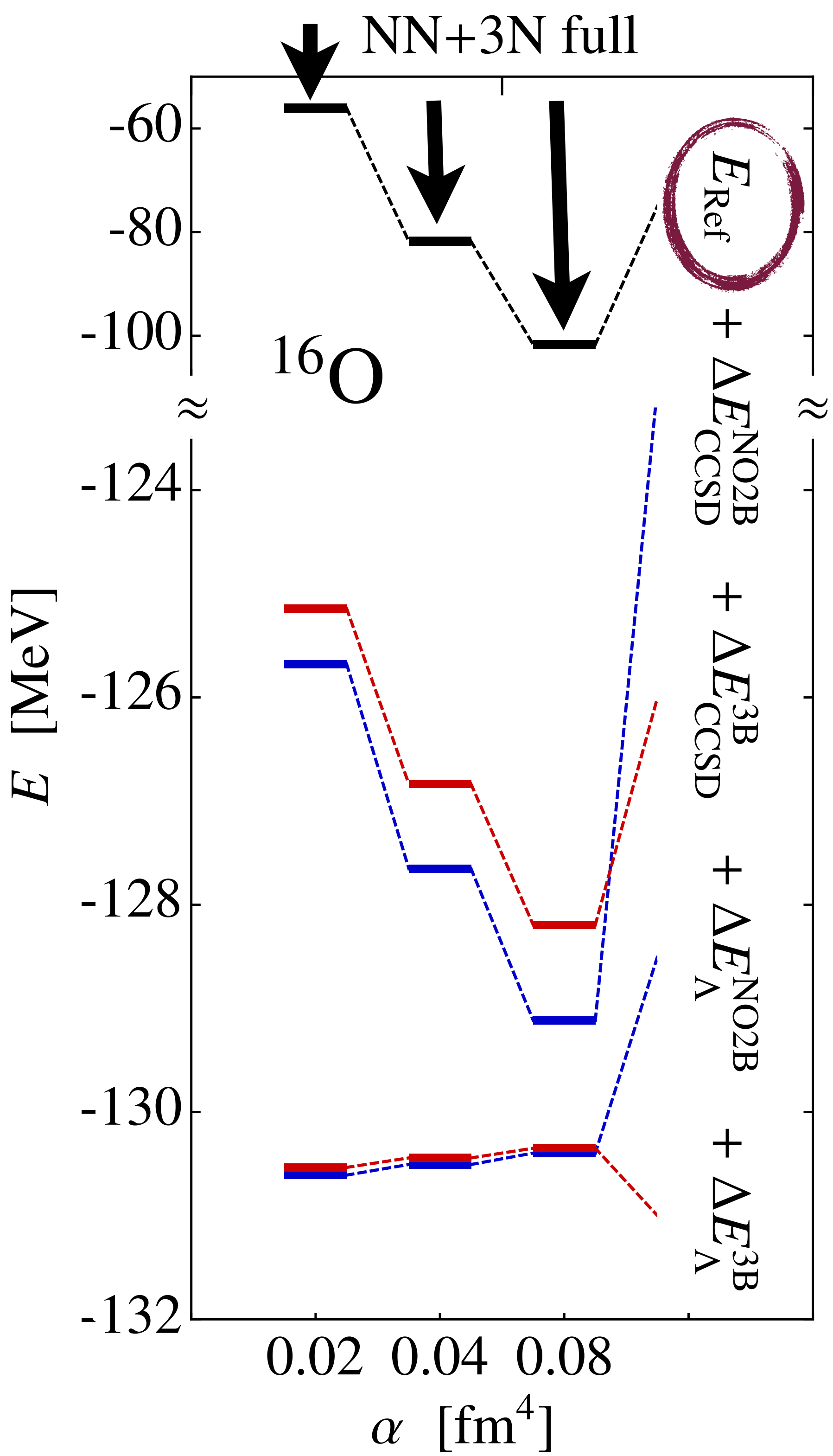


- NO2B shows **excellent agreement** also for ΛCCSD(T)
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

$$\Delta E_{\mathrm{CCSD}} = \Delta E^{\mathrm{NO2B}}_{\mathrm{CCSD}} + \Delta E^{\mathrm{3B}}_{\mathrm{CCSD}}\ , \quad \text{etc.}$$

- significant contribution of residual 3N **only for ΔE_{CCSD}**
- **soft interactions**: contributions from residual 3N to ΔE_{CCSD} comparable to contribution from ΛCCSD(T) correction

ΛCCSD(T) with Explicit 3N Interaction



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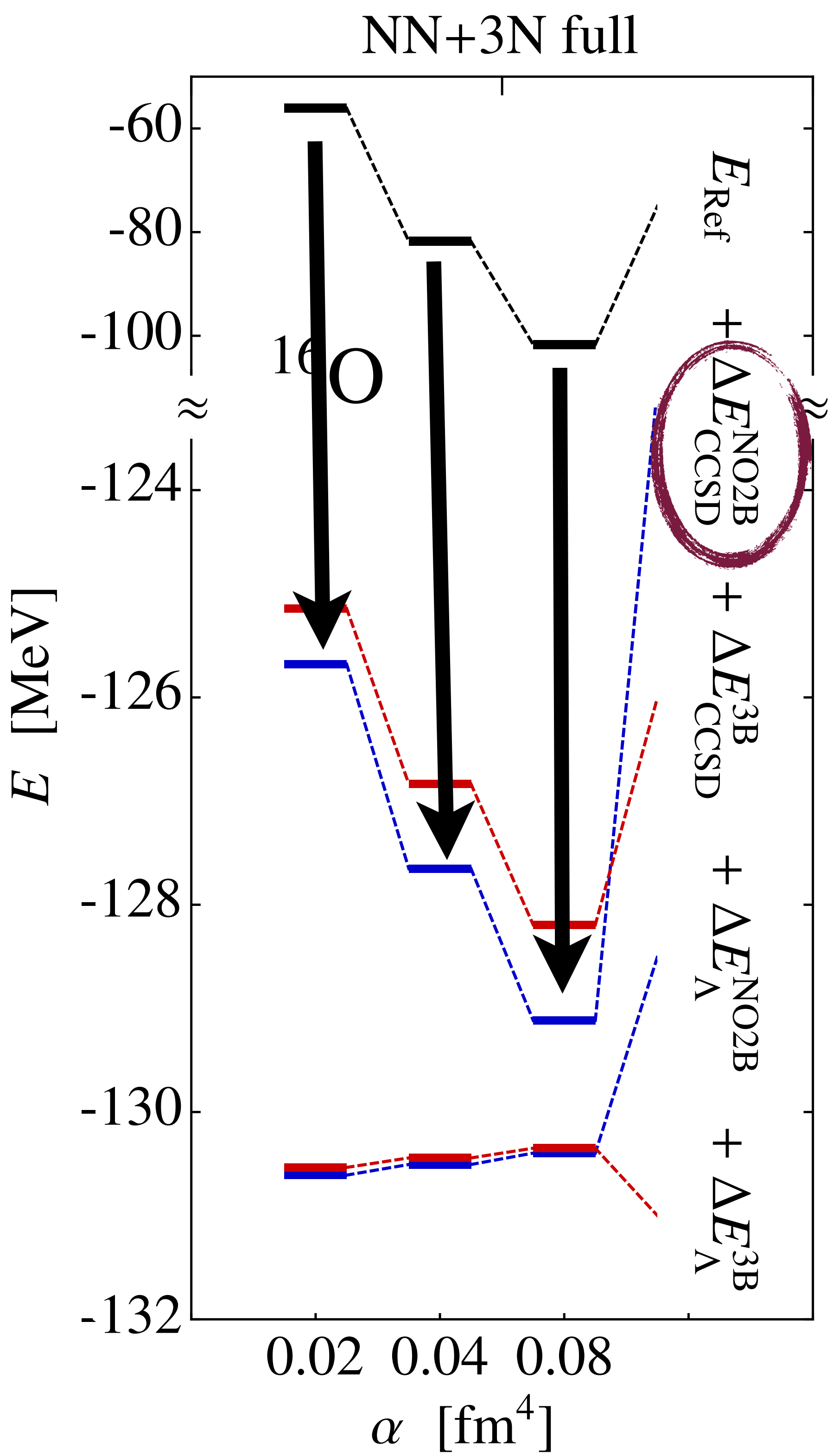

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- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

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- significant contribution of residual 3N **only for ΔE_{CCSD}**

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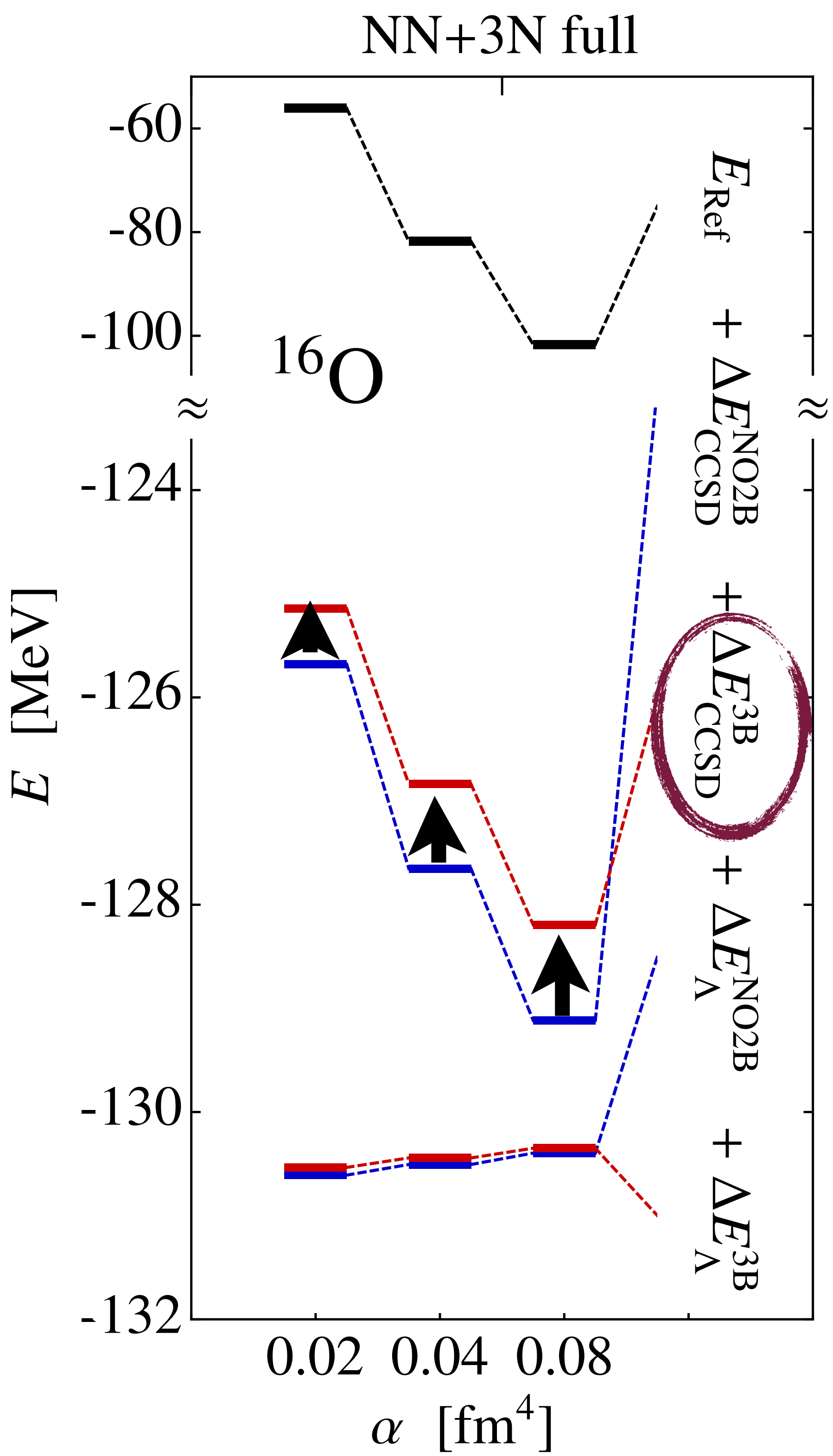
ΛCCSD(T) with Explicit 3N Interaction



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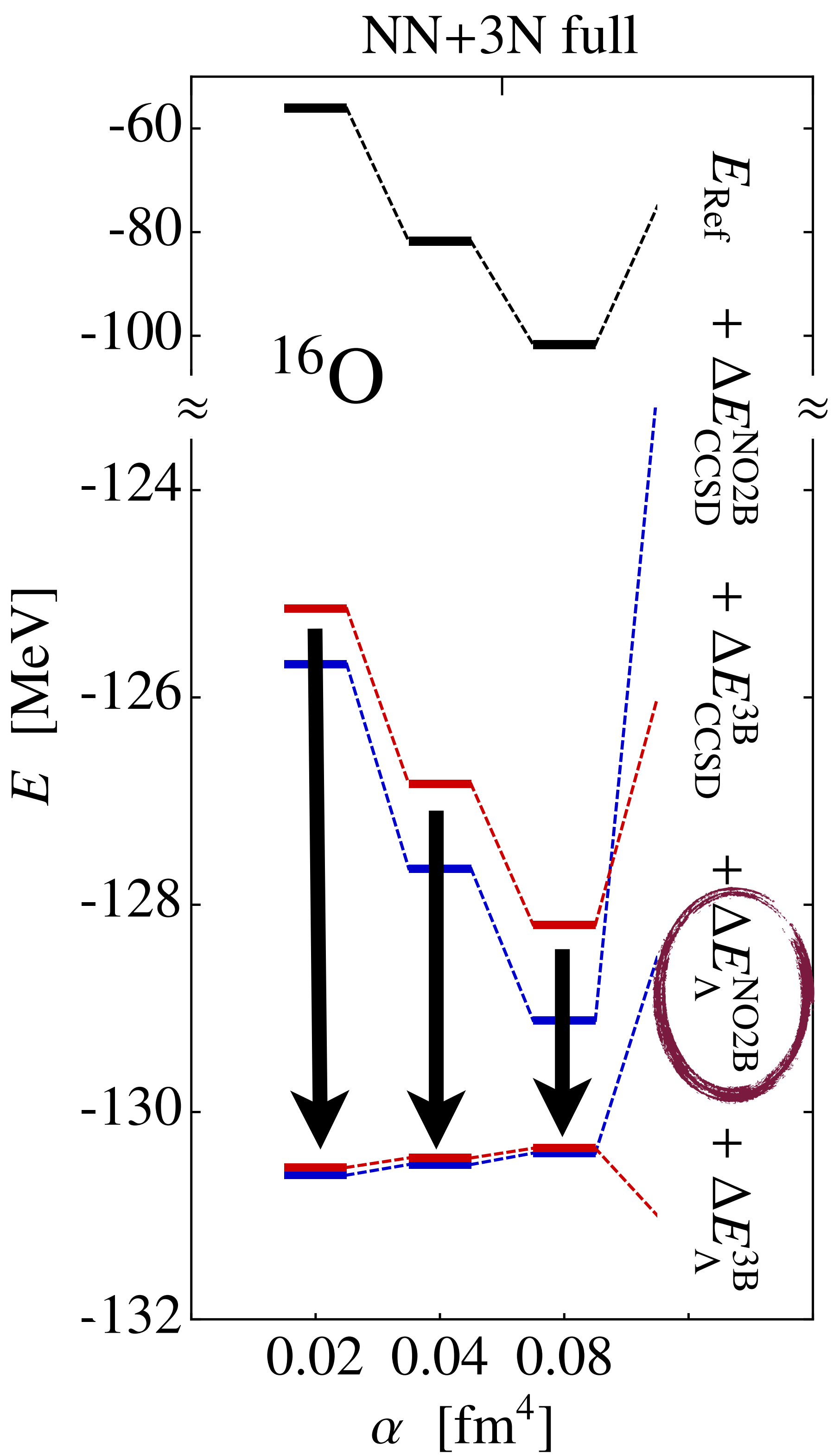

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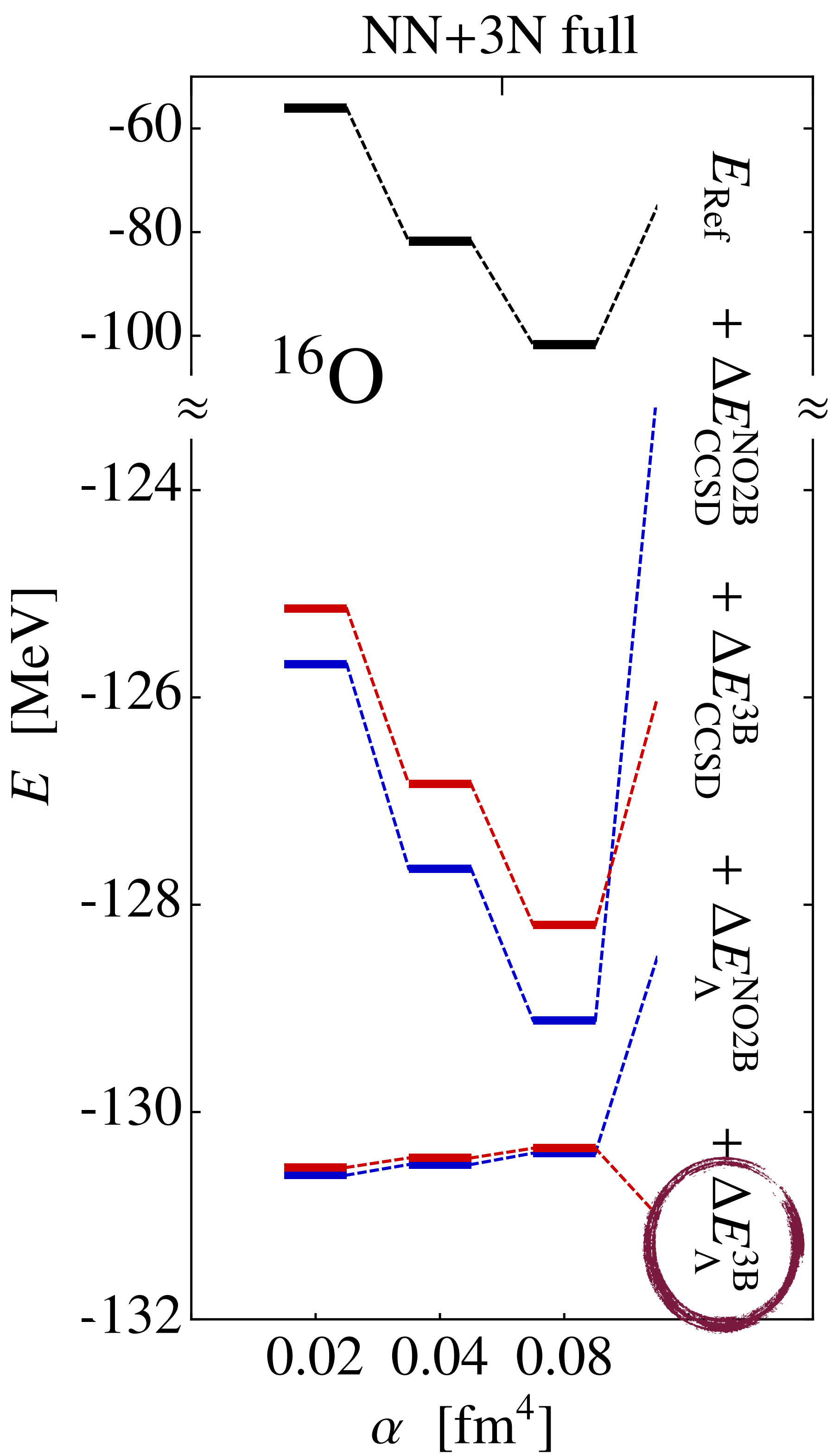

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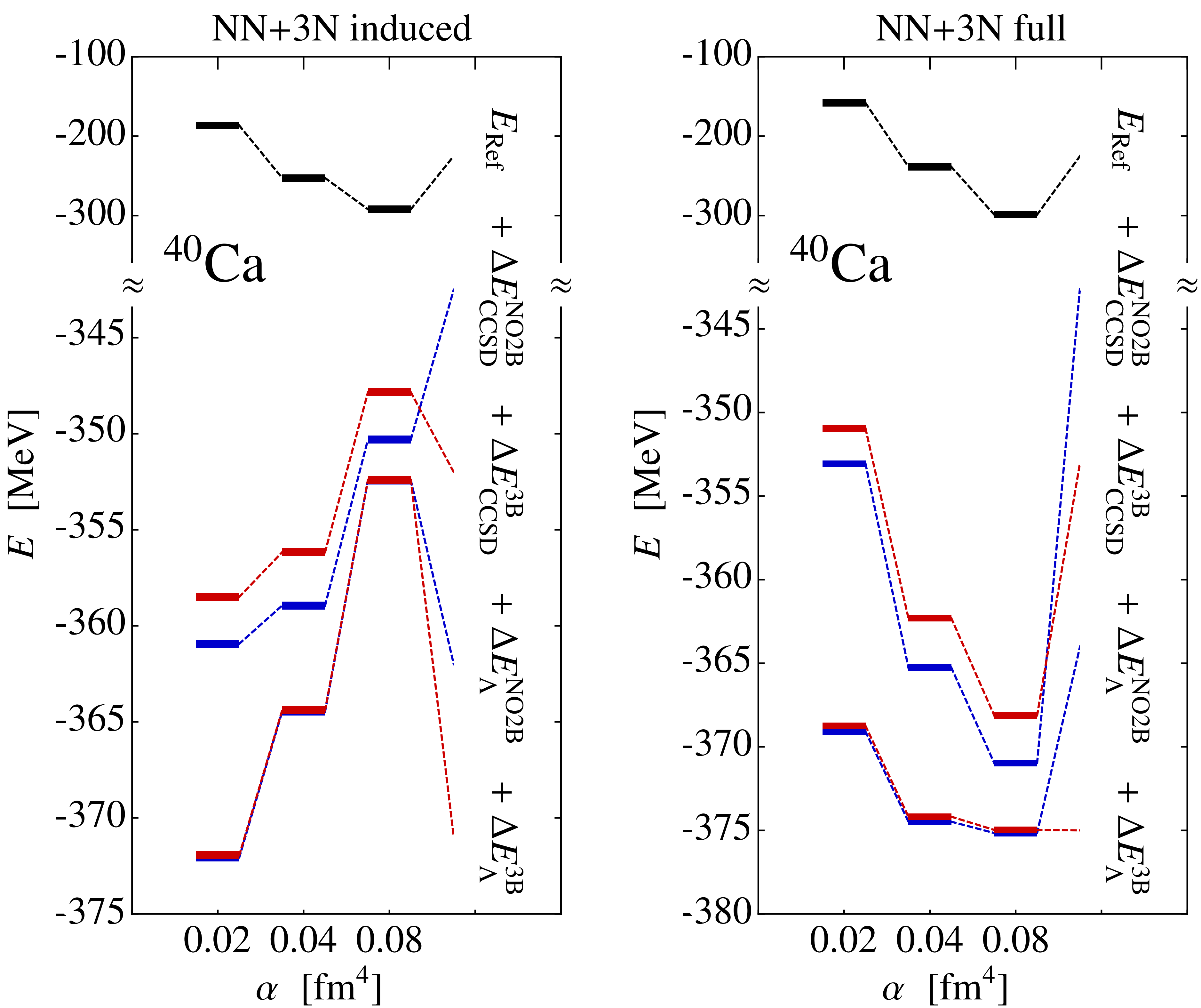

ΛCCSD(T)3B

HF basis
e_{max} = 10
E_{3max} = 12
$\hbar\Omega$ = 24 MeV

Uncertainty Summary

- **Similarity Renormalization Group**
  - ☑ α-dependence: low-cutoff 3N interaction
- **Normal-Ordering 2B Approximation**
  - ☑ error in light nuclei: 1-2%,
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  - ☑ error independent of mass number etc.
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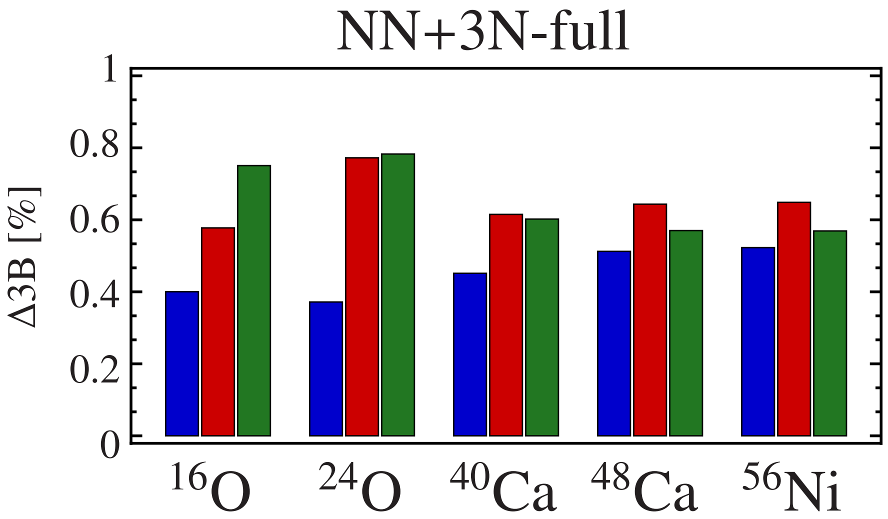
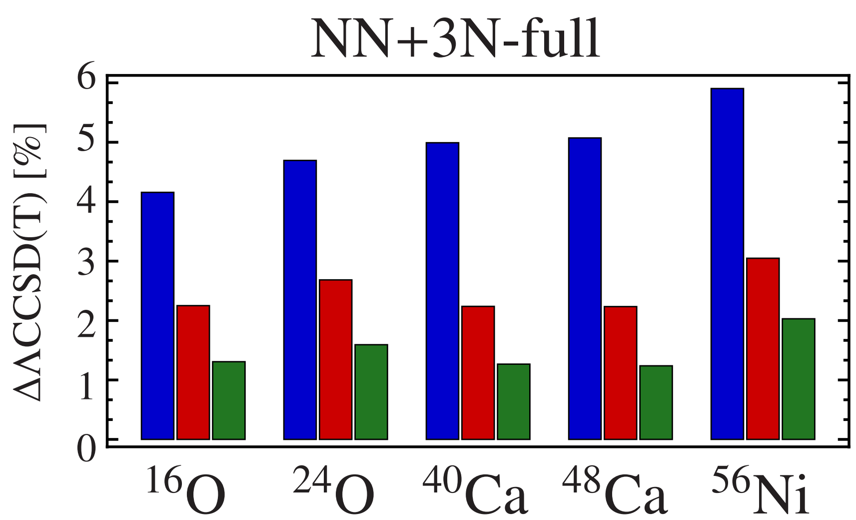


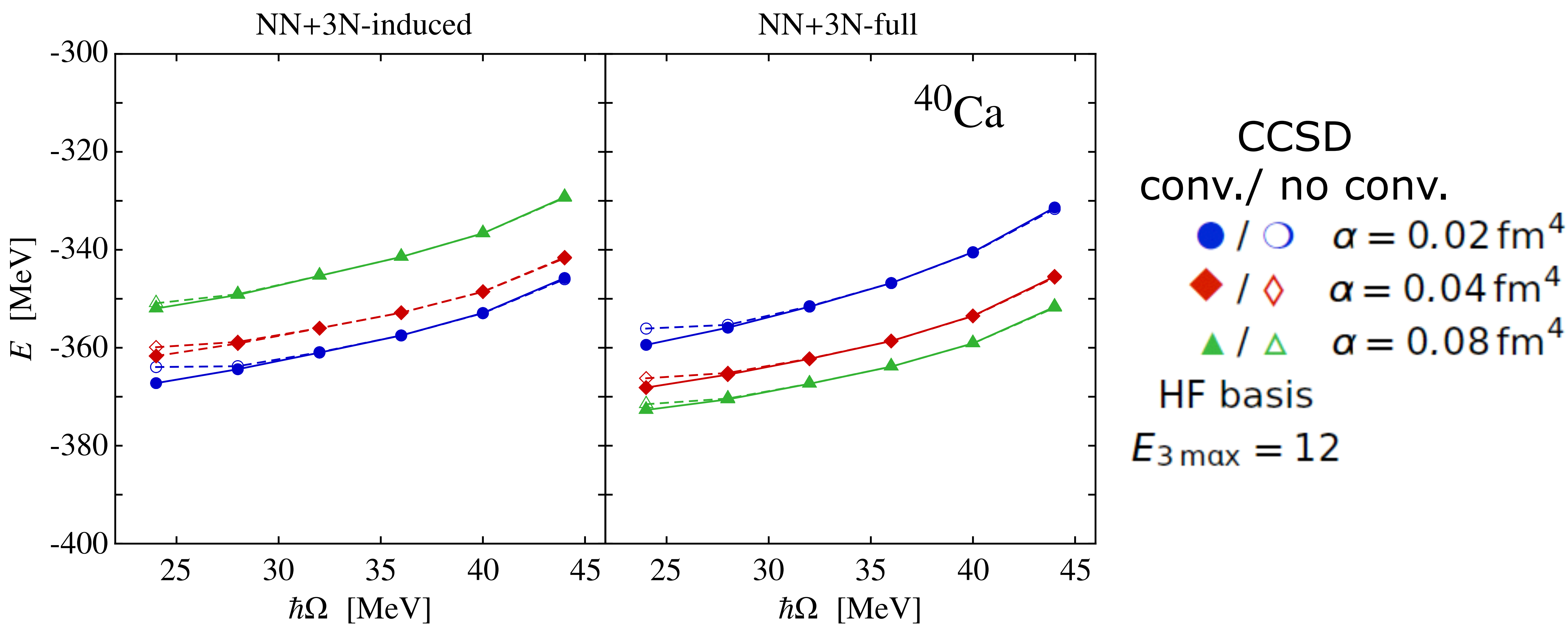


Frequency Conversion

R. Roth, A. Calci, J. Langhammer, S. Binder --- in prep.

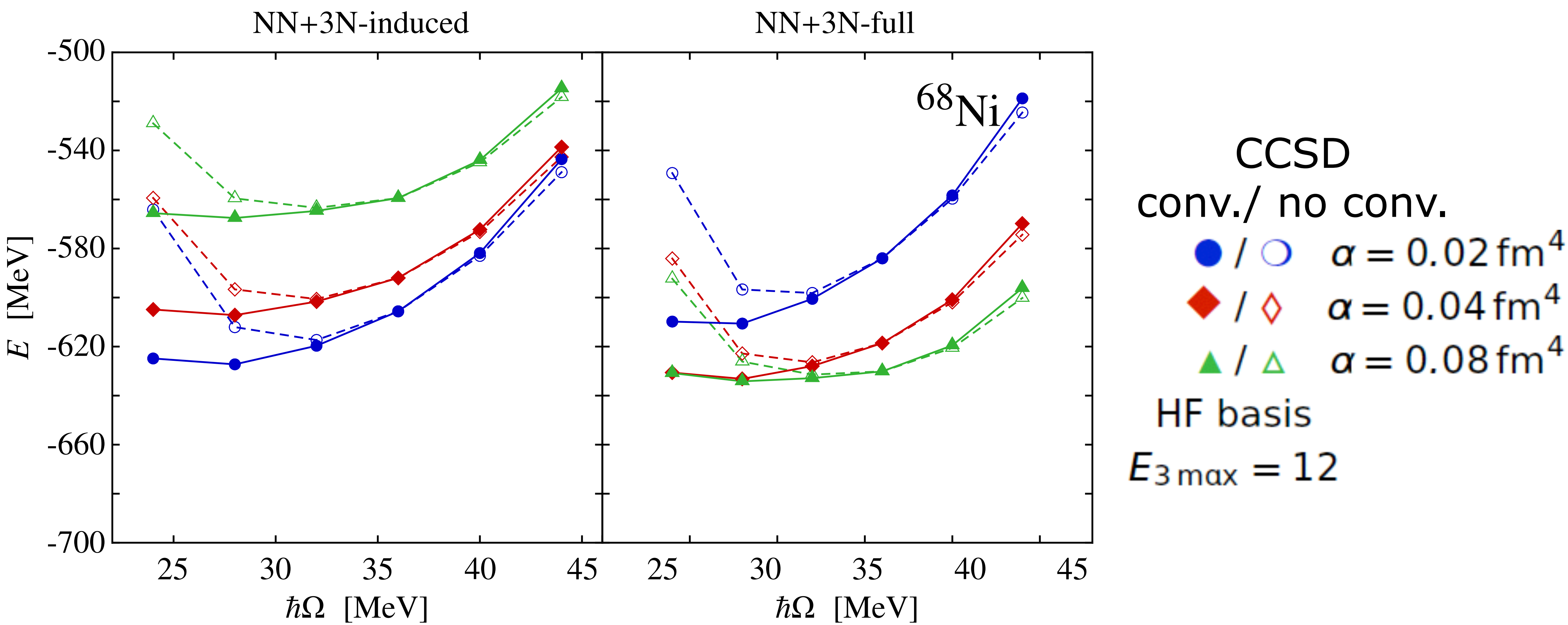
Frequency Conversion

- current SRG model spaces **not appropriate** for small frequencies
  ⇒ **frequency conversion** (see talk by **Angelo Calci**)



- $\hbar\Omega = 36$ MeV used for conversion

Frequency Conversion



- without conversion: **energy minimum** artificially shifted towards larger frequencies

- **frequency conversion** mandatory for heavier nuclei

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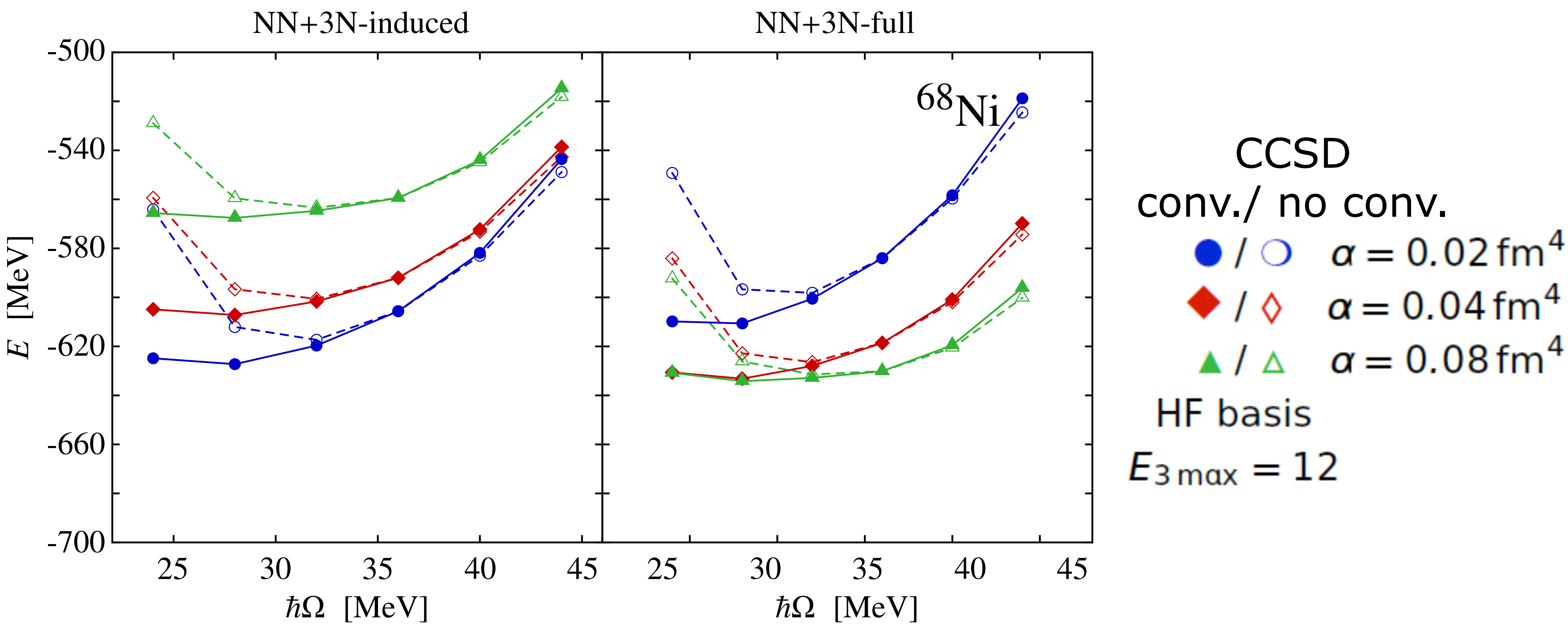

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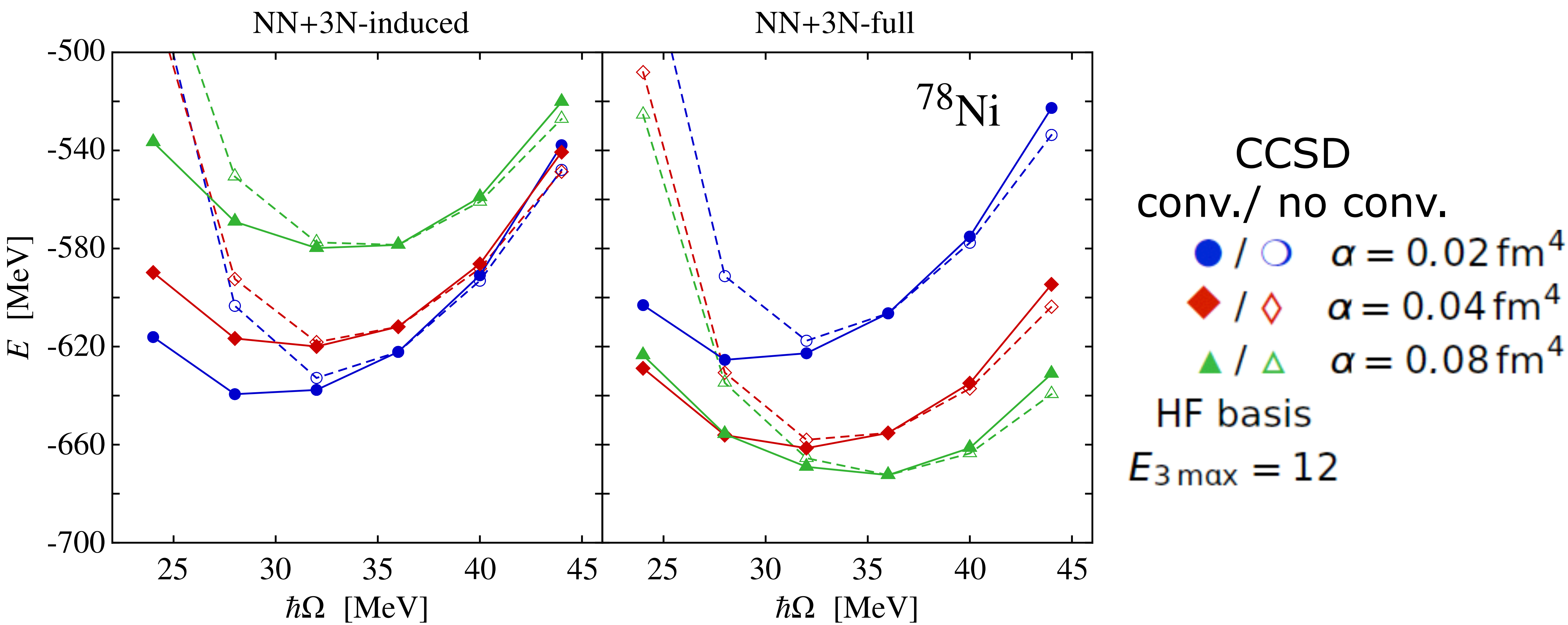

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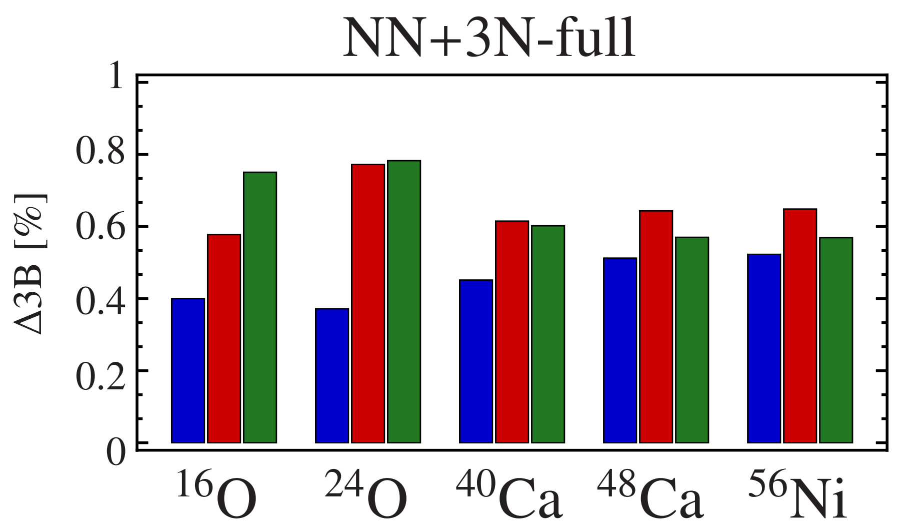
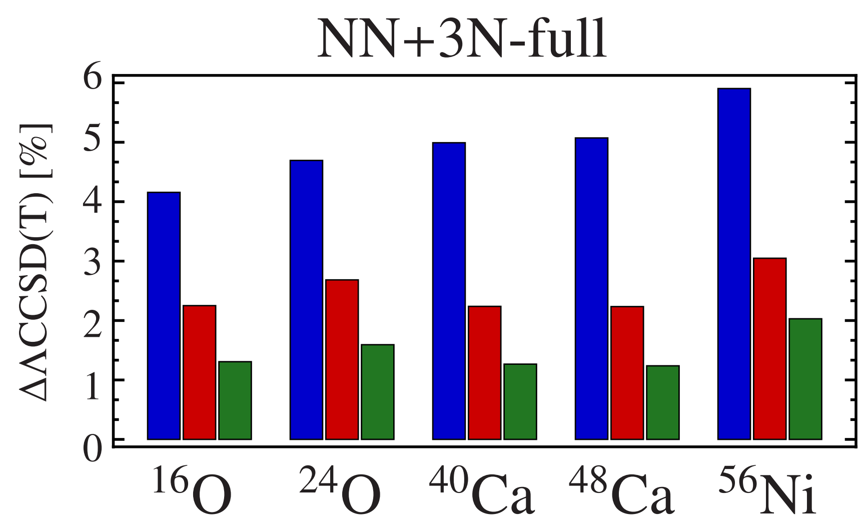




E3Max Truncation

$\mathrm{E_{3max}}$ Truncation

- full $\hat{W}_{3\mathrm{B}}$ matrix **too large** to handle

- **$\mathrm{E_{3max}}$ truncation**: use $\hat{W}_{3\mathrm{B}}$ matrix elements $\langle pqr|\hat{W}_{3\mathrm{B}}|stu\rangle$ with

$$e_p + e_q + e_r \;\leq E_{3\mathrm{max}} \;\vee\; e_s + e_t + e_u \;\leq E_{3\mathrm{max}}$$

$$e_p = 2n_p + l_p$$

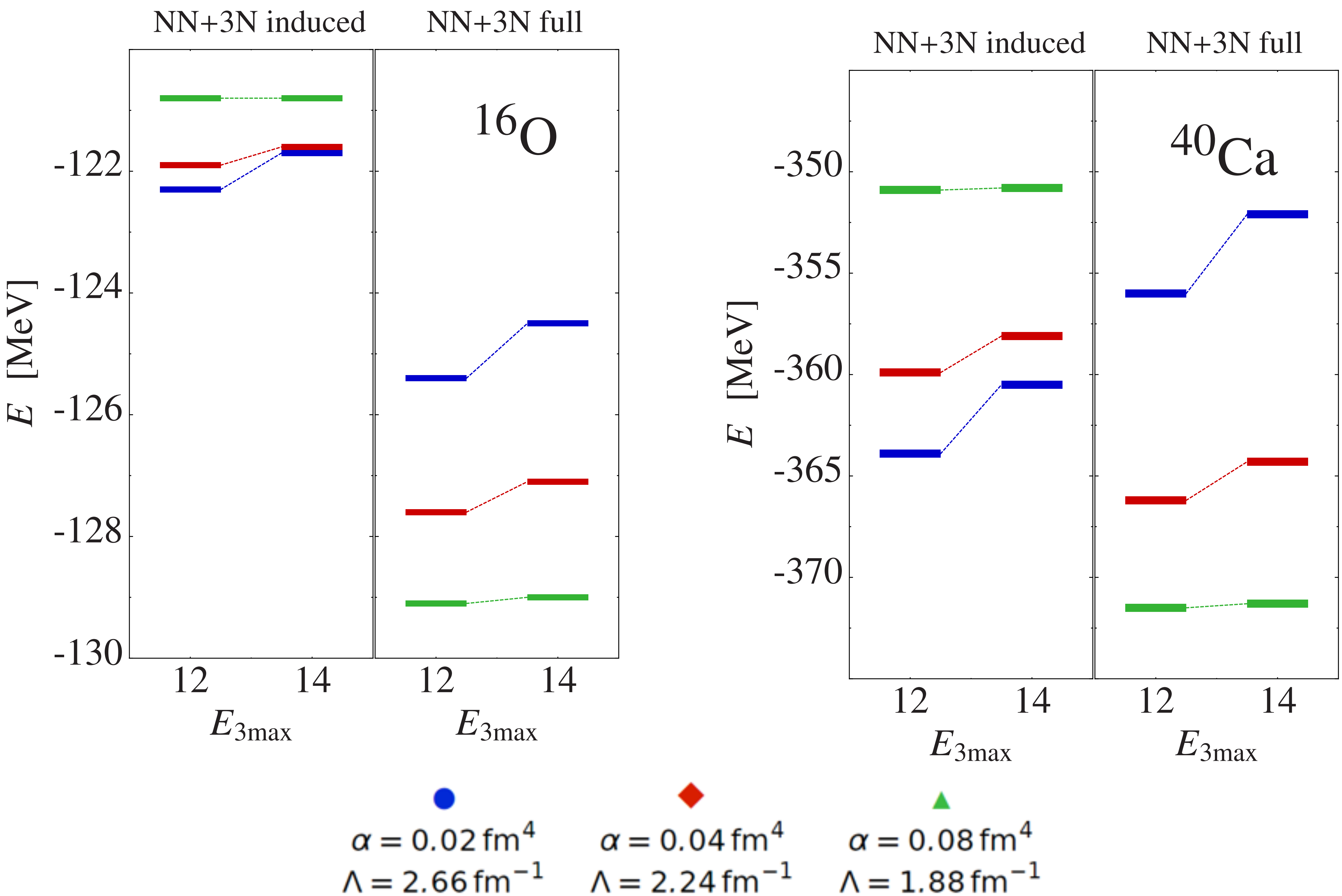
- **current limits**:

$$E_{3\mathrm{max}} \leq \begin{cases} 14 & : \quad \mathrm{CC}, \quad \text{explicit 3N} \\ 16 & : \quad \mathrm{NCSM}, \quad \text{explicit 3N} \\ 20 & : \quad \mathrm{CC,NCSM} \quad \mathrm{NO2B} \end{cases}$$

storage

production

E_{3max} Dependence ($CCSD_{NO2B}$)



E_{3max} Dependence ($CCSD_{NO2B}$)

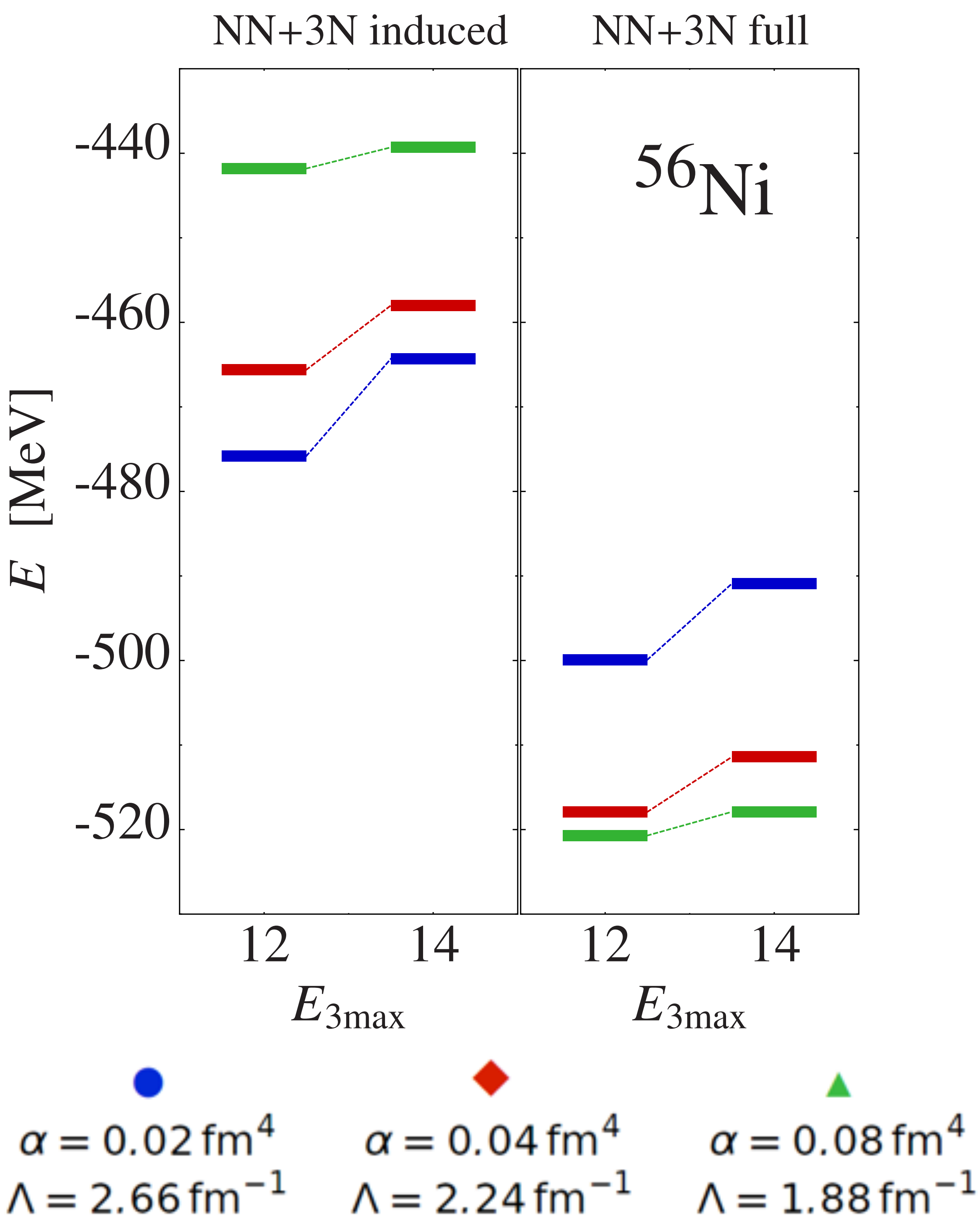
- E_{3max} not significant for **soft interactions** up to A<50
- **harder interactions**: up to 2% change in g.s. energies for E_{3max} 12 → 14
- α-dependence for **NN+3N induced** gets **reduced** for larger E_{3max}
- α-dependence for **NN+3N full** gets **enhanced** for larger E_{3max}

$\alpha = 0.02\,\mathrm{fm}^4$, $\Lambda = 2.66\,\mathrm{fm}^{-1}$

$\alpha = 0.04\,\mathrm{fm}^4$, $\Lambda = 2.24\,\mathrm{fm}^{-1}$

$\alpha = 0.08\,\mathrm{fm}^4$, $\Lambda = 1.88\,\mathrm{fm}^{-1}$

E_{3max} Dependence ($CCSD_{NO2B}$)



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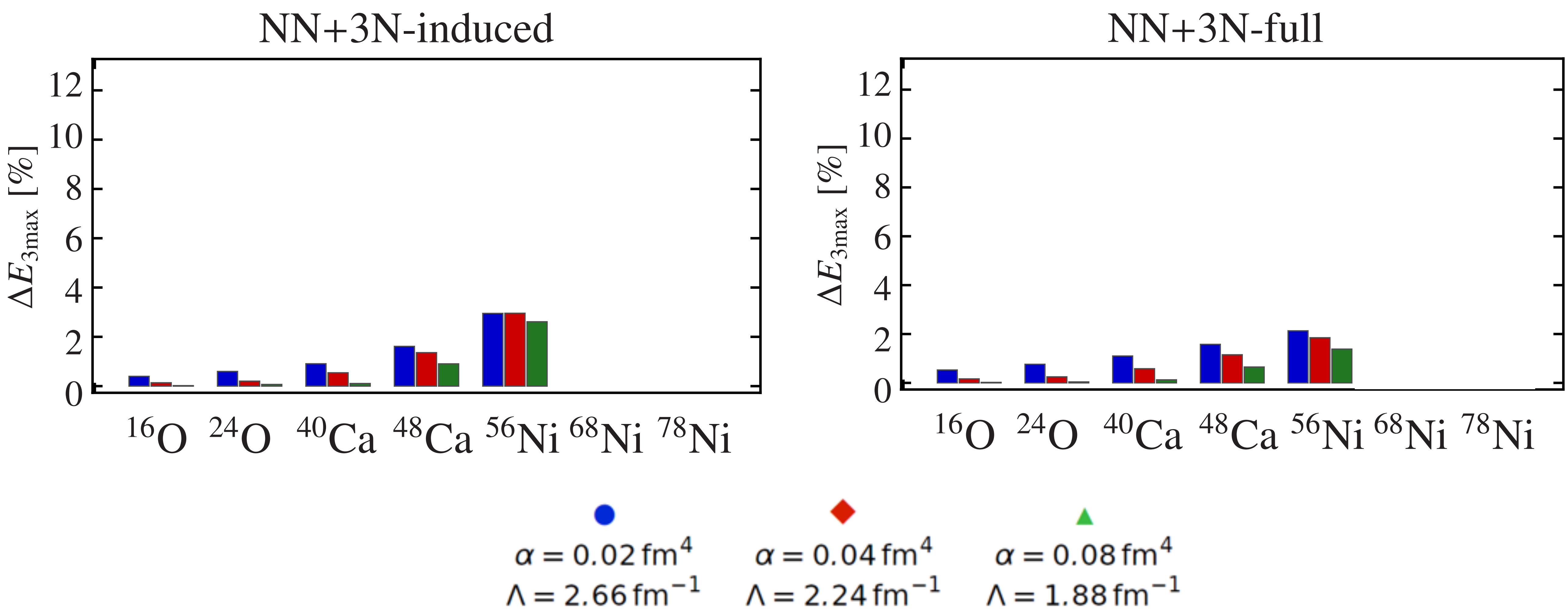
- $E_{3Max}=12$ vs. $E_{3Max}=14$



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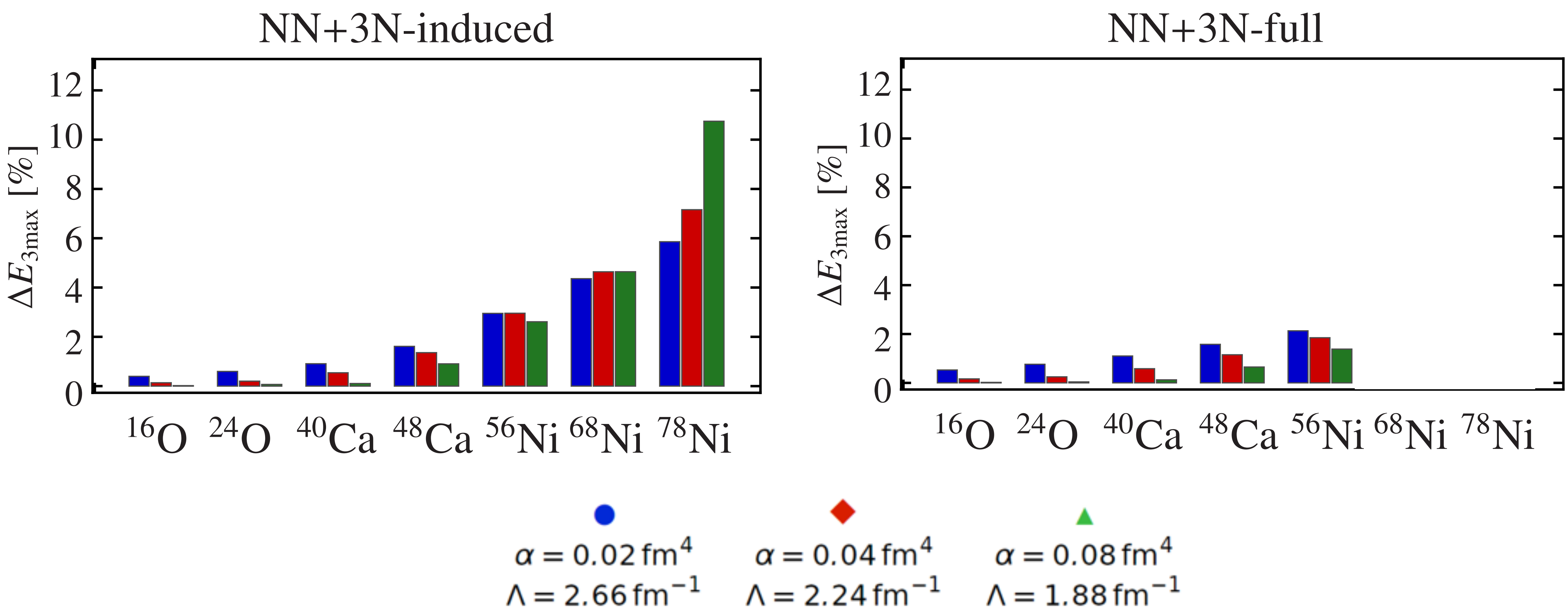

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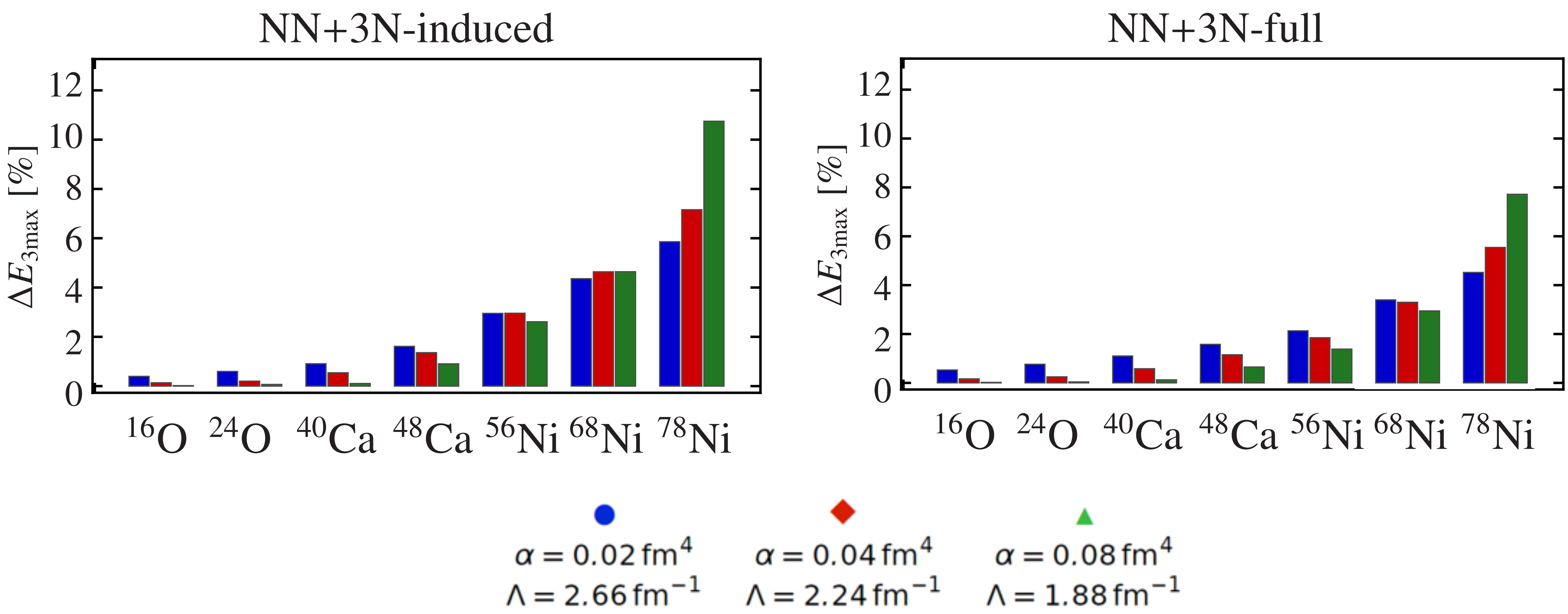

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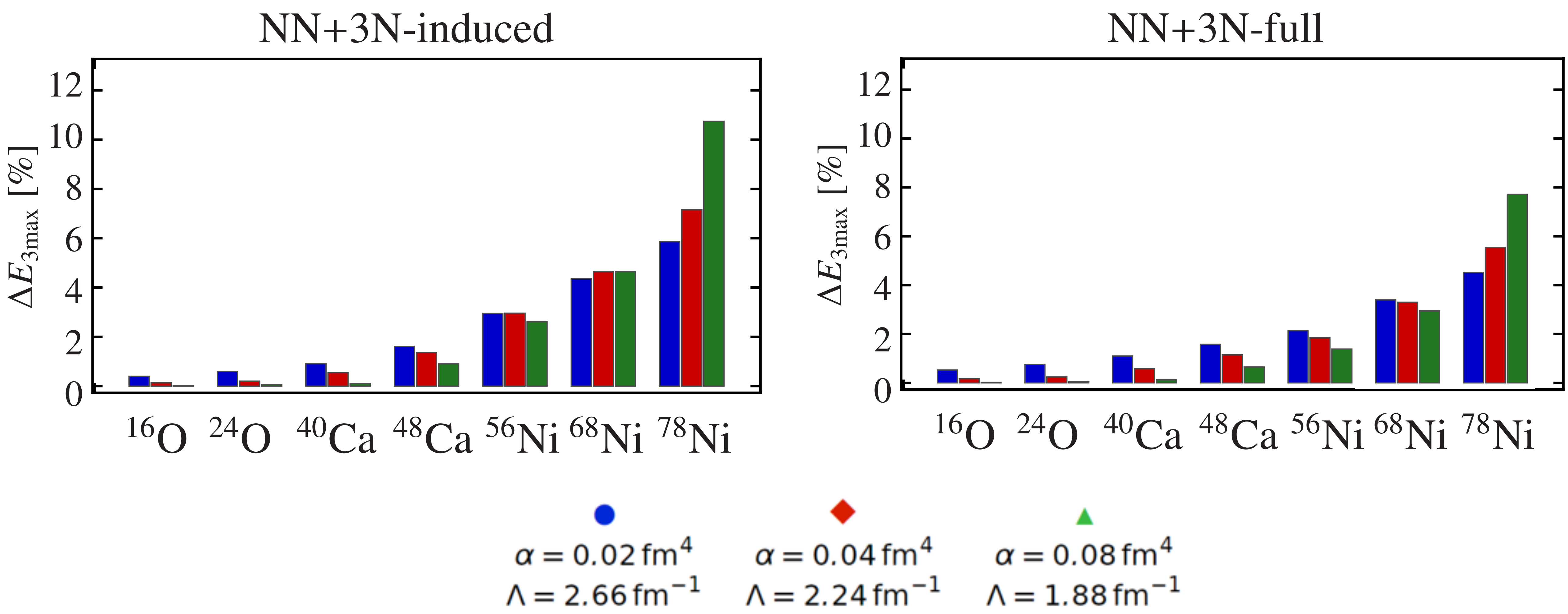

- Relevance of E_{3Max} grows rapidly with **mass number**

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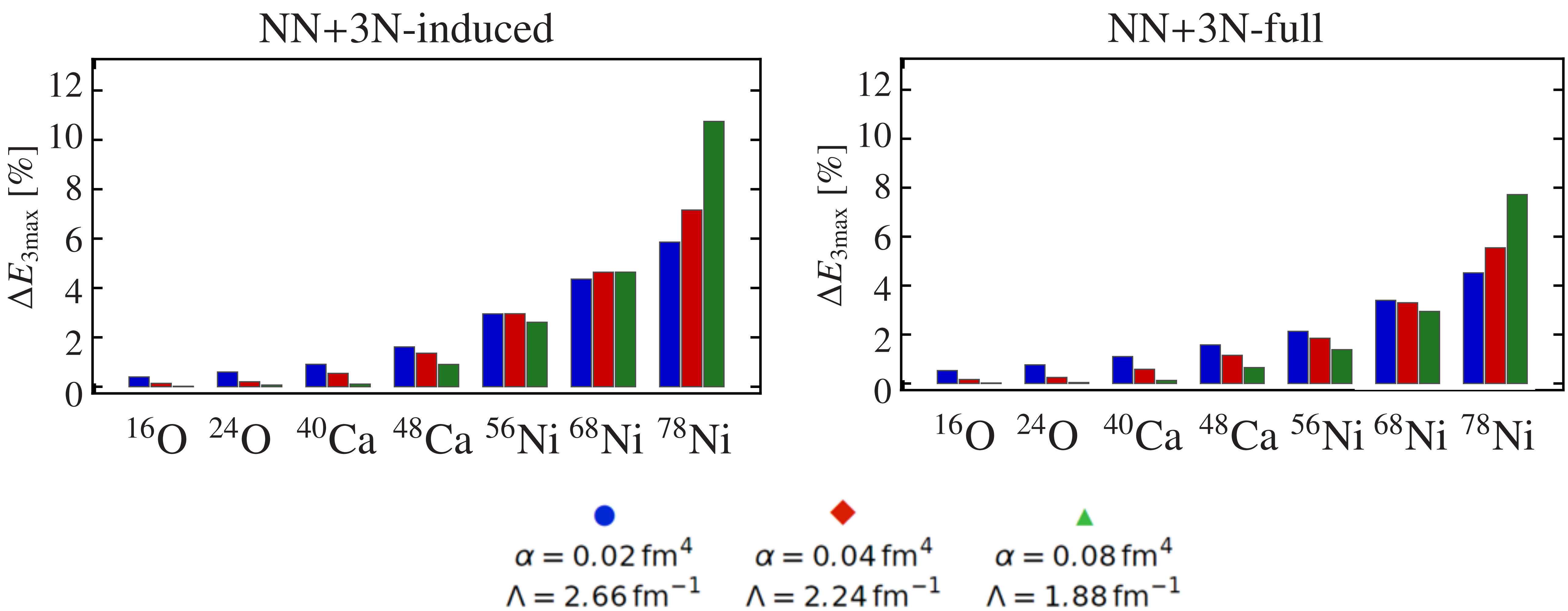

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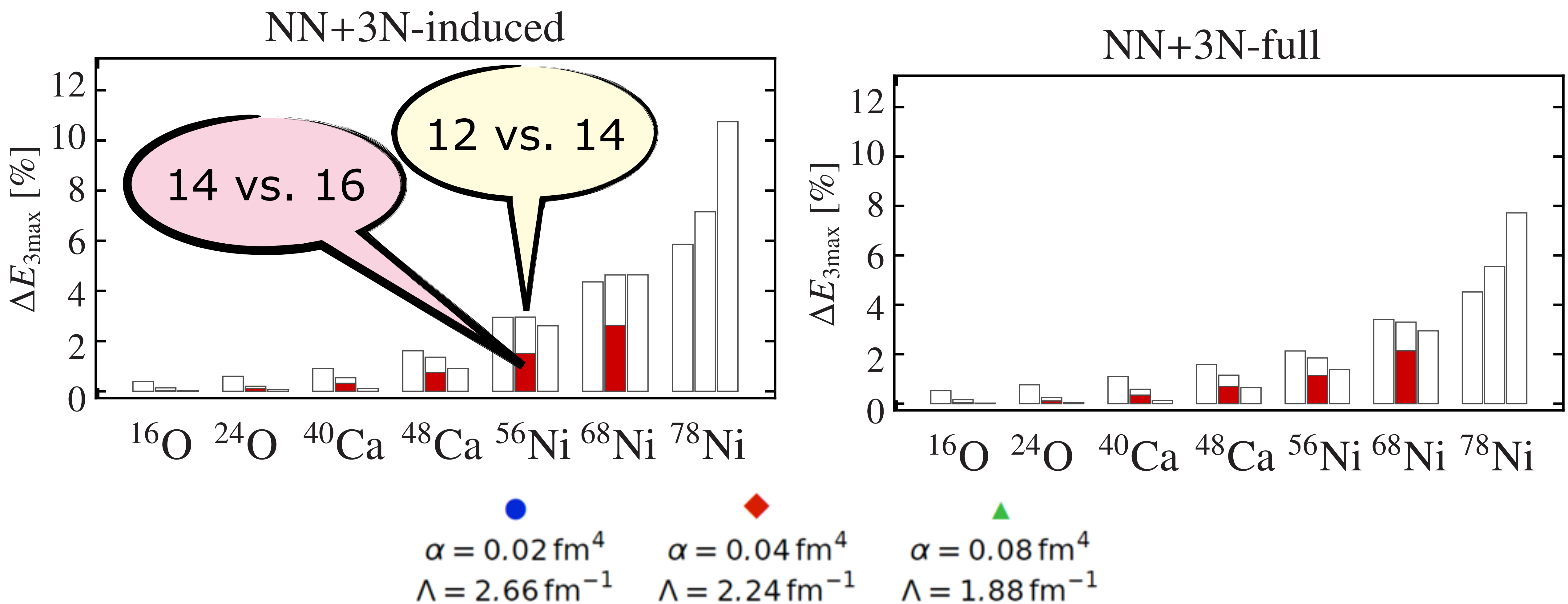
E_{3max} Dependence ($CCSD_{NO2B}$)

- E_{3Max}=14 vs. E_{3Max}=16 (HF reference state with explicit E_{3Max}=14 used)



- E_{3Max}=16 **not sufficient** beyond ^{56}Ni

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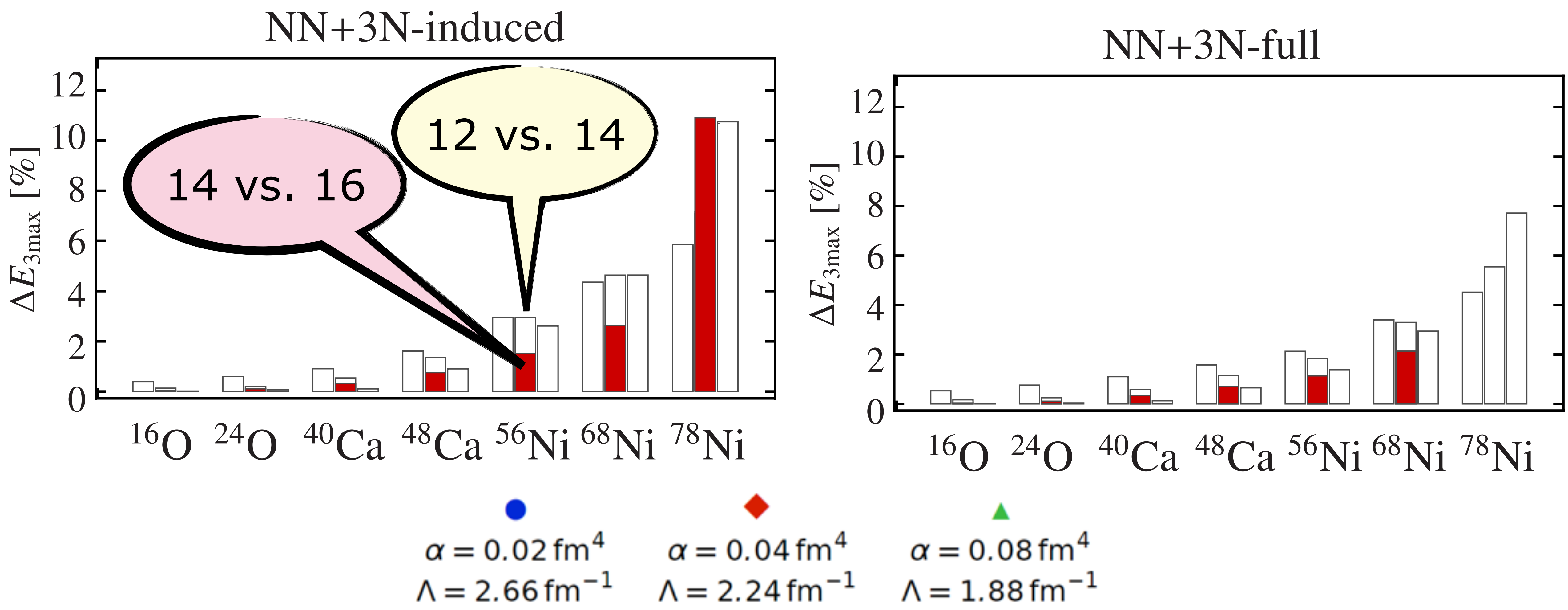

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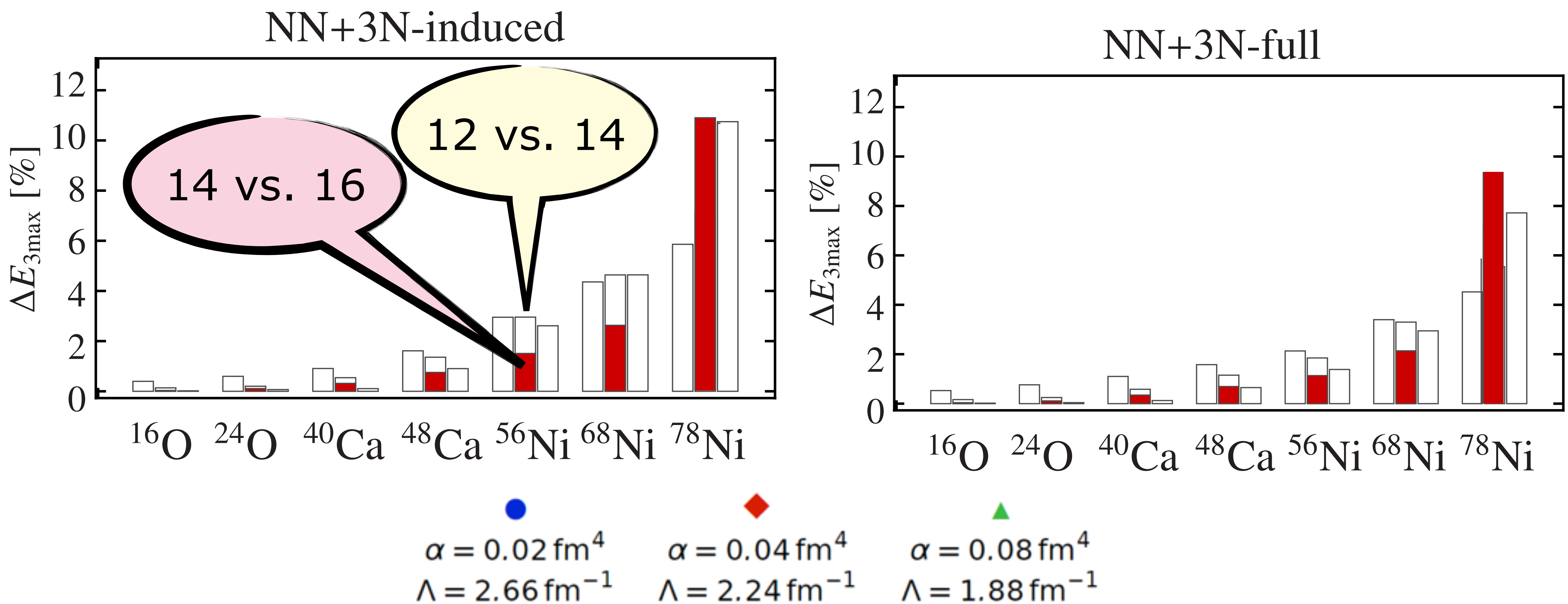

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Uncertainty Summary

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- **Normal-Ordering 2B Approximation**
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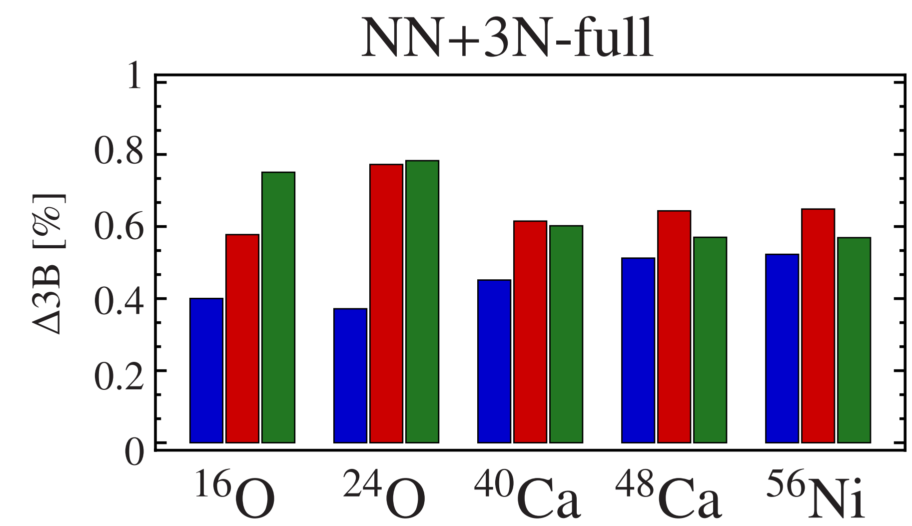
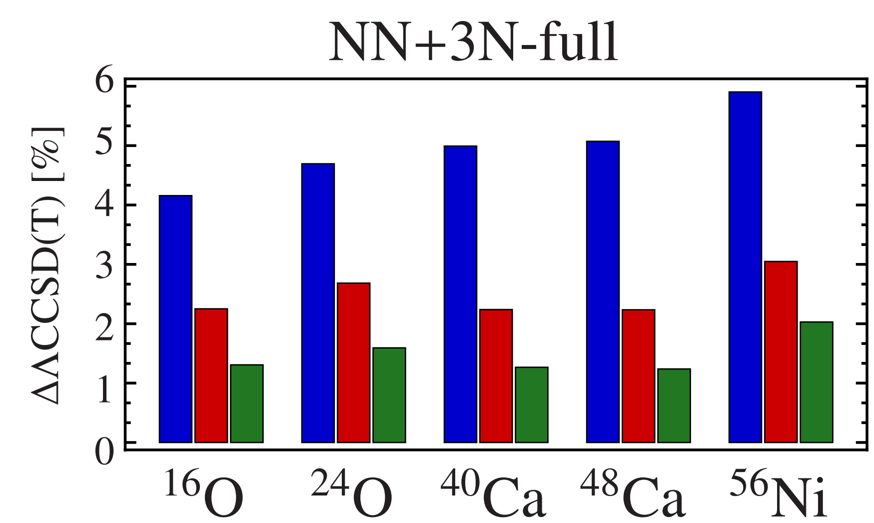
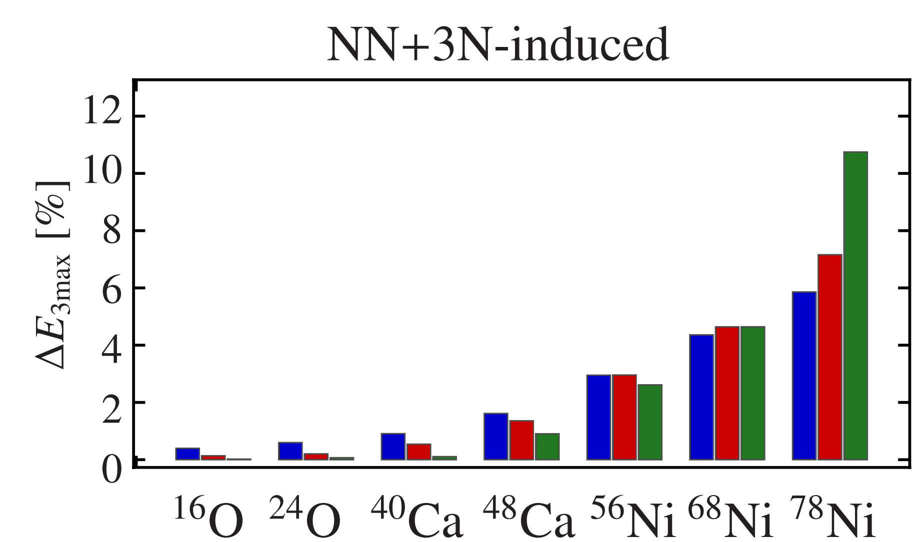
  - [ ] up to 6% contributions from ΛCCSD(T)
  - [x] soft interactions: only 1-2%
  - [x] no strong increase with mass number
- **E_{3Max} Cutoff**
  - [ ] up to ^{56}Ni: 2-3% effect for E_{3Max}=12-14
  - [x] 0.5% for soft interaction
  - [ ] rapid increase with mass number
  - [ ] E_{3Max}=16 not sufficient for A>60







Conclusions

- **medium-mass nuclei** are accessible with **ab initio methods**
- various **truncations** involved $\Rightarrow$ **error quantification** necessary
  - many-body methods can provide **accurate solutions** to Schroedinger equation
  - **generation** and **preparation** of the **input** (Hamiltonian) has emerged as the more challenging part:
    - construct interactions from **chiral EFT**
    - soften Hamiltonians through **SRG**
    - high-**E3Max** normal-ordering
    - **frequency conversion**

Epilogue

- **thanks to my group & collaborators**
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- H. Feldmeier, T. Neff
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- P. Papakonstantinou
  IPN Orsay, France

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Thanks for your attention!

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