Ab Initio Coupled-Cluster Calculations of Medium-Mass Nuclei

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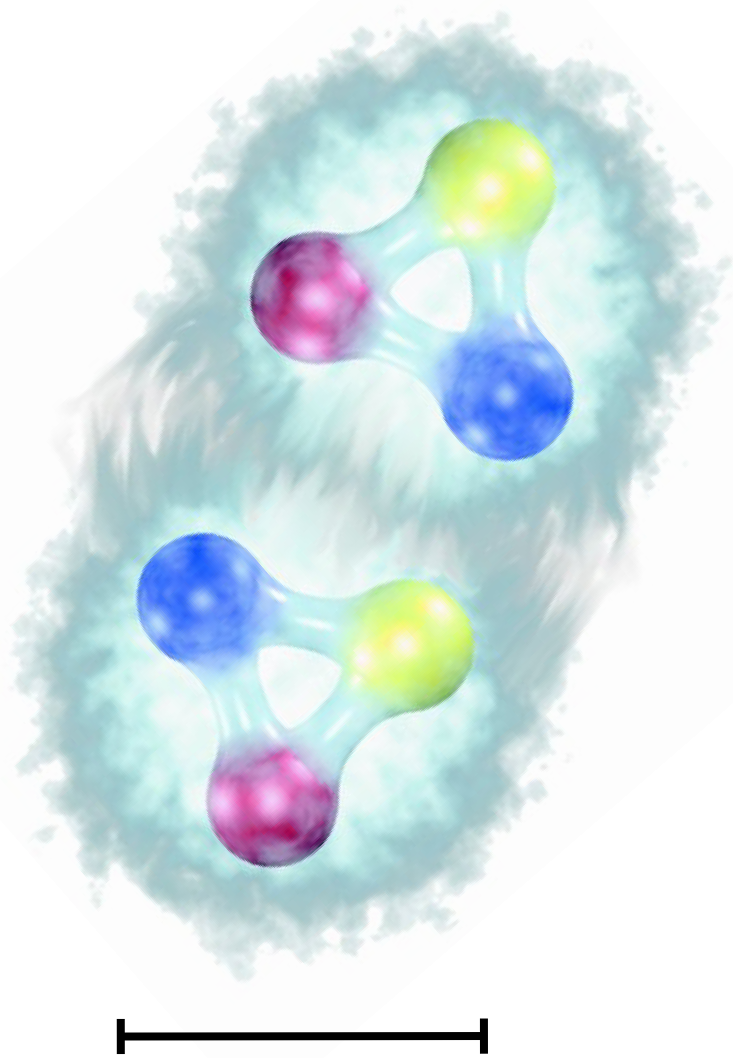
Nature of Nuclear Interaction



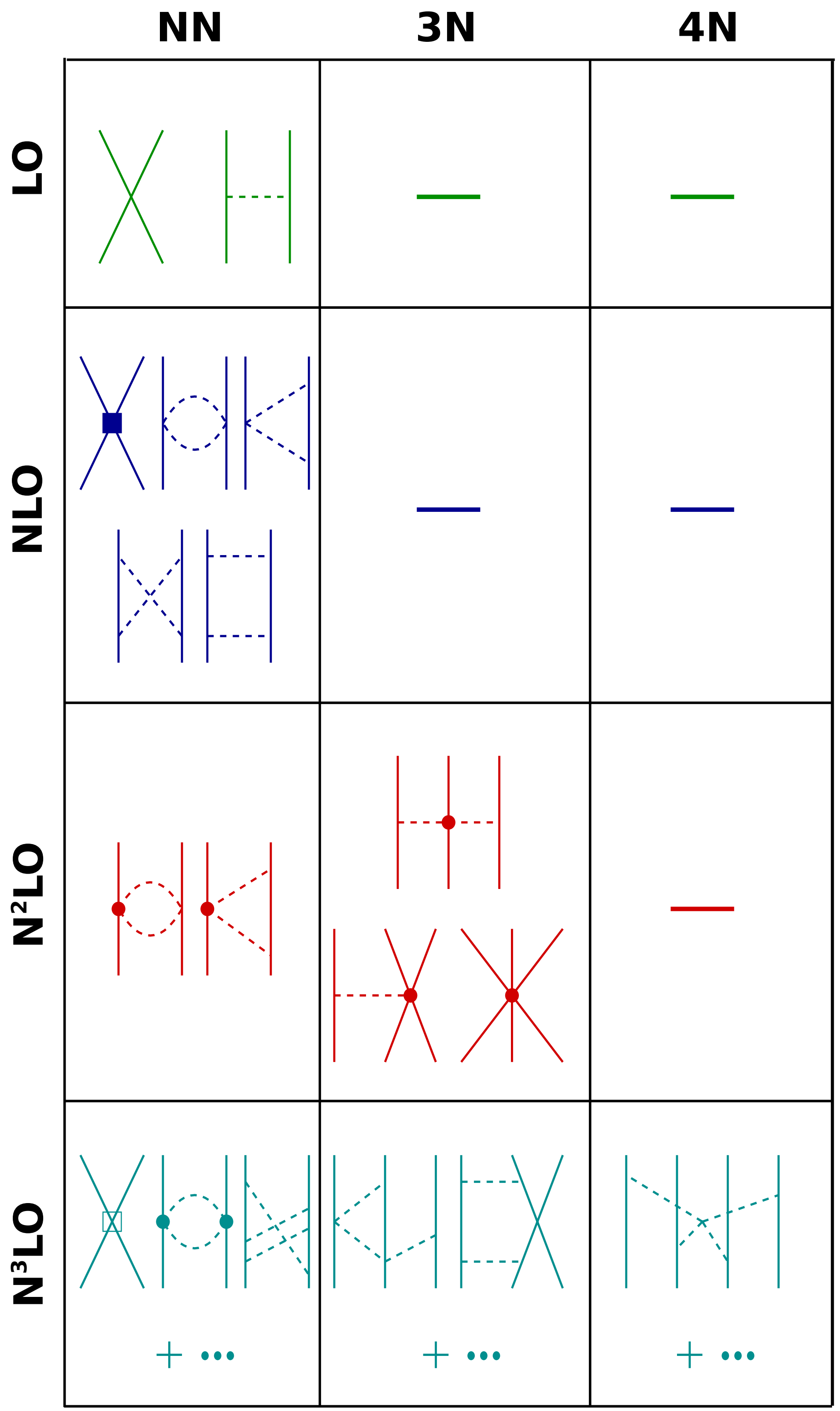
$\sim 1.6\ \text{fm}$

$\rho_0^{-1/3} = 1.8\ \text{fm}$

- NN-interaction is **not fundamental**
- analogous to **van der Waals** interaction between neutral atoms
- induced via mutual **polarization** of quark and gluon distributions
- acts only if the nucleons overlap, i.e., at **short ranges**
- genuine **3N-interaction** is important

Nuclear Interactions from Chiral EFT

- QCD **non-perturbative** at low energies
- low-energy **effective field theory** for relevant degrees of (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)



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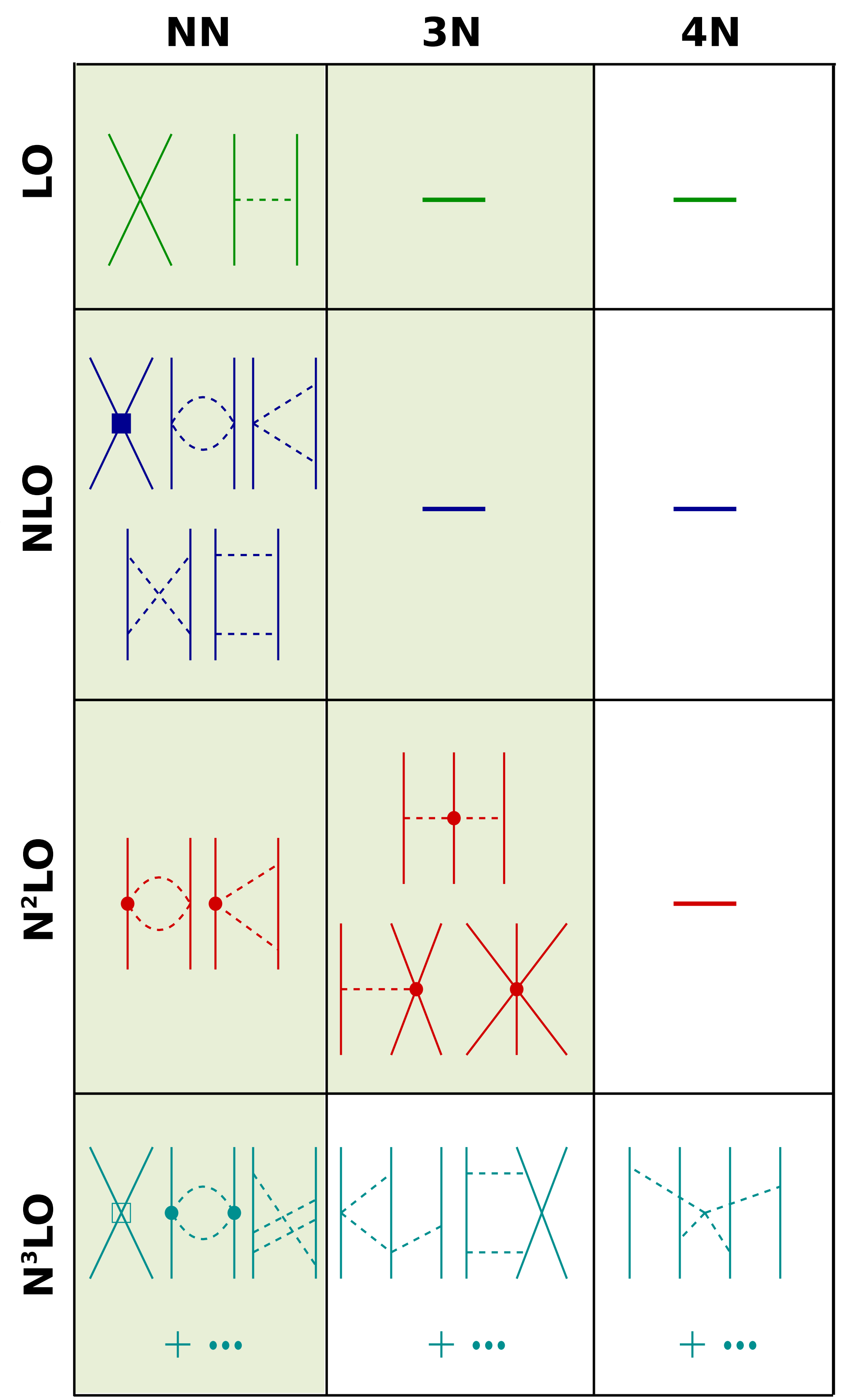


From QCD to Nuclear Structure

Nuclear Structure

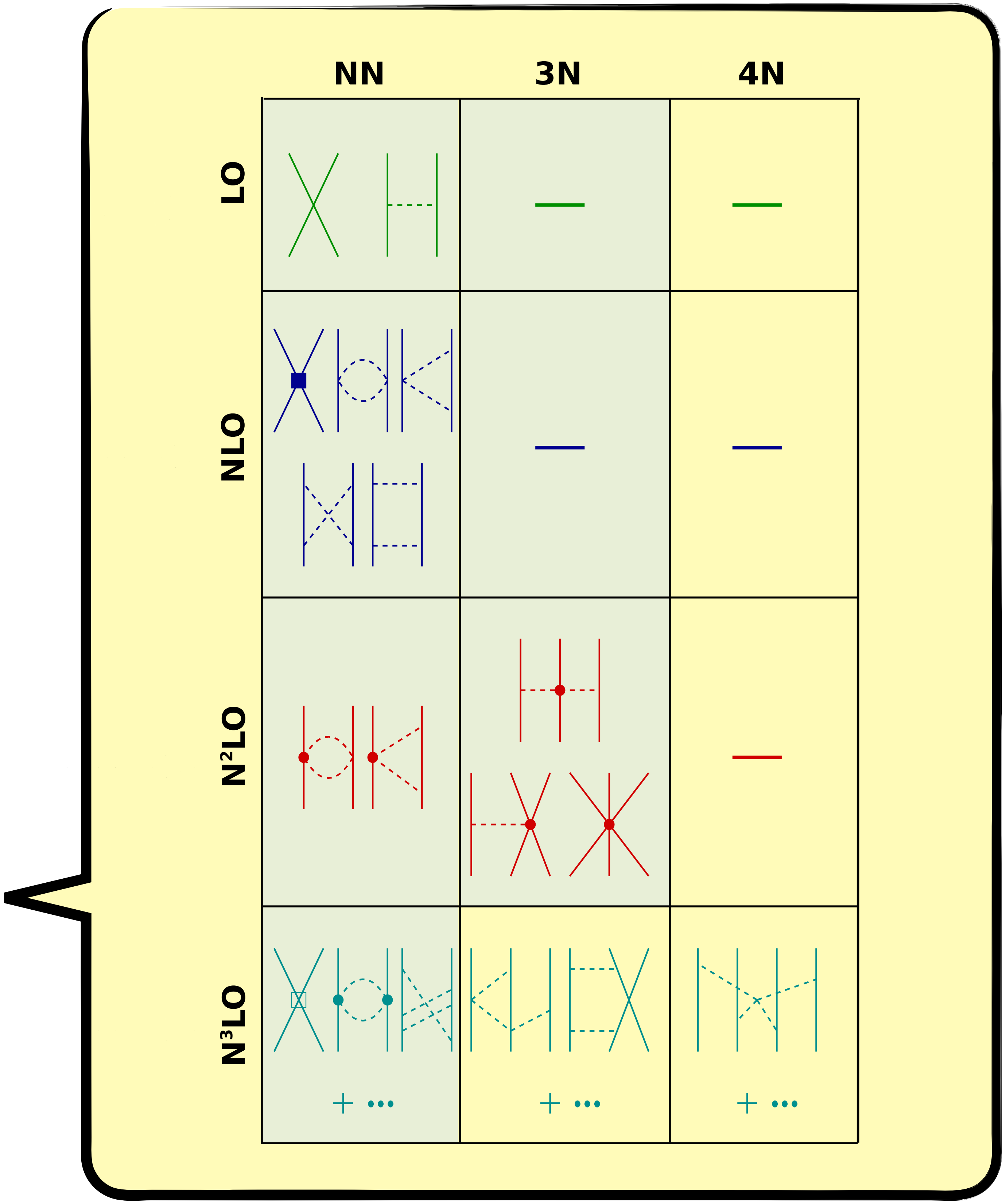
Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

NN+3N interaction
from Chiral EFT

Low-Energy QCD



From QCD to Nuclear Structure

Nuclear Structure

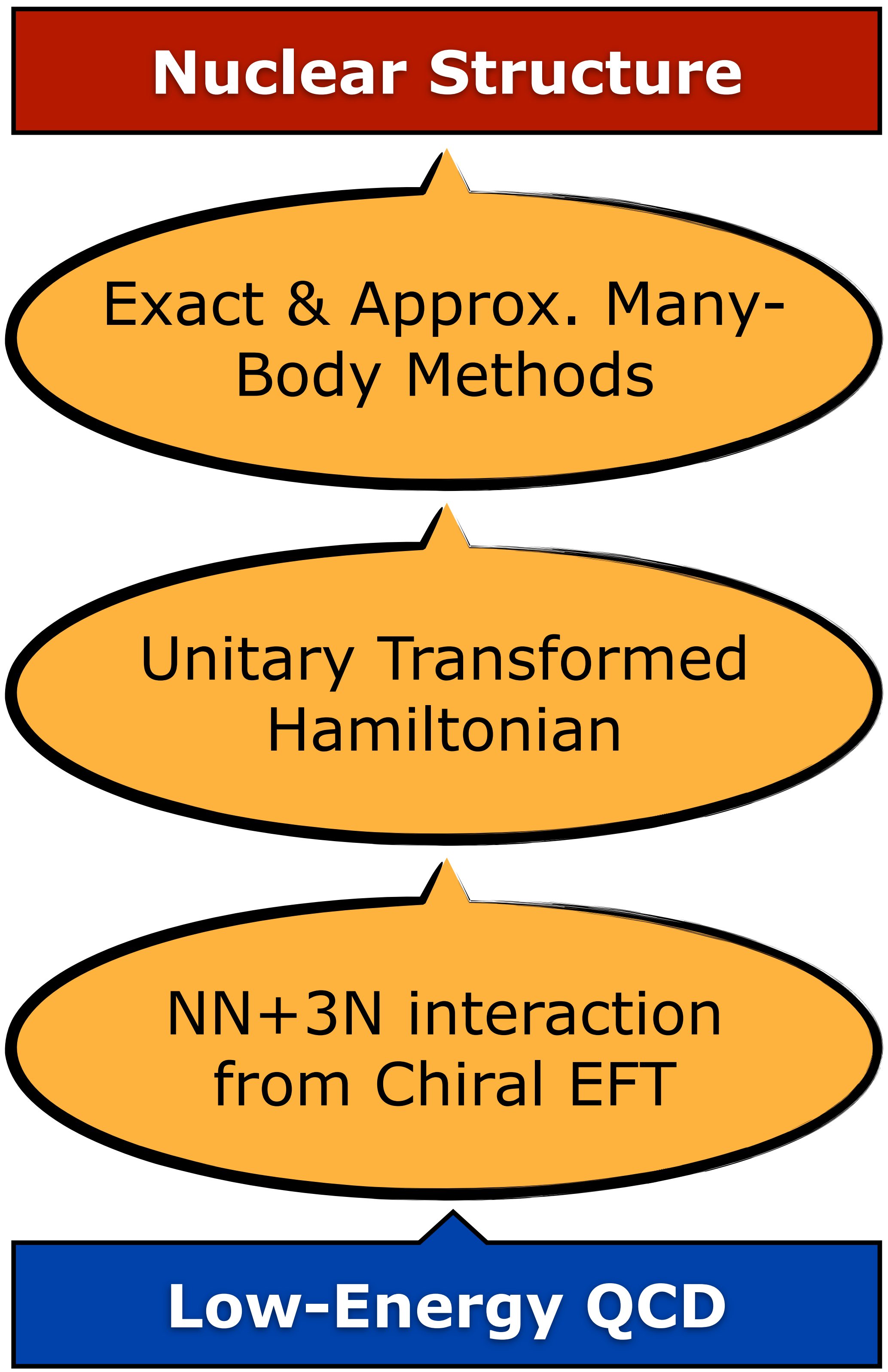
Unitary Transformed Hamiltonian

adapt Hamiltonian to truncated low-energy model spaces

NN+3N interaction from Chiral EFT

Low-Energy QCD

From QCD to Nuclear Structure



- 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

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

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

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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Light Nuclei from the IT-NCSM

R. Roth, J. Langhammer, A. Calci et al. --- Phys. Rev. Lett. 107, 072501 (2011)

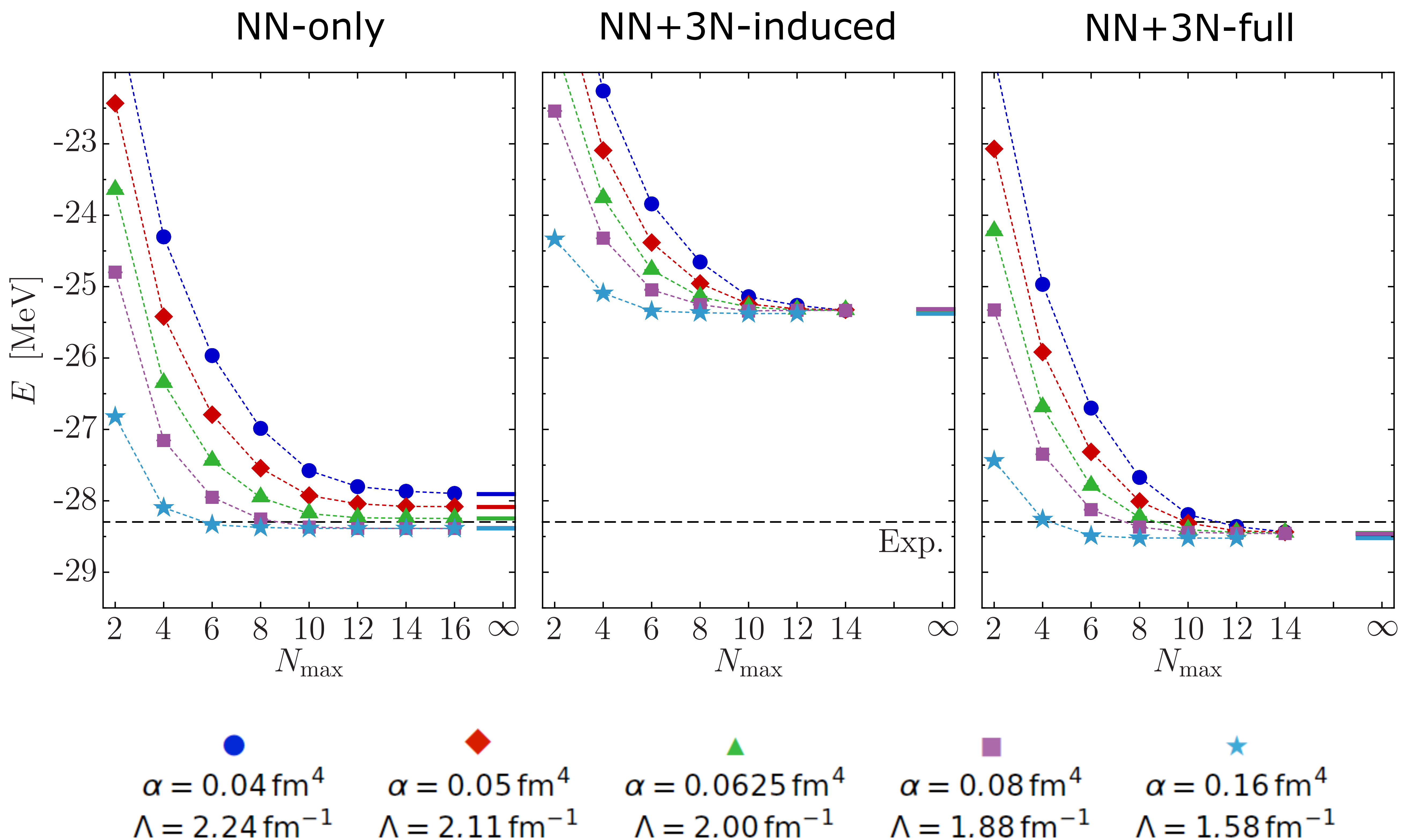
P. Navrátil et al. --- Phys. Rev. C 82, 034609 (2010)

R. Roth --- Phys. Rev. C 79, 064324 (2009)

IT–NCSM

- **CI**: truncate wave operator $\hat{C}$ at some **excitation level**
  - $$\hat{C}_{\text{CISD}} = c_0 + \sum_{ai} c_i^a \; \hat{a}_a^\dagger \hat{a}_i + \sum_{abij} c_{ij}^{ab} \; \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i$$
- **NCSM**: truncate at **excitation energy** $N_{\max}\hbar\Omega$
  - $$\hat{C}_{\text{NCSM}} = c_0 + \sum_{ai} c_i^a \; \hat{a}_a^\dagger \hat{a}_i + \sum_{abij} c_{ij}^{ab} \; \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i + \ldots$$
    $$\Big(e_a + e_b \cdots - e_i - e_j \leq N_{\max}\Big)$$
  - **center-of-mass** part factorizes in the wave function
- **IT-NCSM**: extend range of NCSM by selective inclusion of basis states according to their individual importance for the problem at hand

^{4}He: Ground–State Energies



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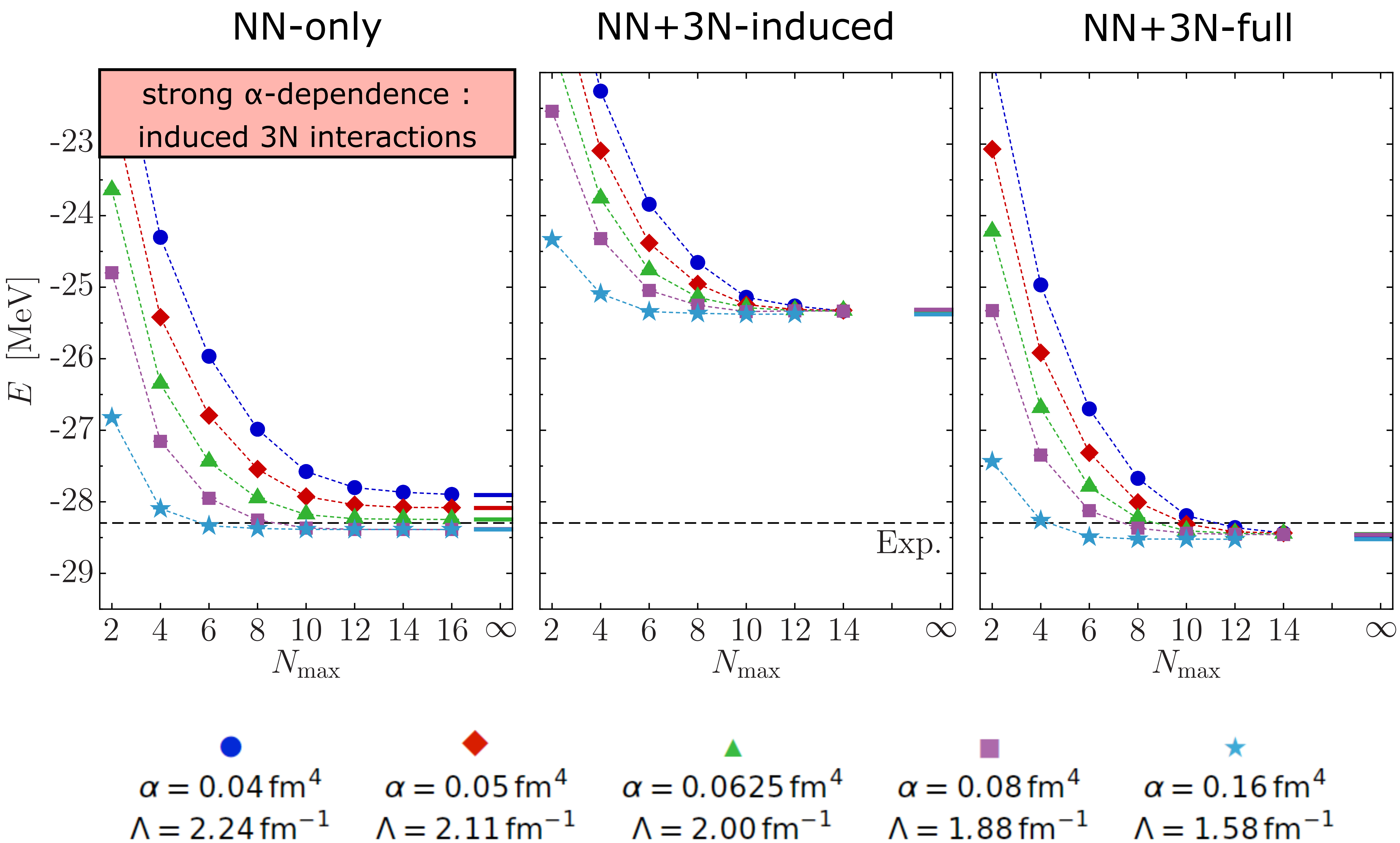

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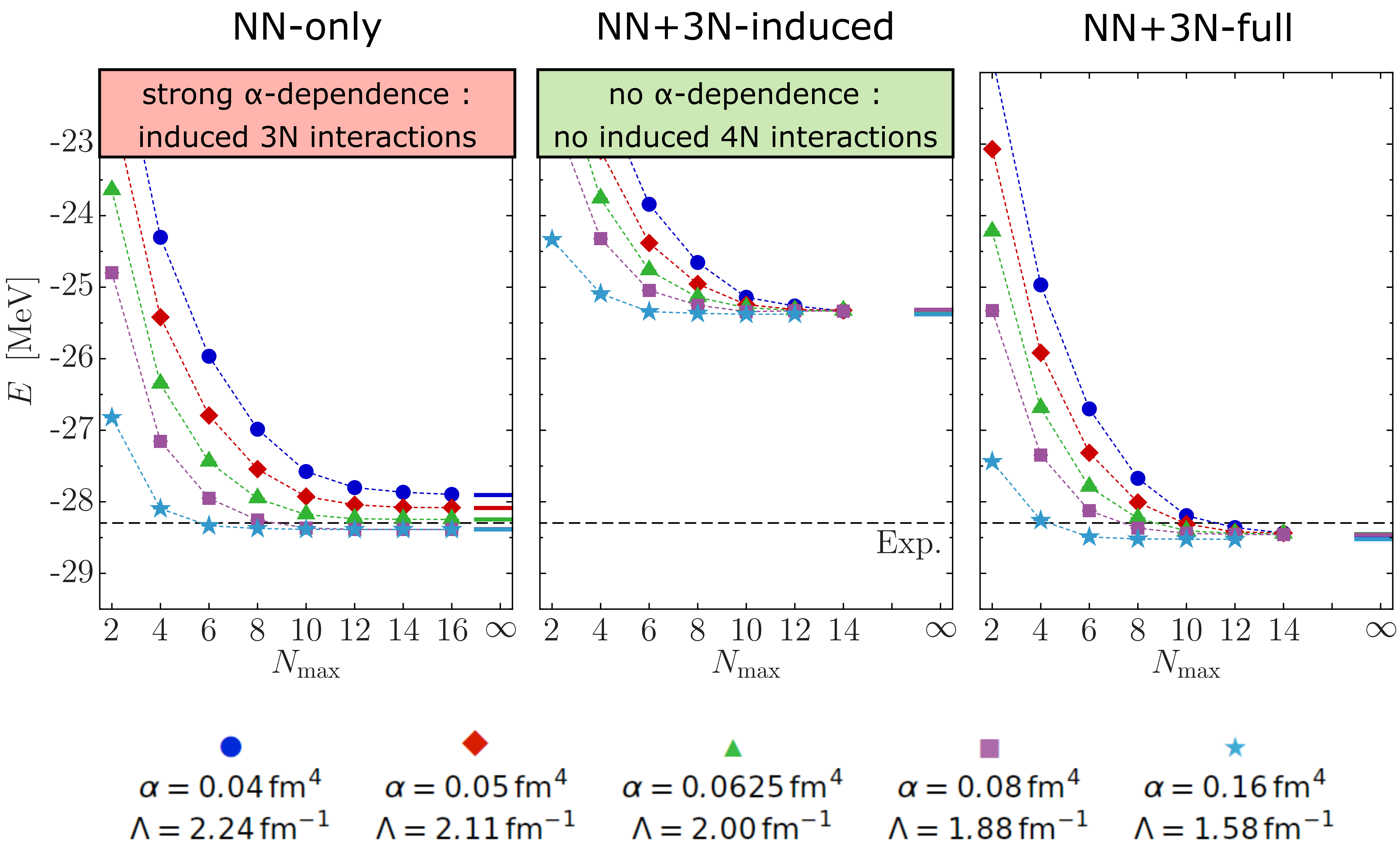

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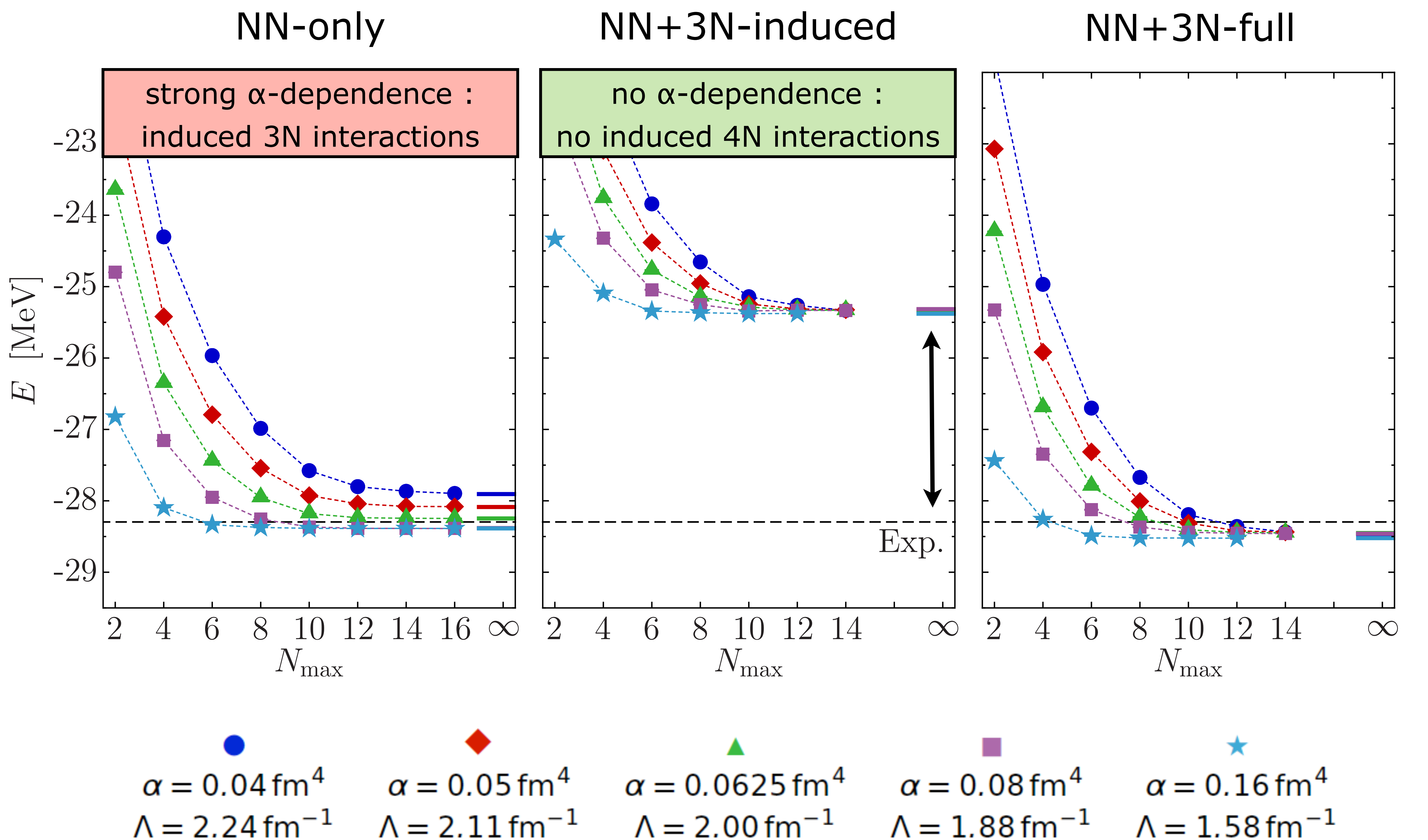

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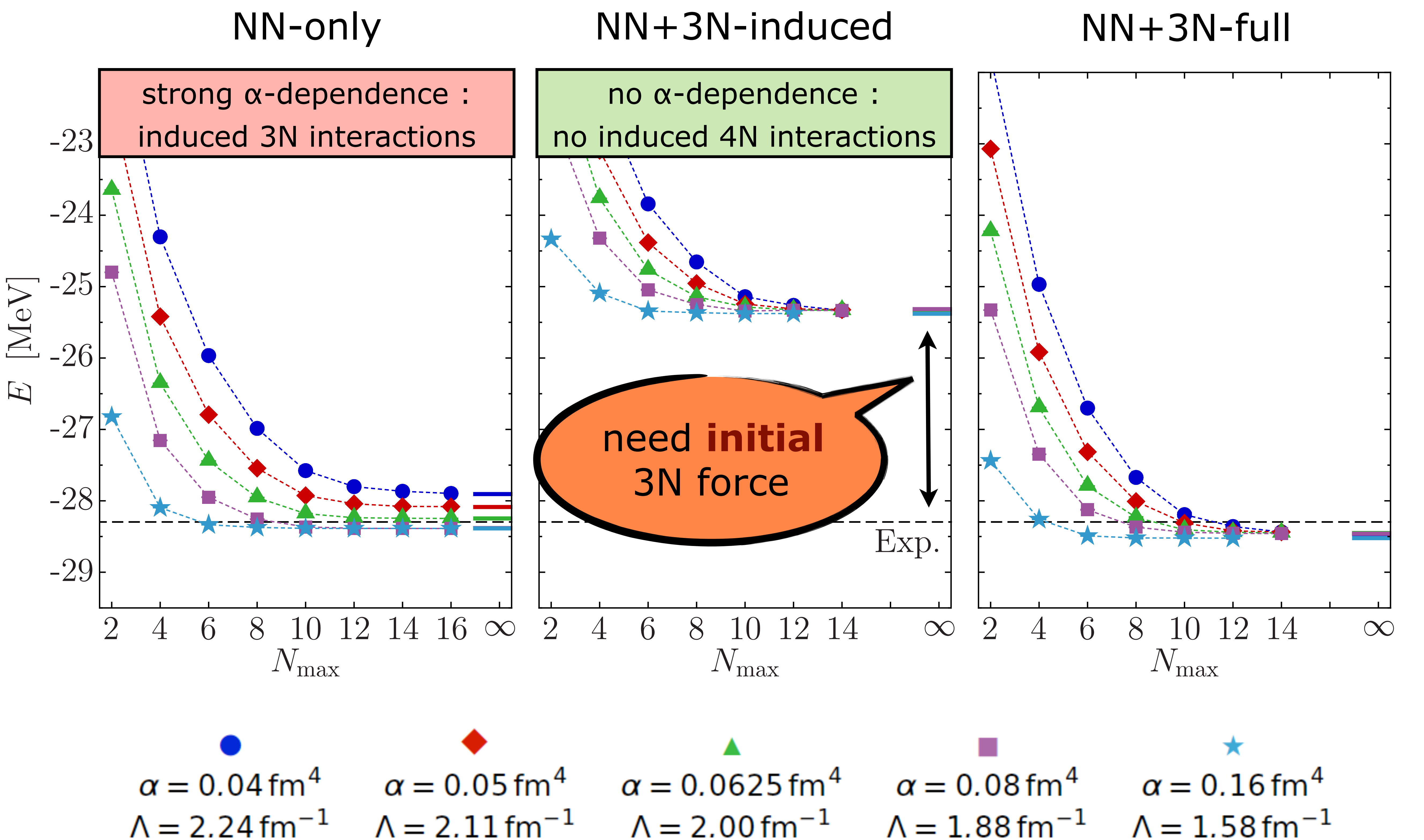

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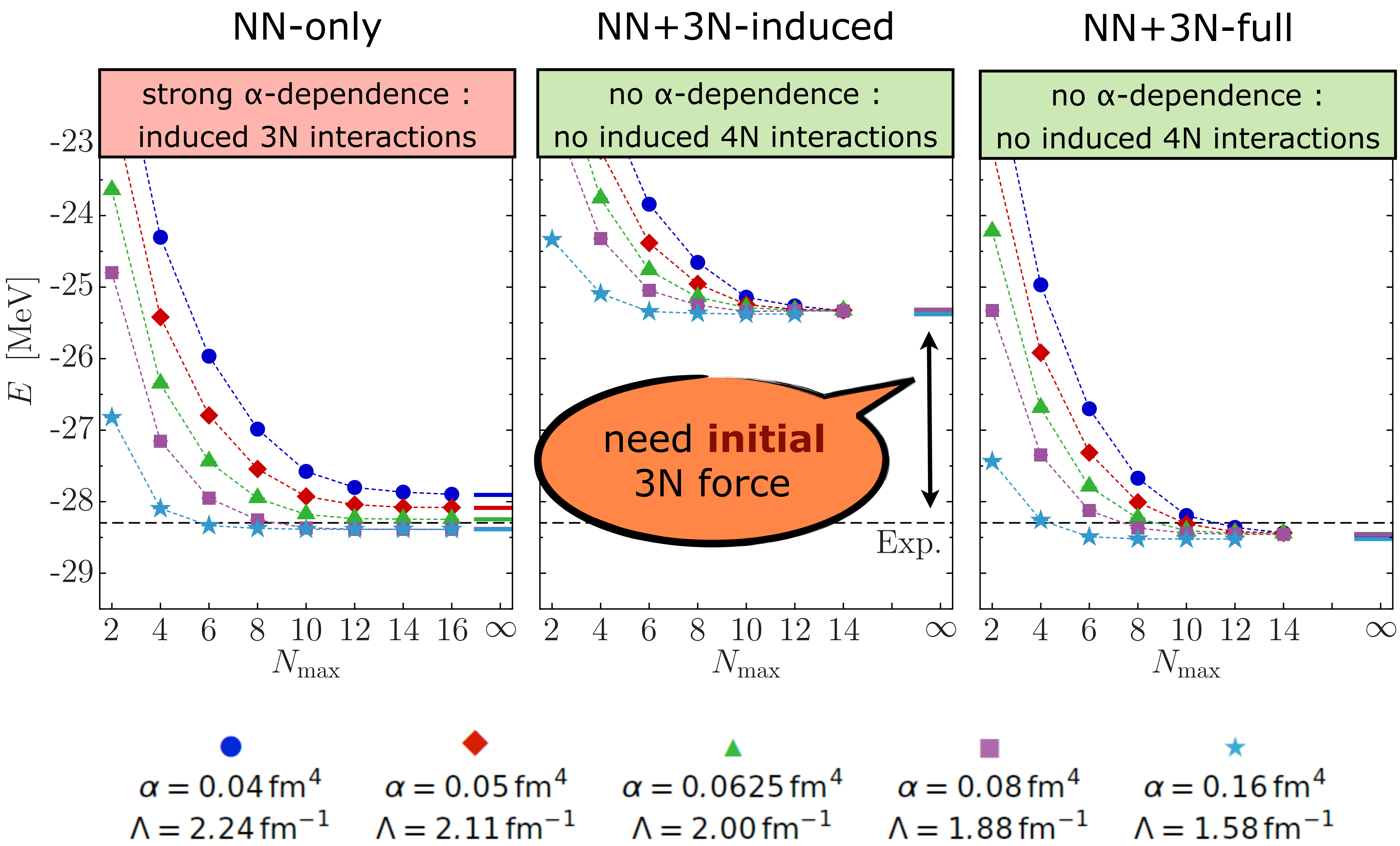
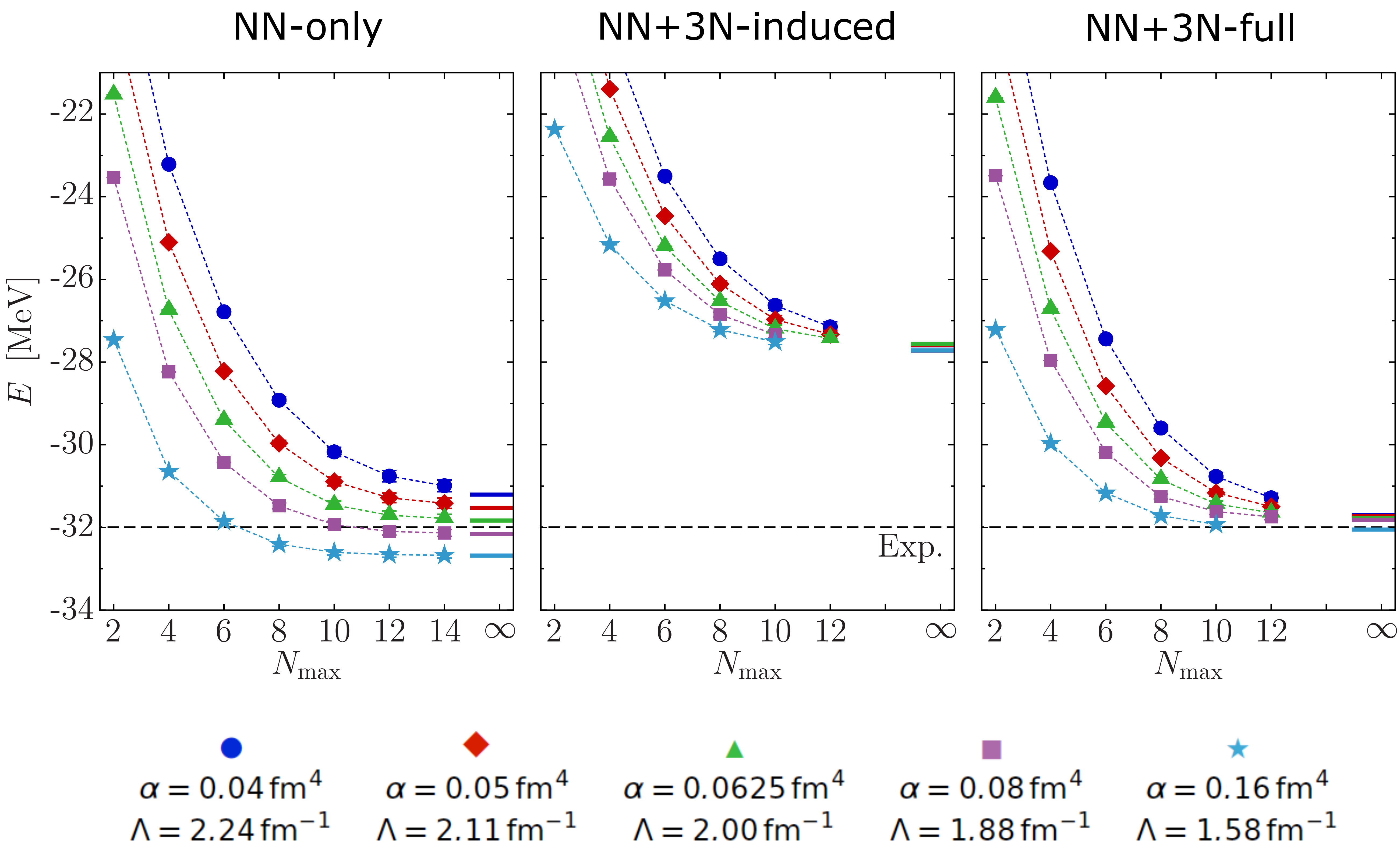
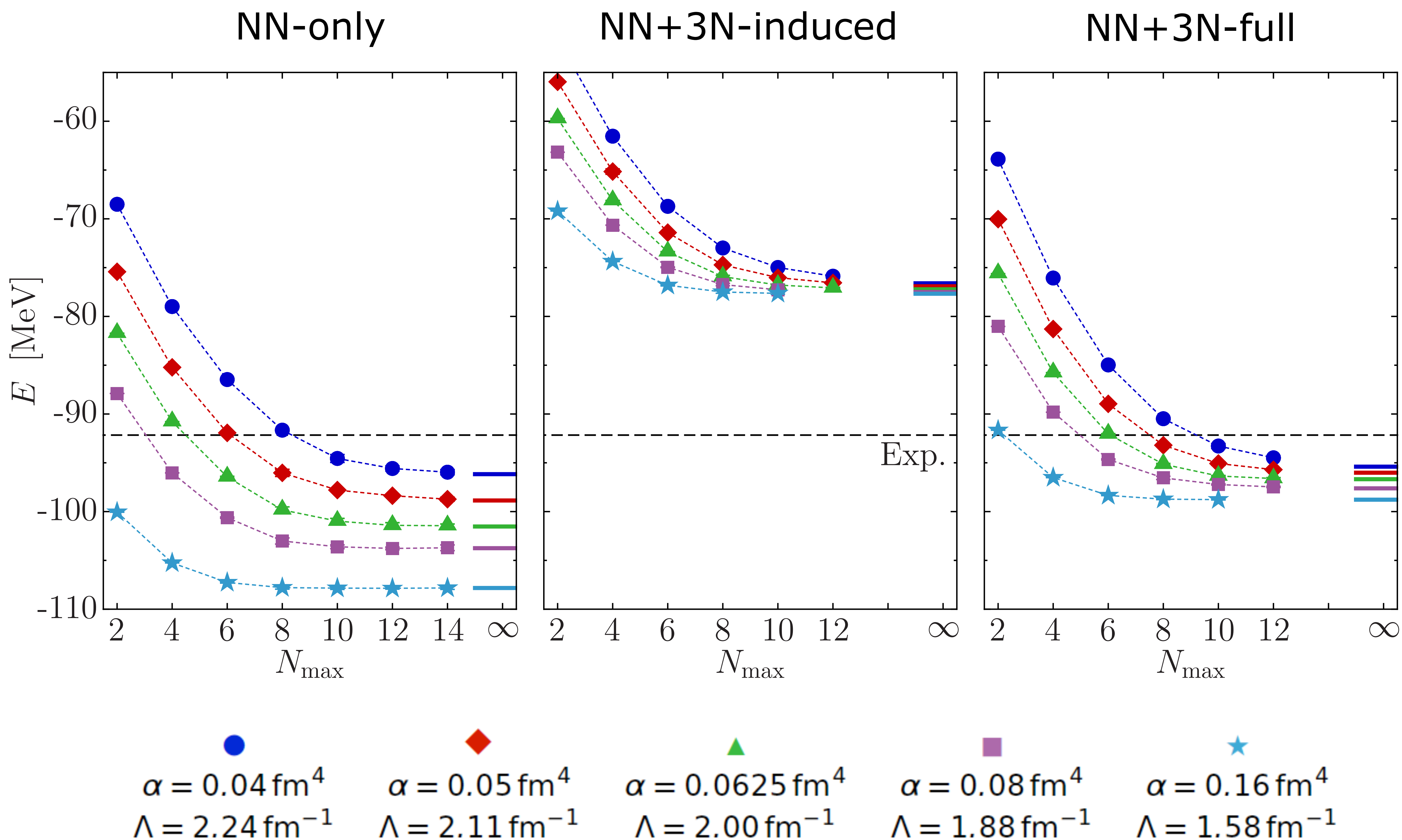


^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies



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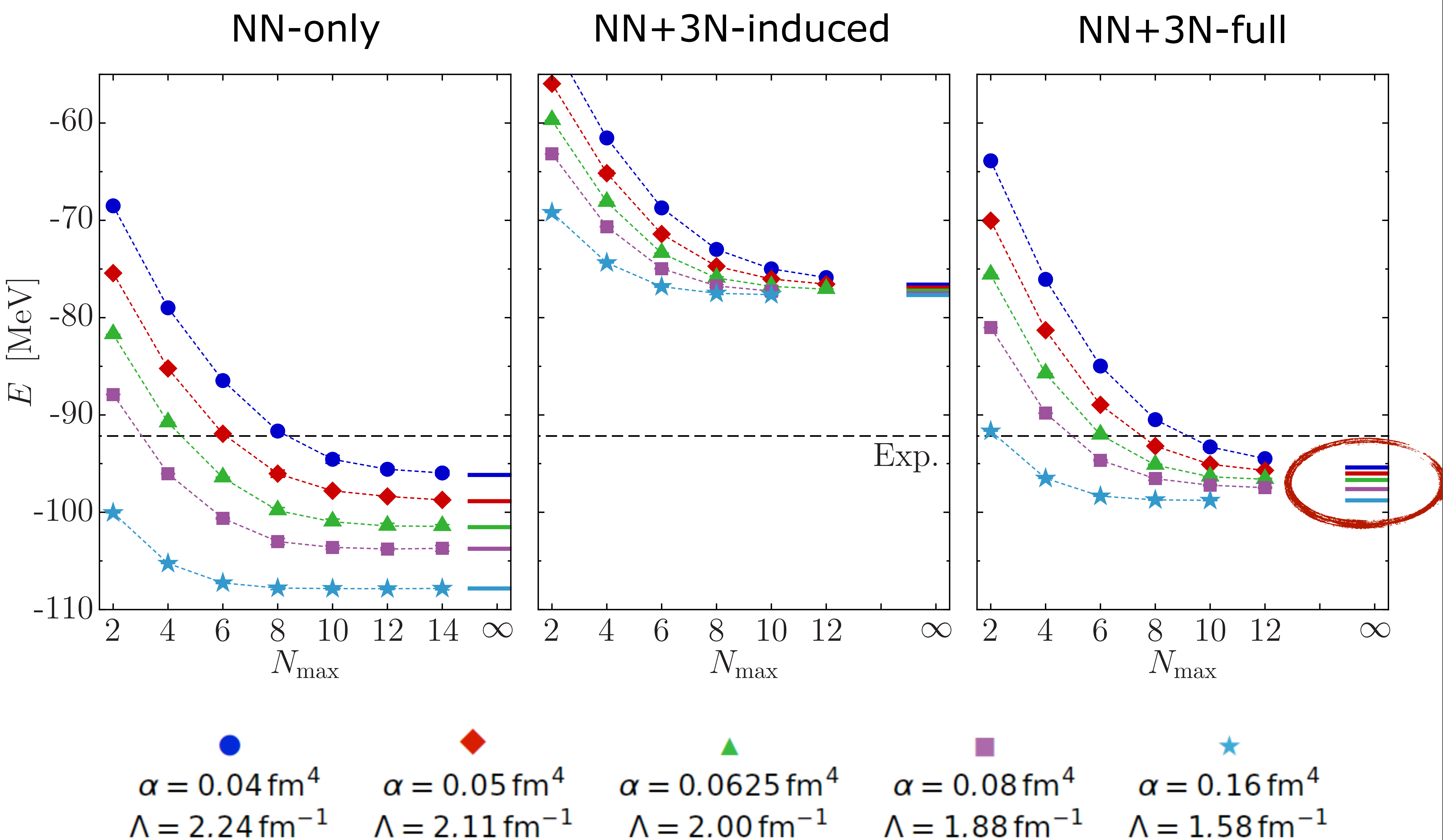

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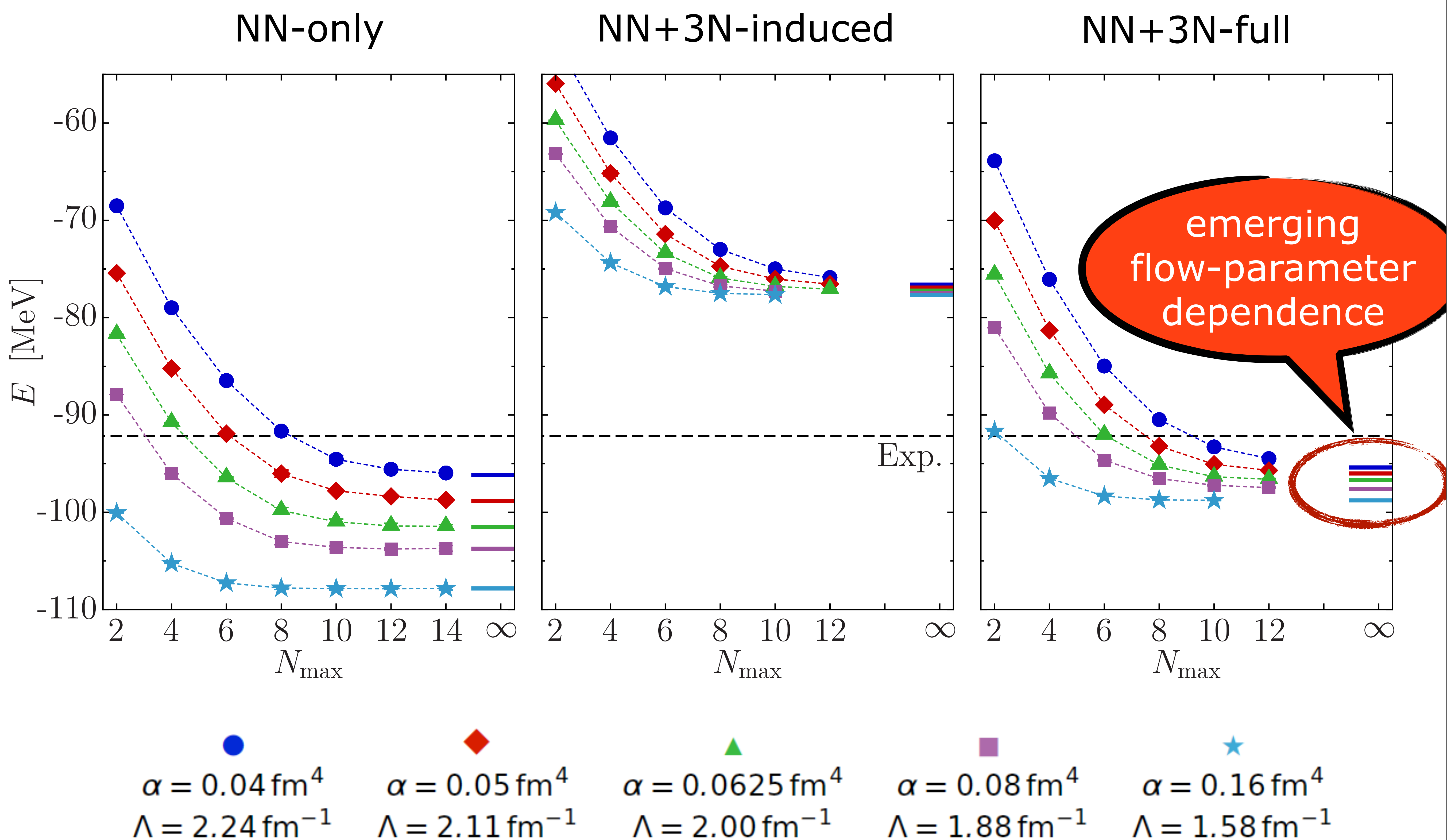
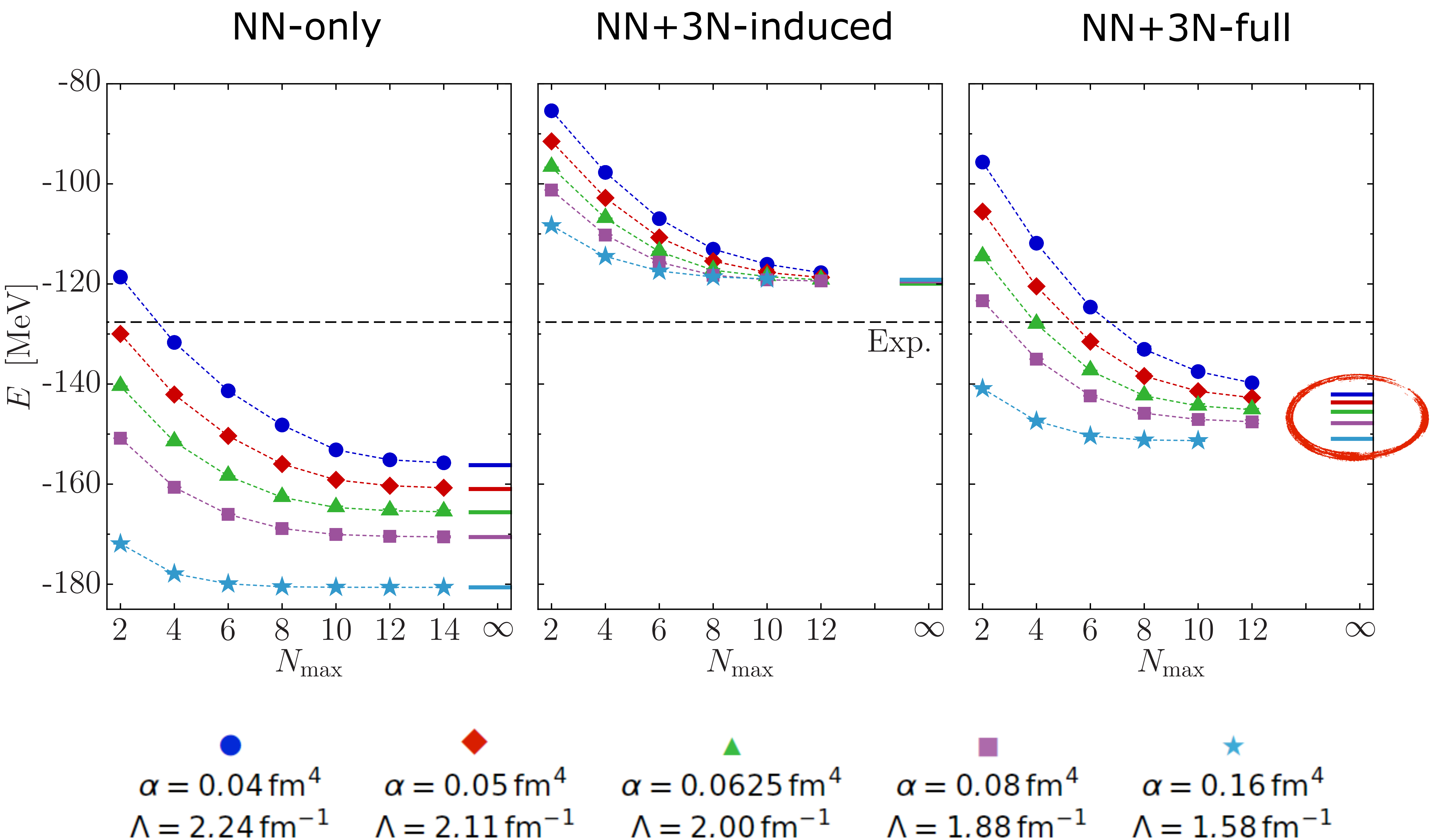


^{16}O: Ground-State Energies



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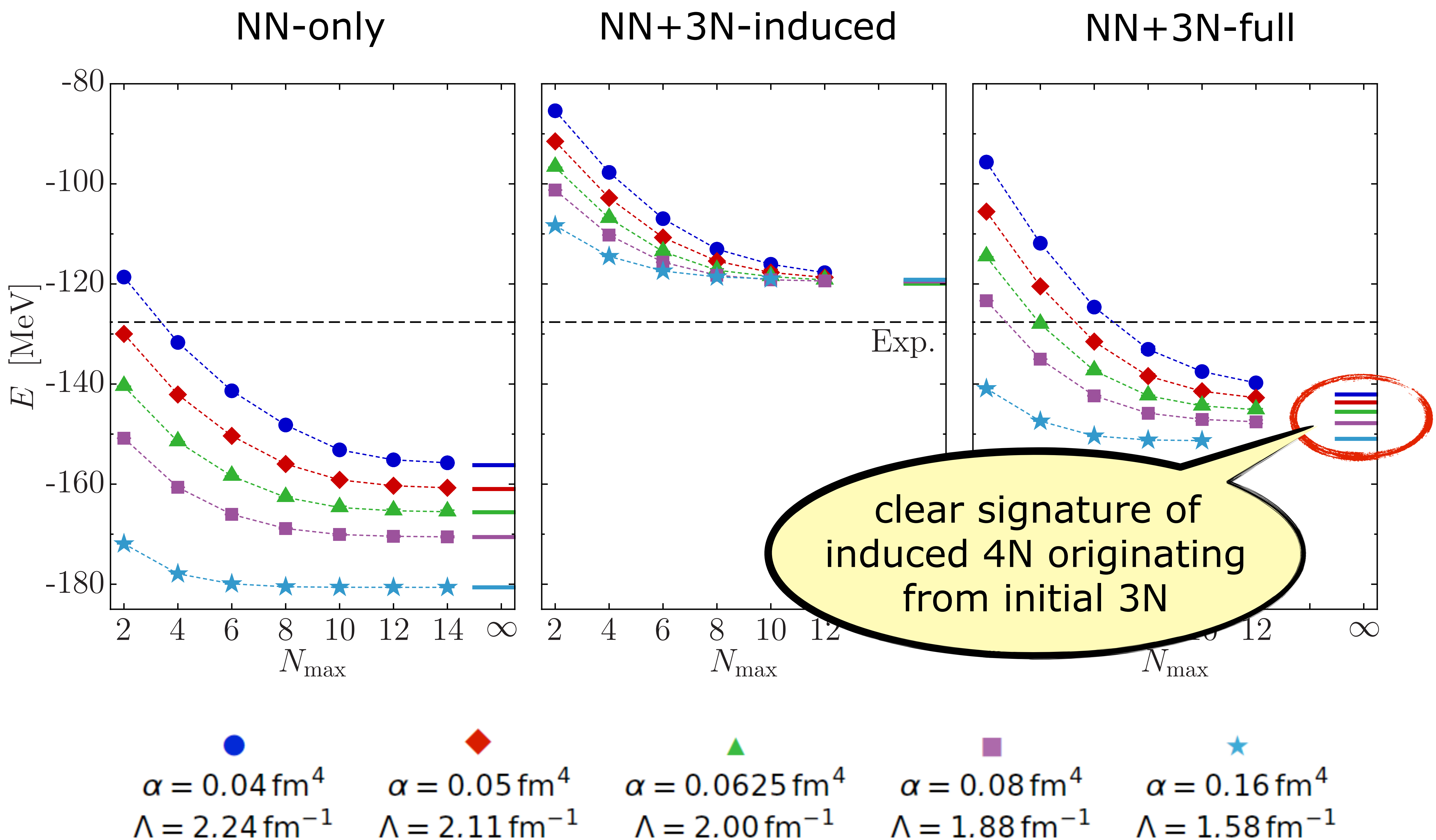

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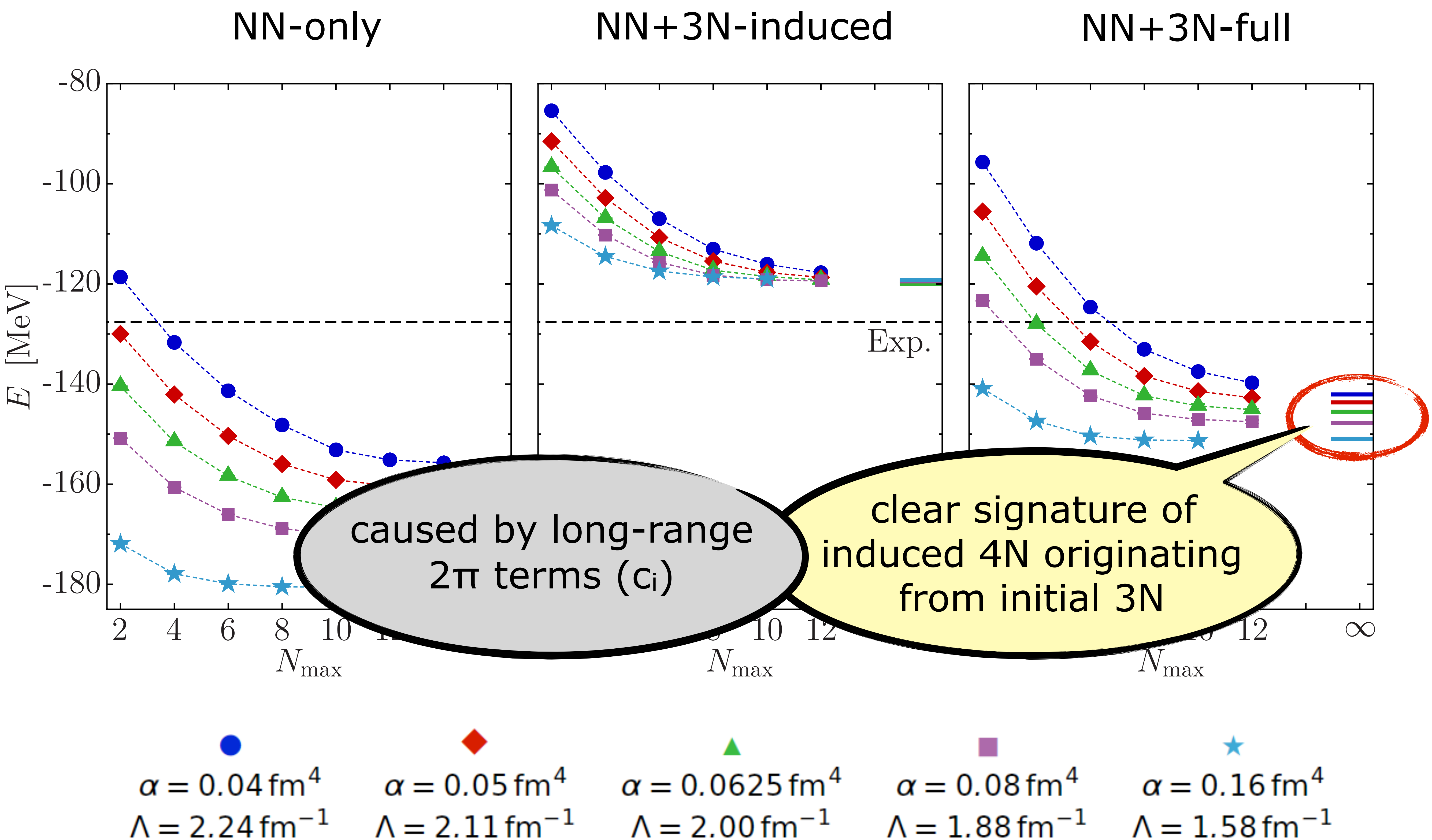

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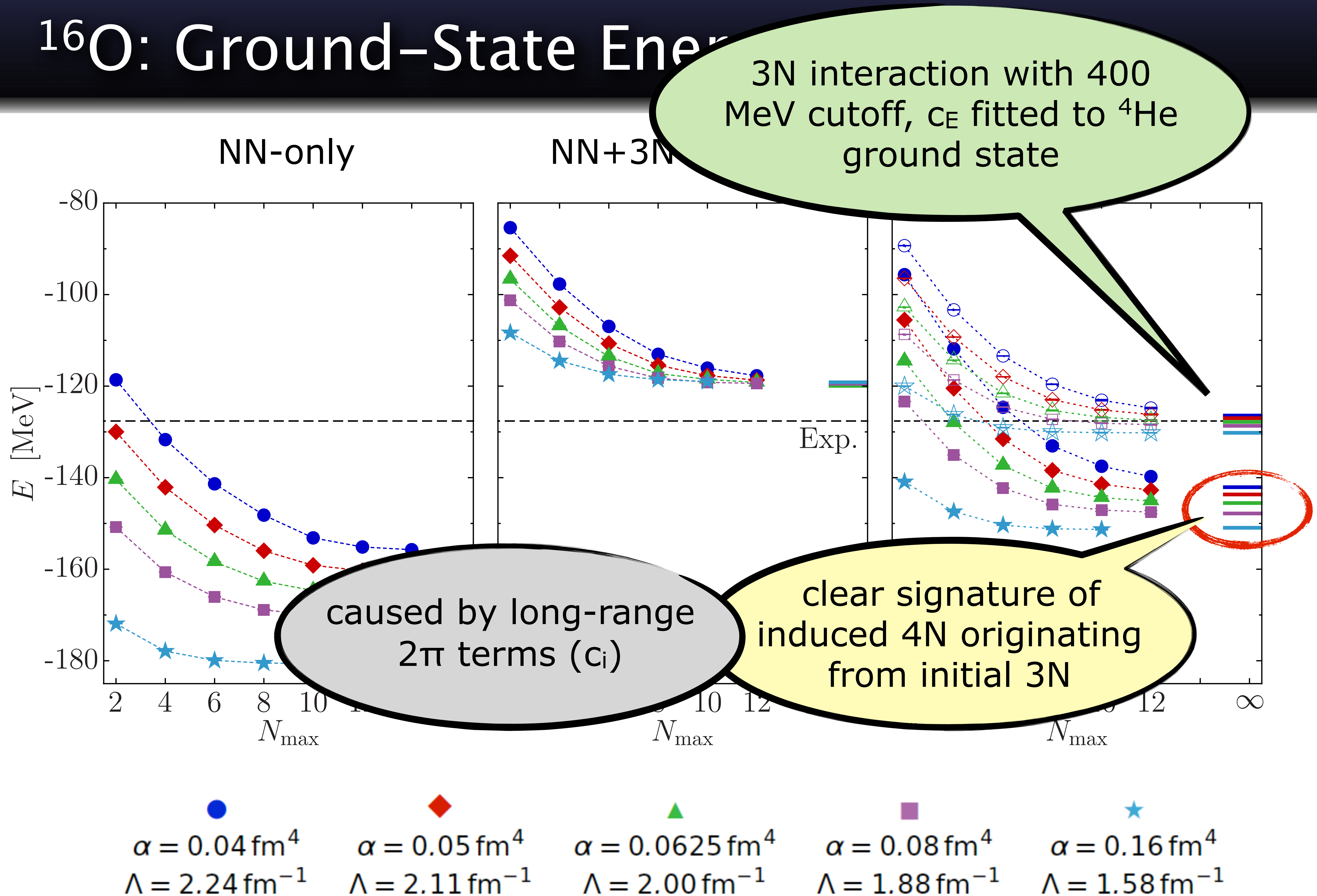

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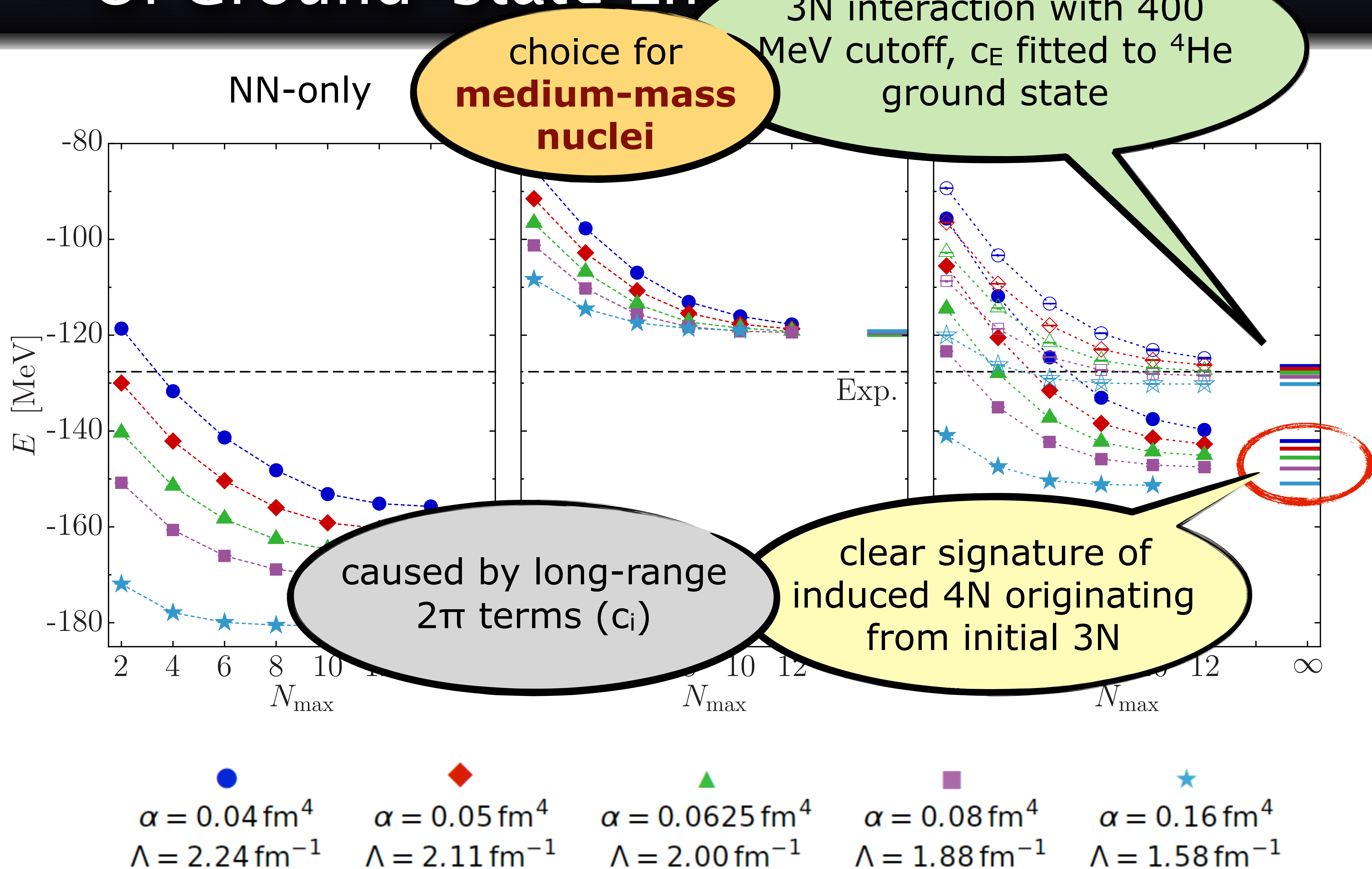

Coupled Cluster Method

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

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

- $\hat{T}_n$: ***n*p*n*h 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**

Coupled Cluster Approach

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

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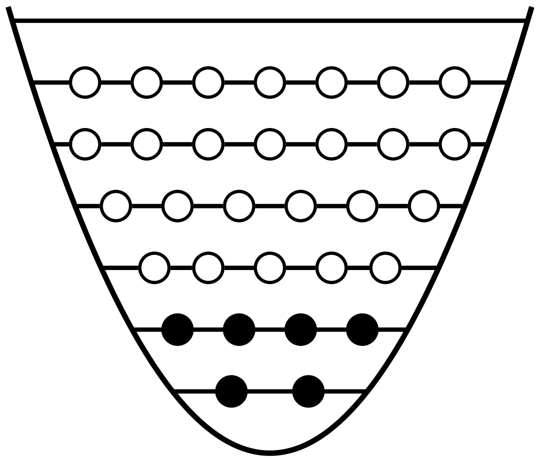

$|\Phi_0\rangle$

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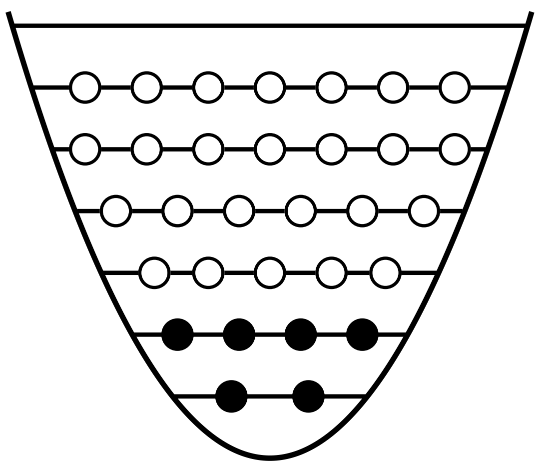

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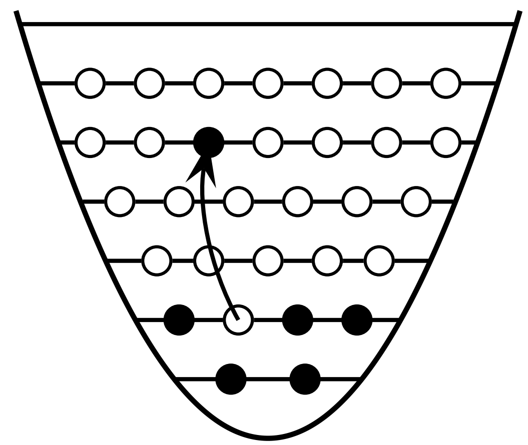

$\hat{T}_1 \, |\Phi_0\rangle$

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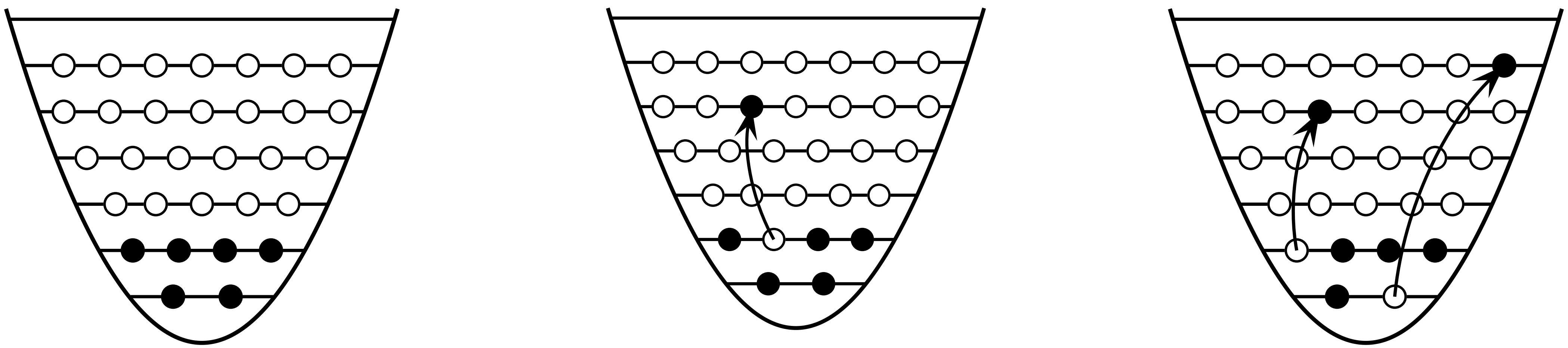

$|\Phi_0\rangle$ $\hat{T}_1 |\Phi_0\rangle$ $\hat{T}_2 |\Phi_0\rangle$

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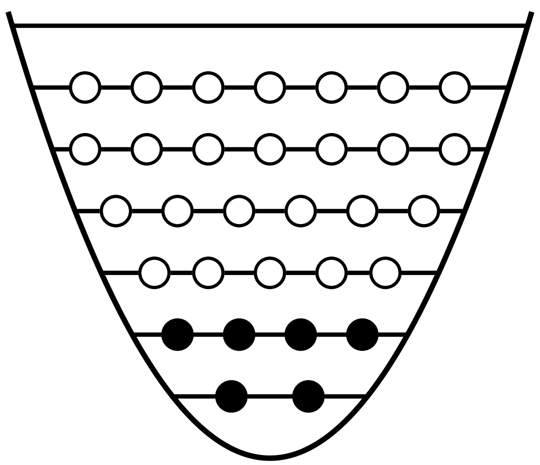

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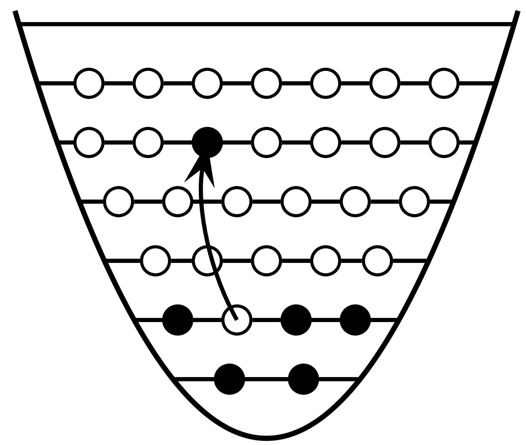
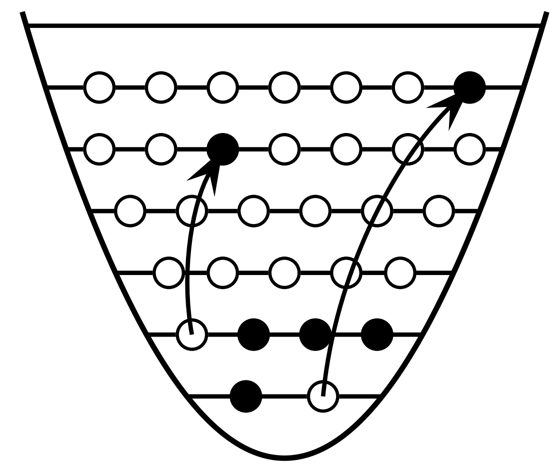
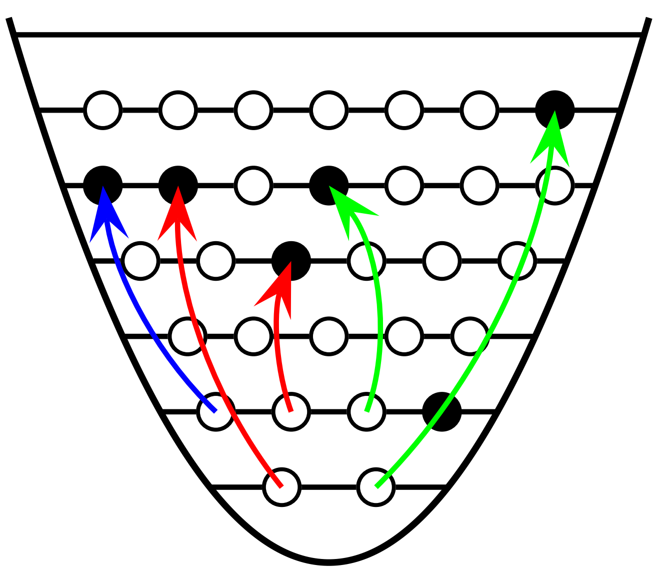


$\hat{T}_1\,|\Phi_0\rangle$



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



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

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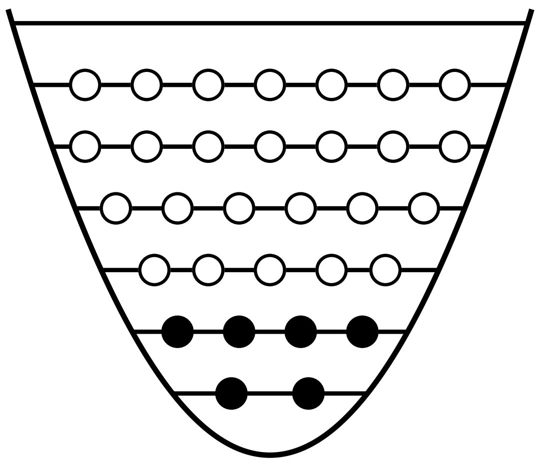
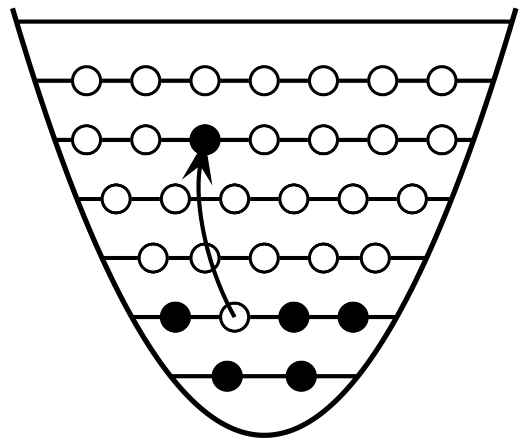


$|\Phi_0\rangle$



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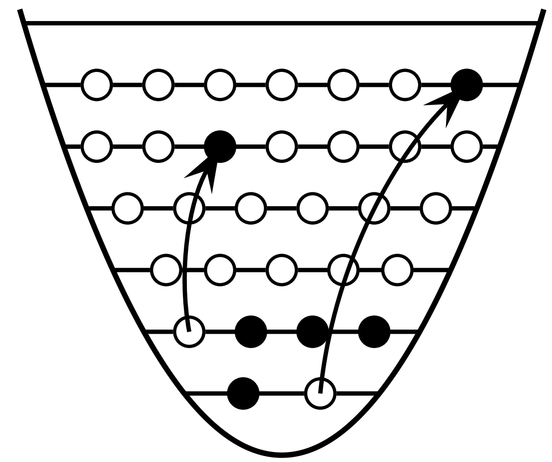

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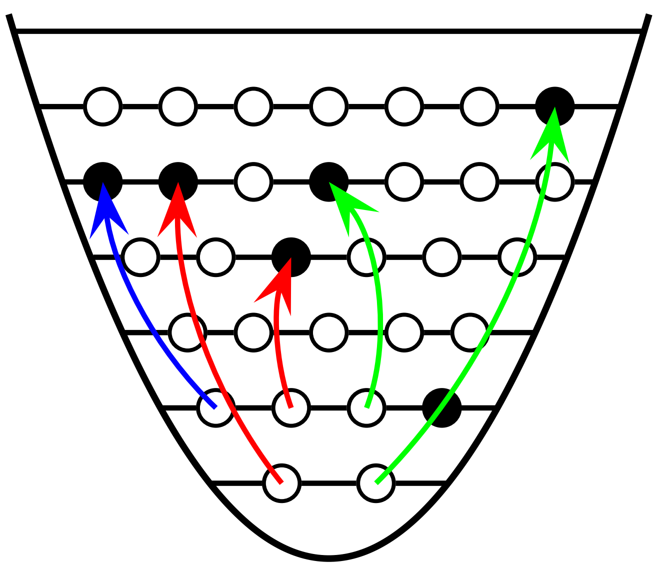


$\hat{T}_1 \, \hat{T}_2 \, \hat{T}_2 \, |\Phi_0\rangle$

- CCSD equations

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

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

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

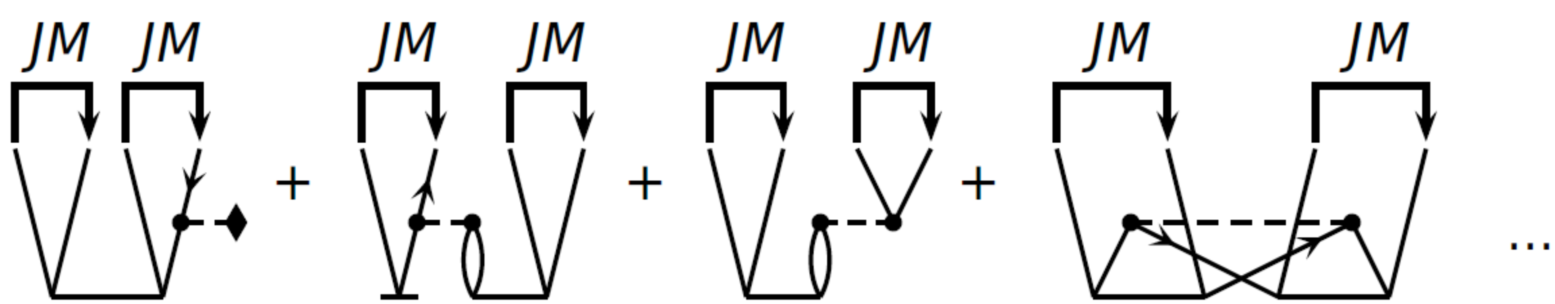
Coupled Cluster – Spherical Scheme

- exploit **spherical symmetry** for closed-shell nuclei, use spherical tensor operator formulation

$$\hat{T}_1 = \sum_{ai} t_i^a \left\{ \hat{a}_a^\dagger \otimes \hat{\tilde{a}}_i \right\}_0^{(0)}$$

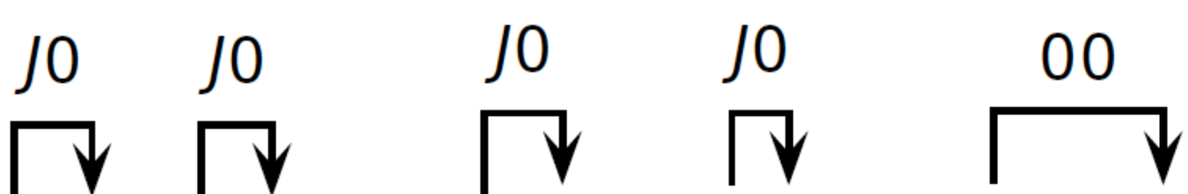
$$\hat{T}_2 = \sum_{abij} \sum_{J} t_{ij}^{ab}(J) \left\{ \left\{ \hat{a}_a^\dagger \otimes \hat{a}_b^\dagger \right\}^{(J)} \otimes \left\{ \hat{\tilde{a}}_j \otimes \hat{\tilde{a}}_i \right\}^{(J)} \right\}_0^{(0)}$$

- **angular-momentum coupling** of external lines

0 = 

etc.

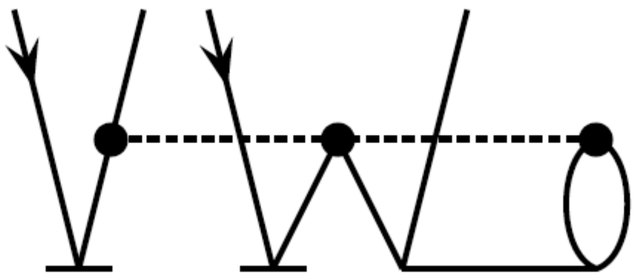
- express CCSD equations in terms of



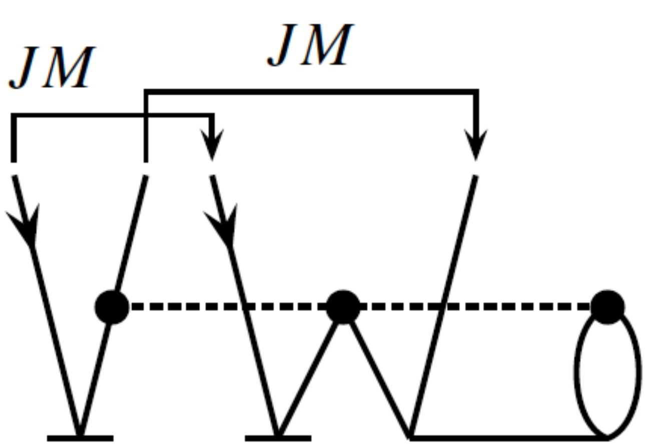
⟨ p q || r s ⟩ , ⟨ a b | t | i j ⟩ , ⟨ ã | t | i ⟩ , *etc.*

Coupled Cluster – Spherical Scheme

- implementation **manually (real labor ⇒ painful)**



$$\frac{1}{4} P_{ab} P_{ij} \sum_{cdekl} \langle kla|w|cde\rangle \langle eb|t_2|kl\rangle \langle c|t_1|i\rangle \langle d|t_1|j\rangle$$



$$-\frac{1}{4} P^{(J)}_{ab} P^{(J)}_{ij} \left(\hat{J}\hat{j}_i\hat{j}_j\right)^{-1} (-1)^{j_a+j_b-J} \sum_{cdekl} \sum_{J'J''} \hat{J}' \hat{J}''$$

$$\times \begin{Bmatrix} J' & J'' & J \\ j_a & j_b & j_e \end{Bmatrix} \langle \overset{J'}{kl} \underbrace{\tilde{a}||w||c}_{J''} \overset{J}{de}\rangle \langle \overset{J'M'}{eb}|t_2|\overset{J'M'}{kl}\rangle \langle \overset{00}{\tilde{c}|t_1|i}\rangle \langle \overset{00}{\tilde{d}|t_1|j}\rangle$$

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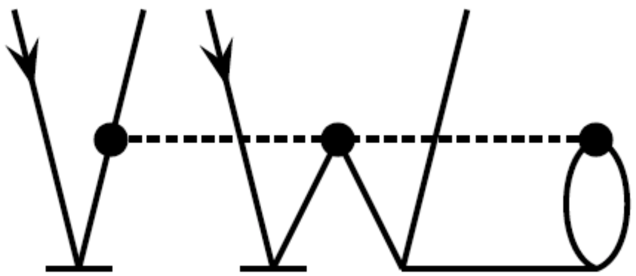

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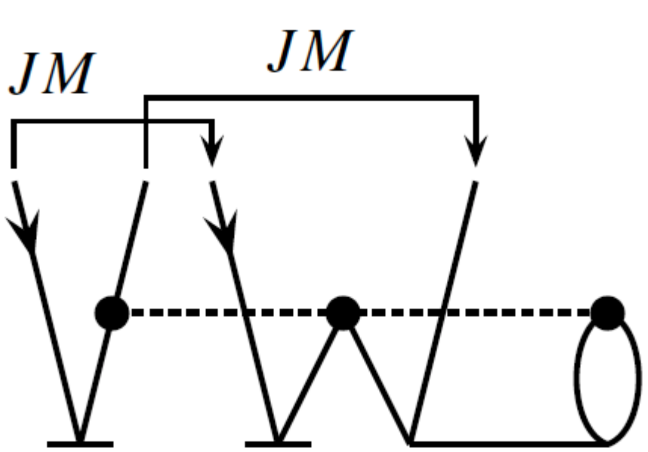
no
automated derivation
and implementation such
as TCE



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Coupled Cluster – Spherical Scheme

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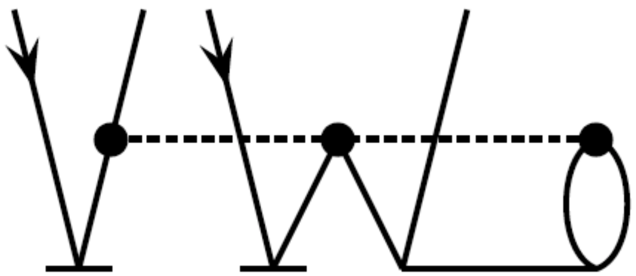

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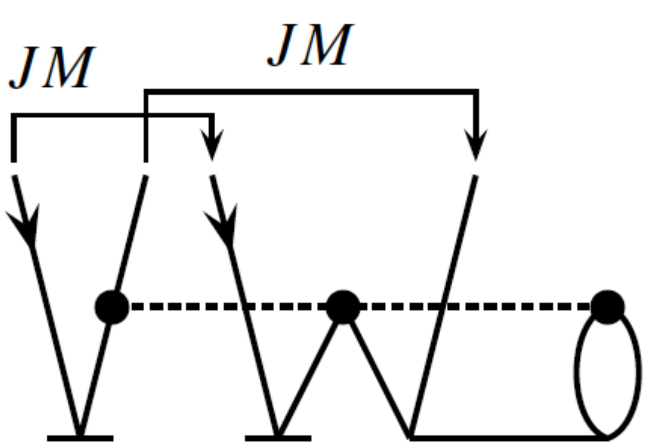
no BLAS



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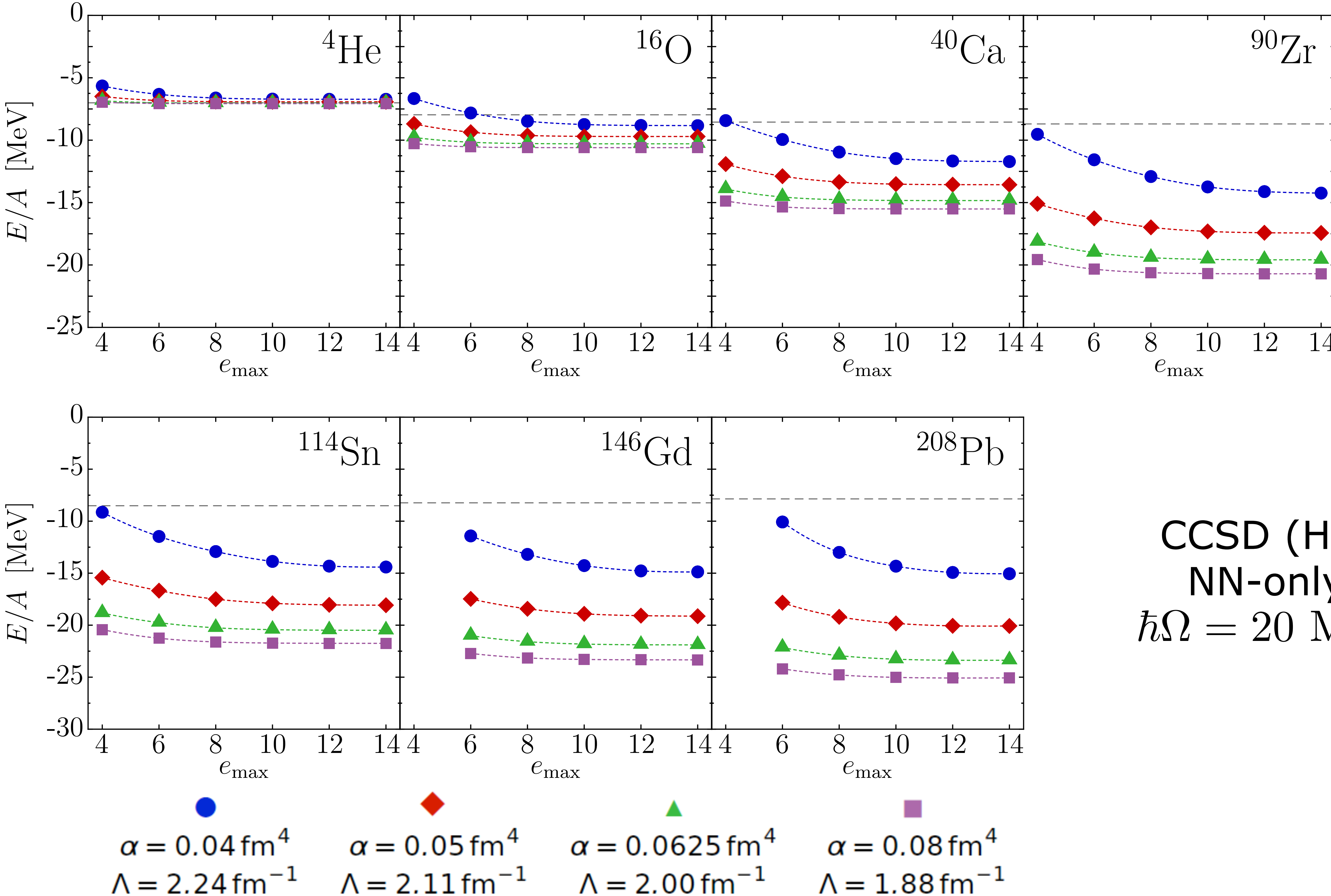
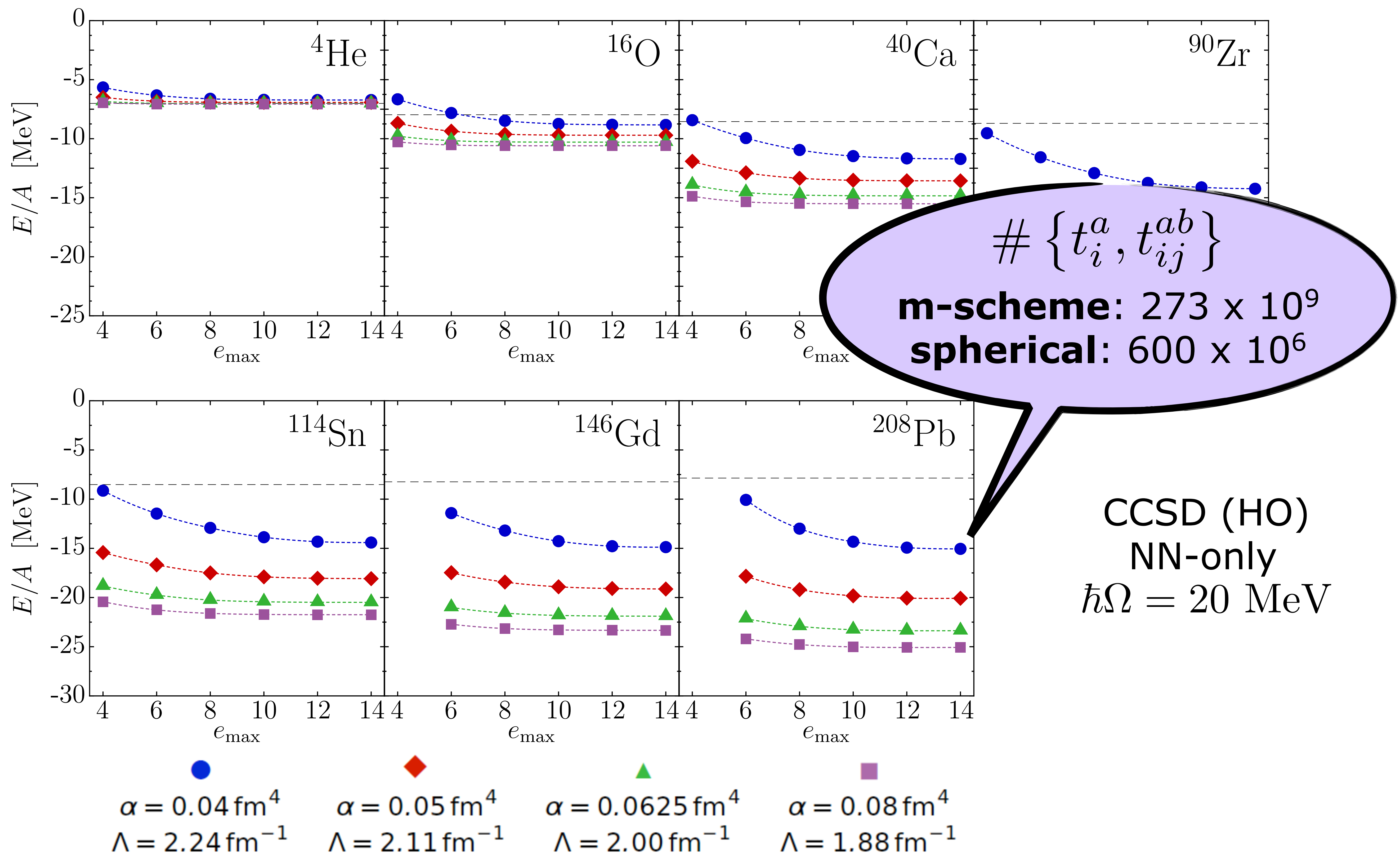
$$\times \begin{Bmatrix} J' & J'' & J \\ j_a & j_b & j_e \end{Bmatrix} \langle \overset{J'}{kl}\tilde{a}||w||\overset{J}{cd}e\rangle_{J''} \langle \overset{J'M'}{eb}|t_2|\overset{J'M'}{kl}\rangle \langle \tilde{c}|t_1|i\rangle^{00} \langle \tilde{d}|t_1|j\rangle^{00}$$

Spherical CCSD – NN only



CCSD (HO)
NN-only
$\hbar\Omega = 20$ MeV

Spherical CCSD – NN only



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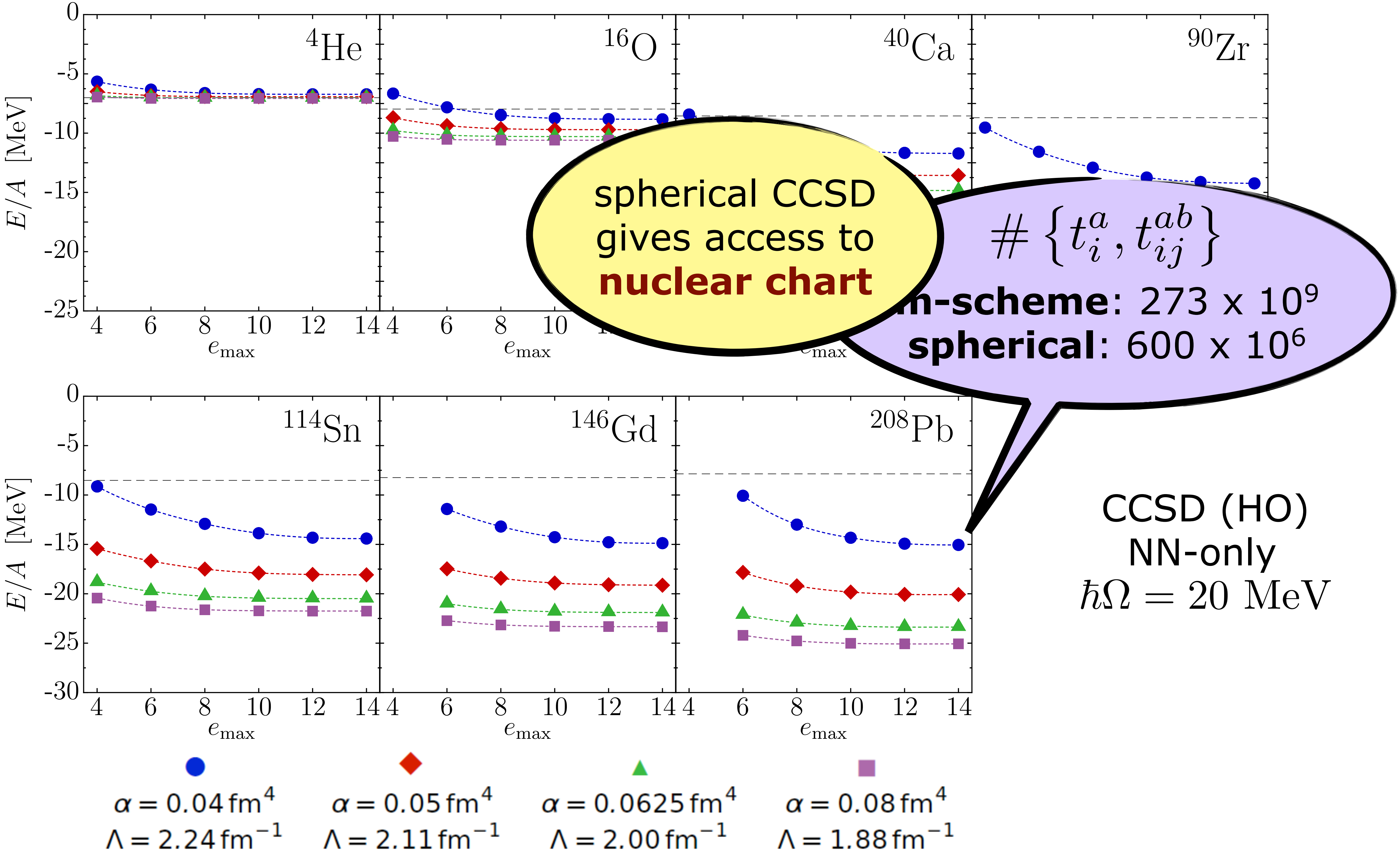
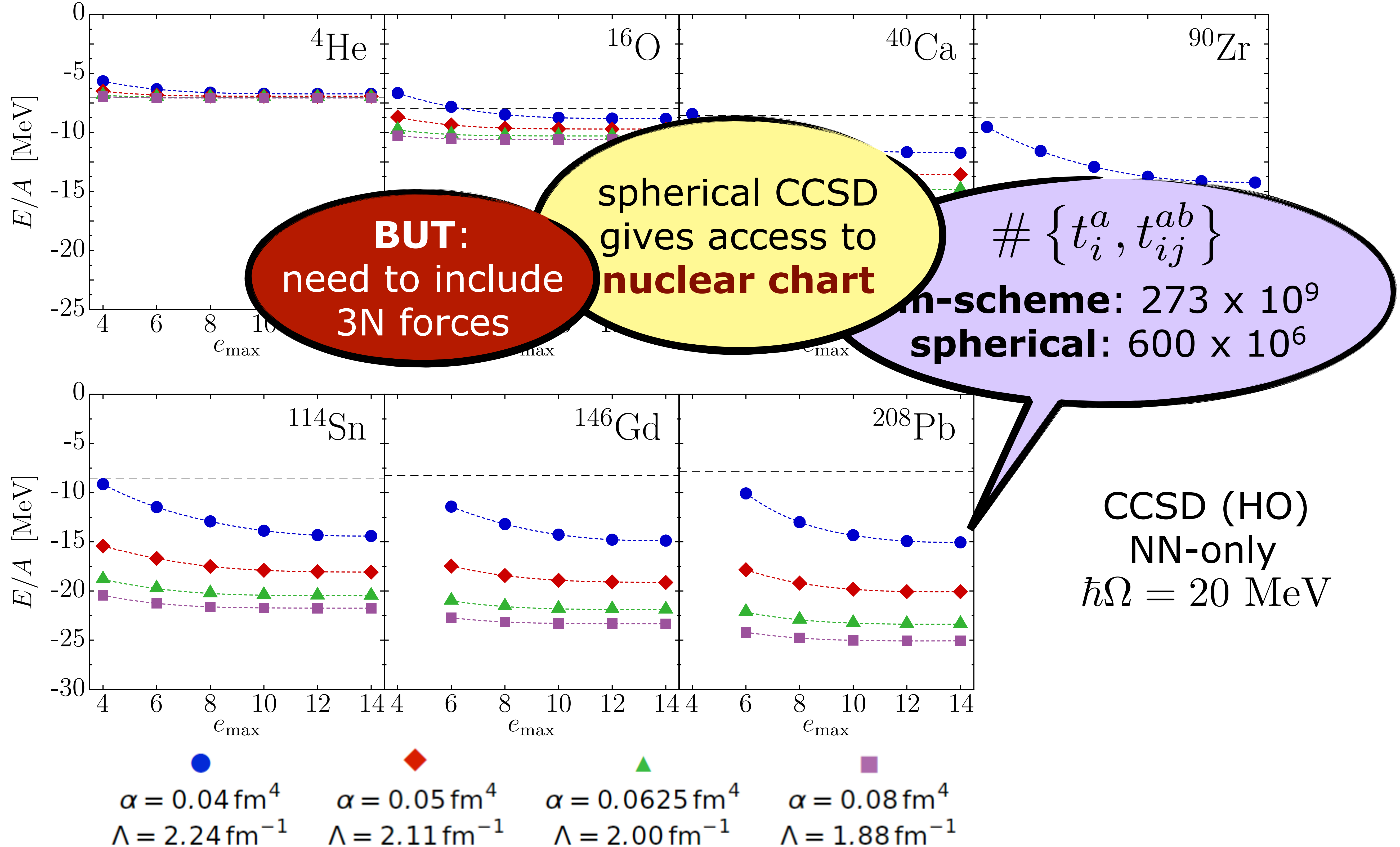


Spherical CCSD – NN only



CCSD (HO)
NN-only
$\hbar\Omega = 20$ MeV

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)

$$\hat{V}_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ} \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

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

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

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

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

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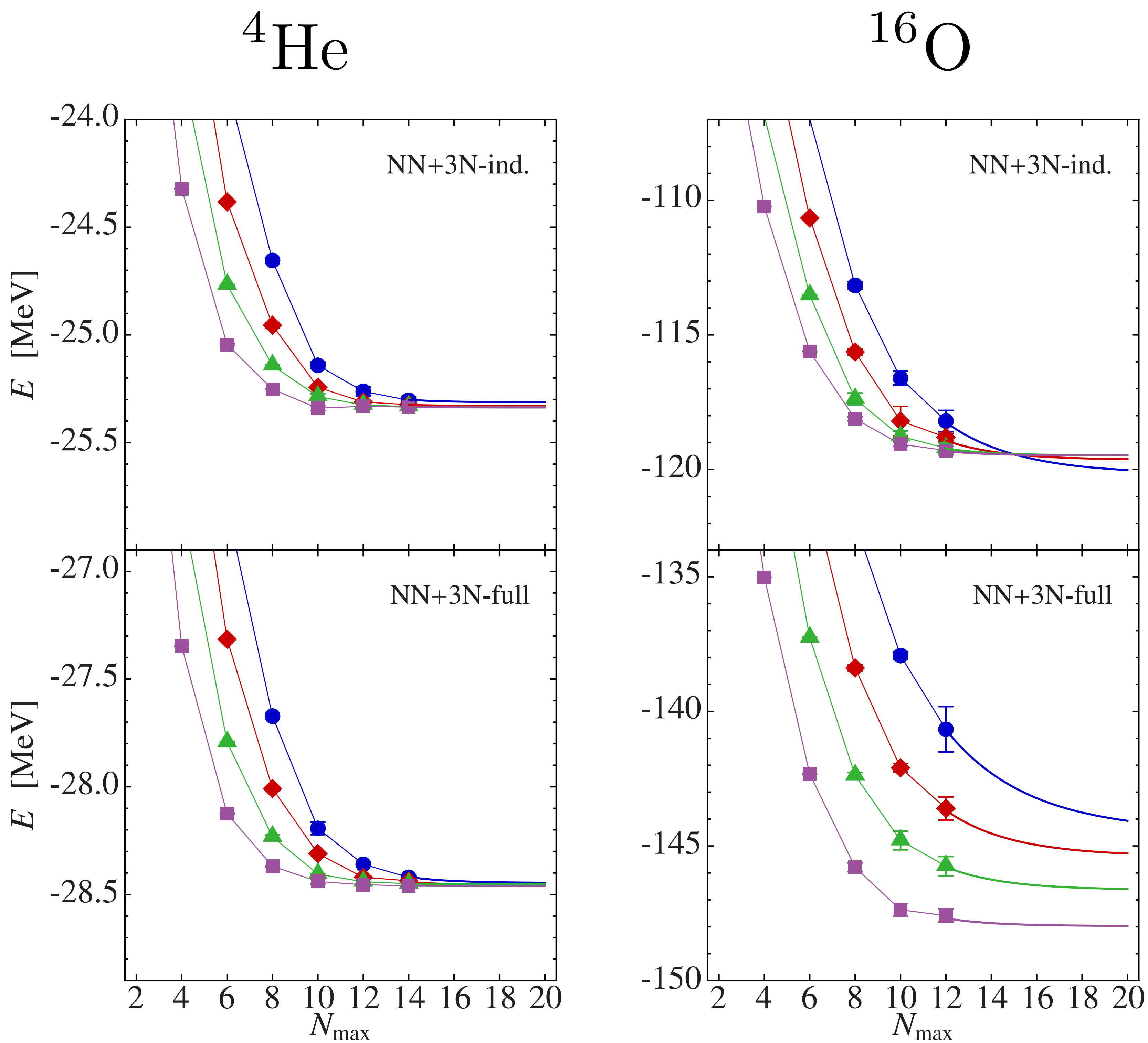
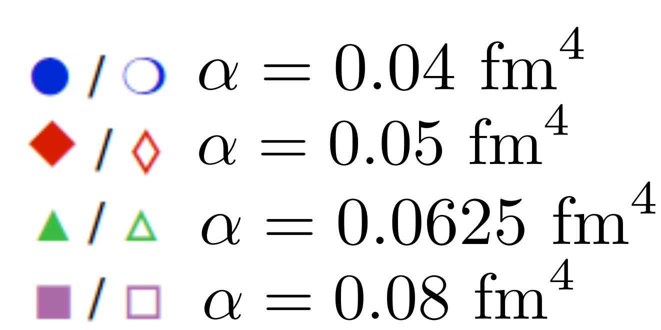
Benchmark of Normal-Ordered 3N

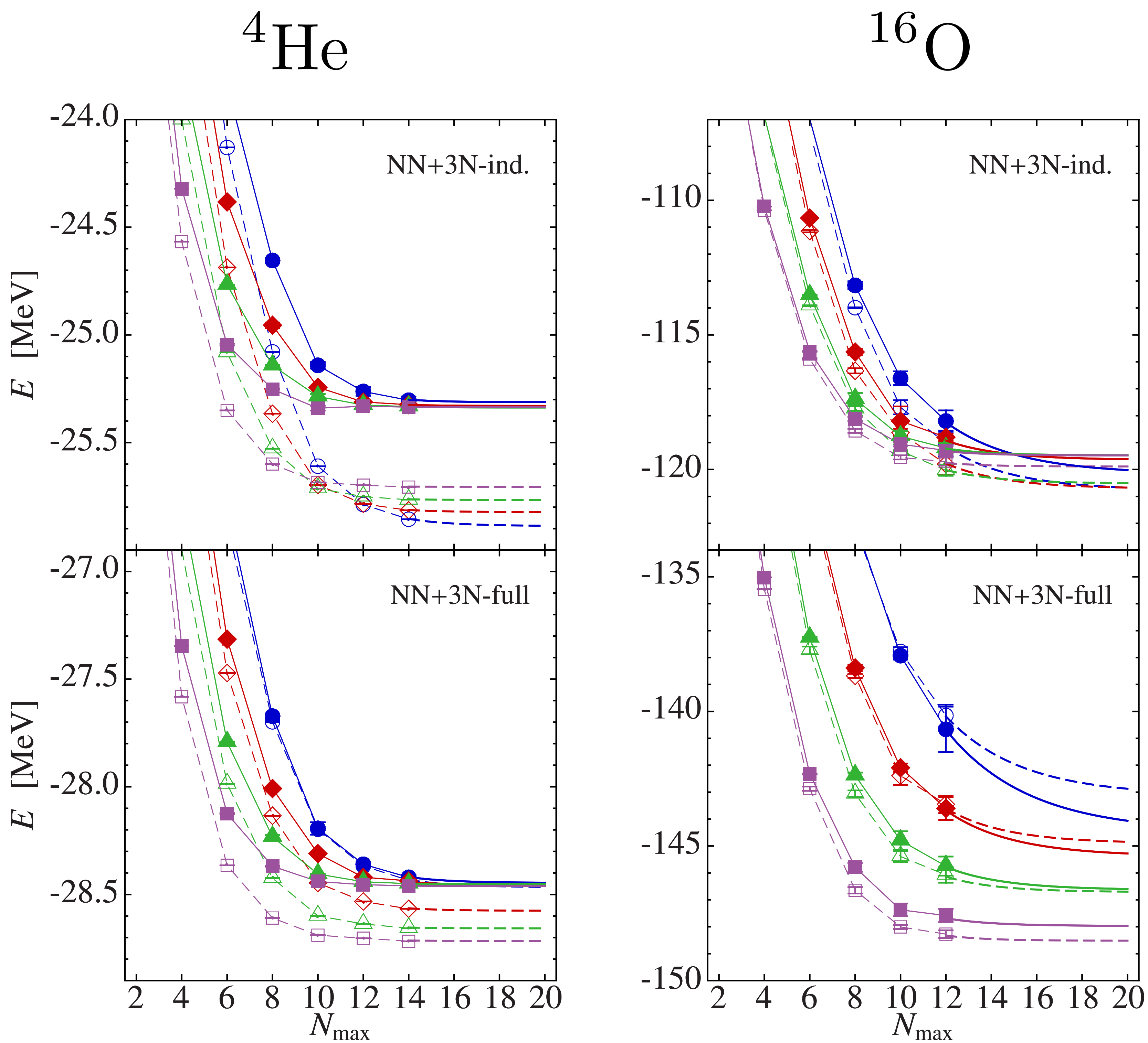


- compare IT-NCSM results with explicit 3N to normal-ordered 3N truncated at the 2B level (NO2B)
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O



$\hbar\Omega = 20\ \text{MeV}$

Benchmark of Normal-Ordered 3N



- compare IT-NCSM results with explicit 3N to normal-ordered 3N truncated at the 2B level (NO2B)
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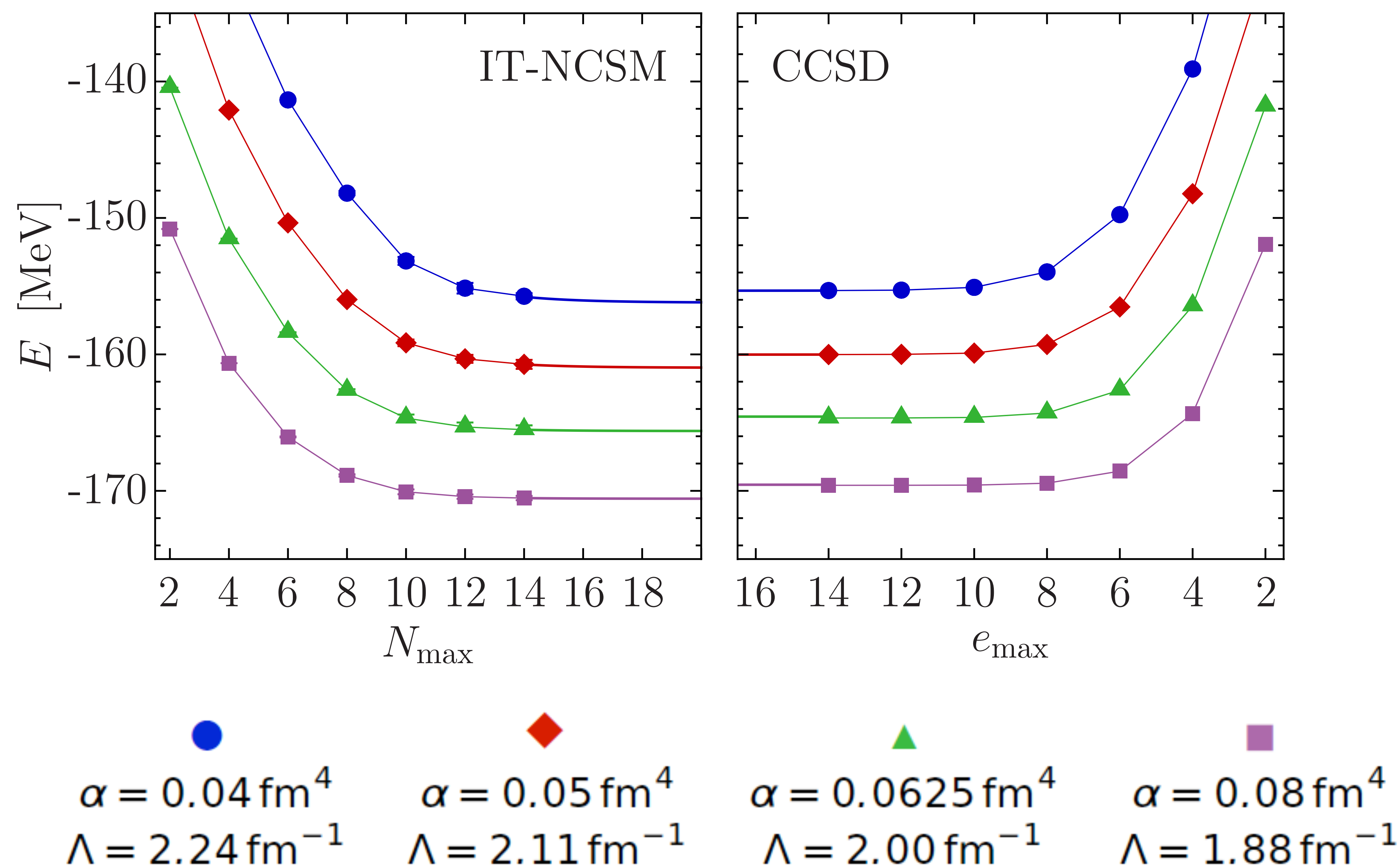
●/○ $\alpha = 0.04\ \mathrm{fm}^4$
◆/◇ $\alpha = 0.05\ \mathrm{fm}^4$
▲/△ $\alpha = 0.0625\ \mathrm{fm}^4$
■/□ $\alpha = 0.08\ \mathrm{fm}^4$

$\hbar\Omega = 20\ \mathrm{MeV}$

^{16}O: IT–NCSM vs. CCSD

NN only (HO)



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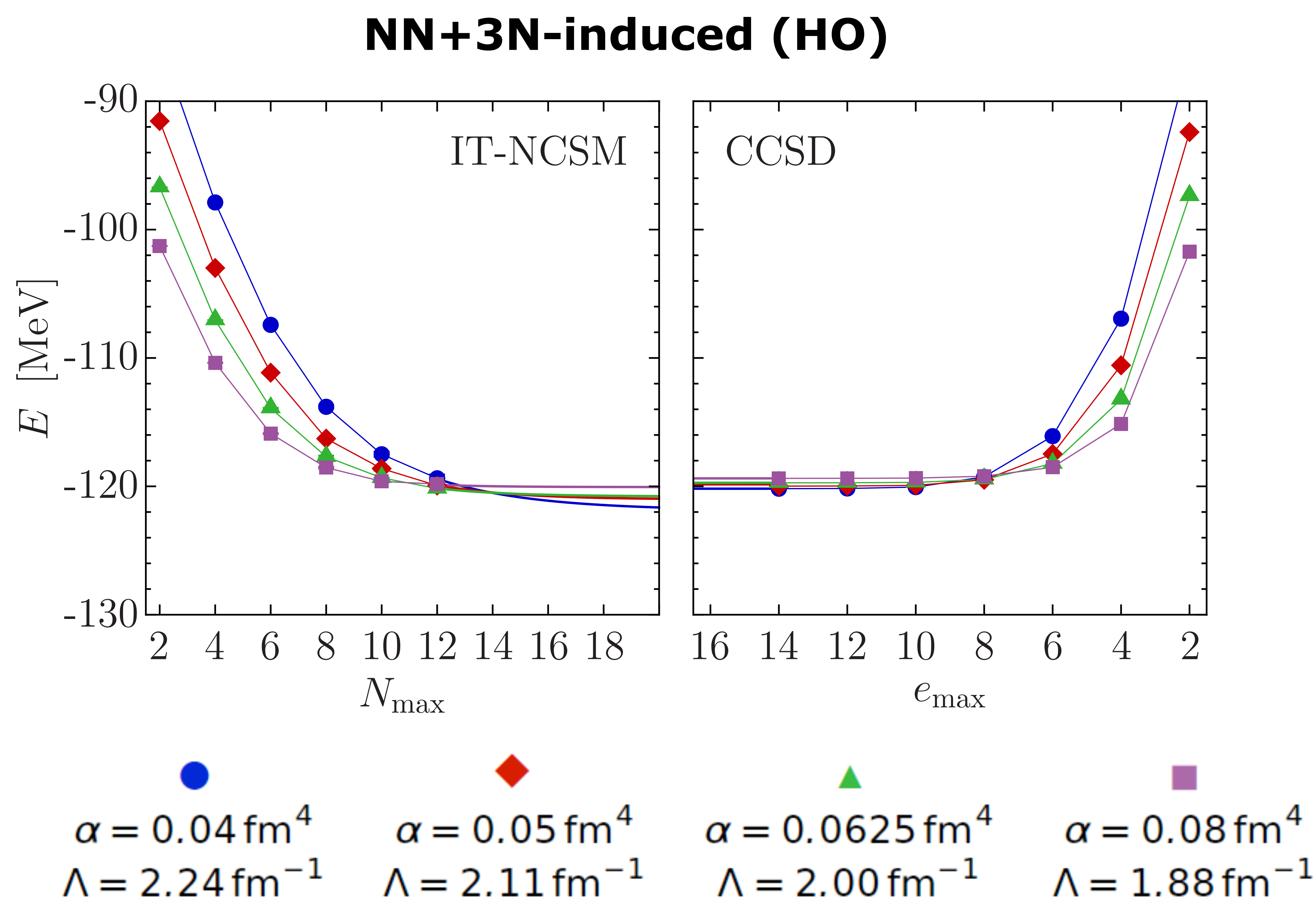

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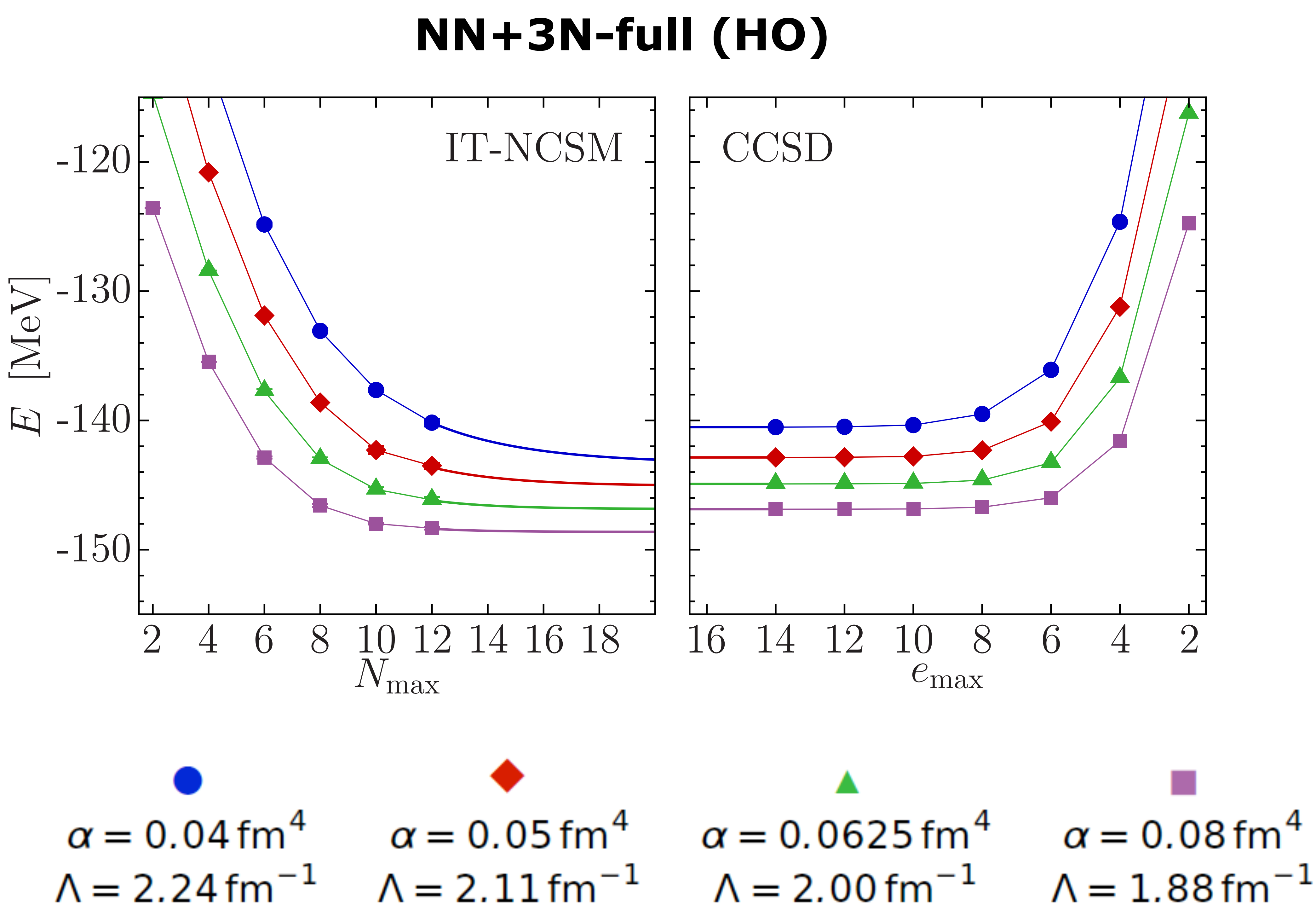
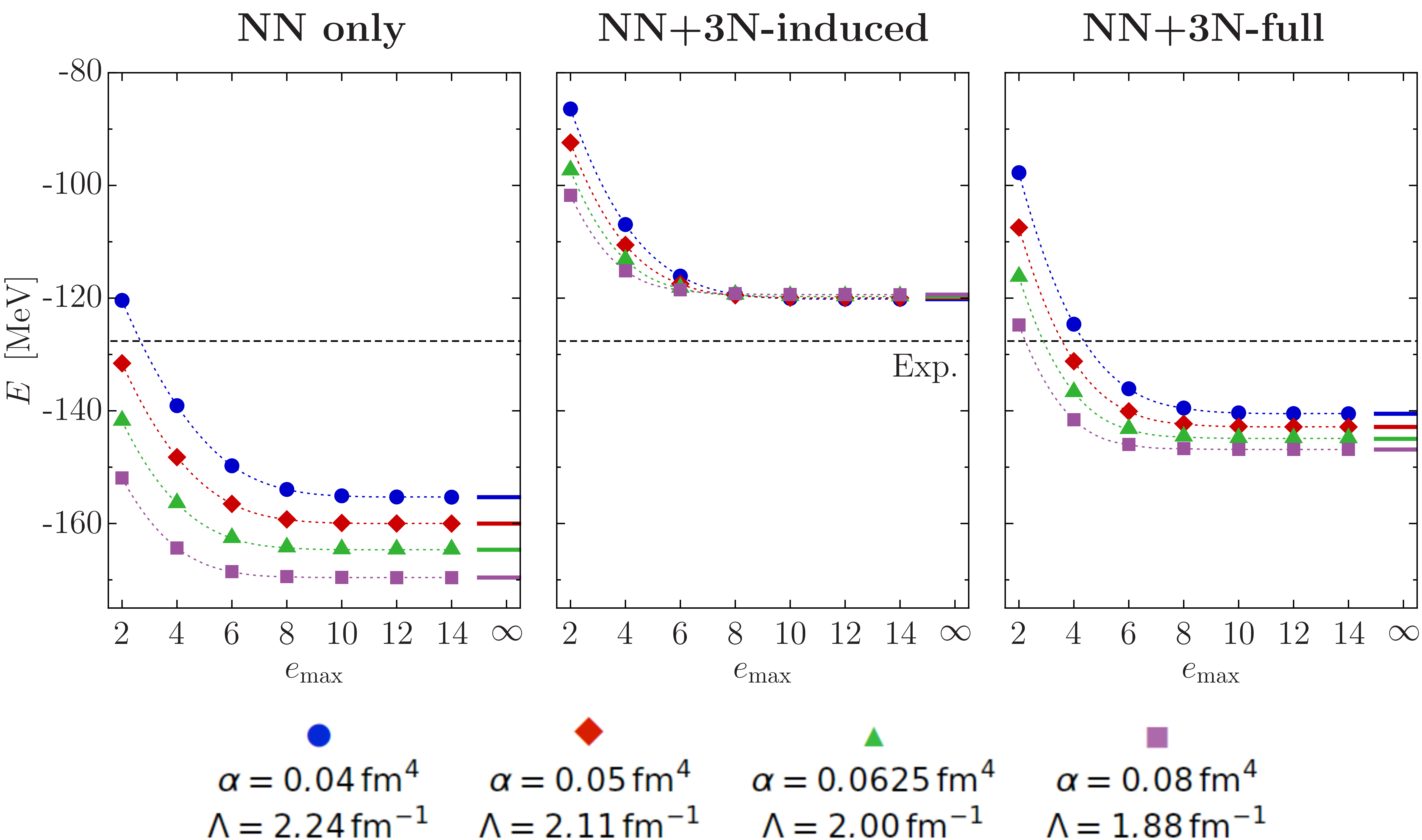


^{16}O: Coupled Cluster with $3N_{NO2B}$



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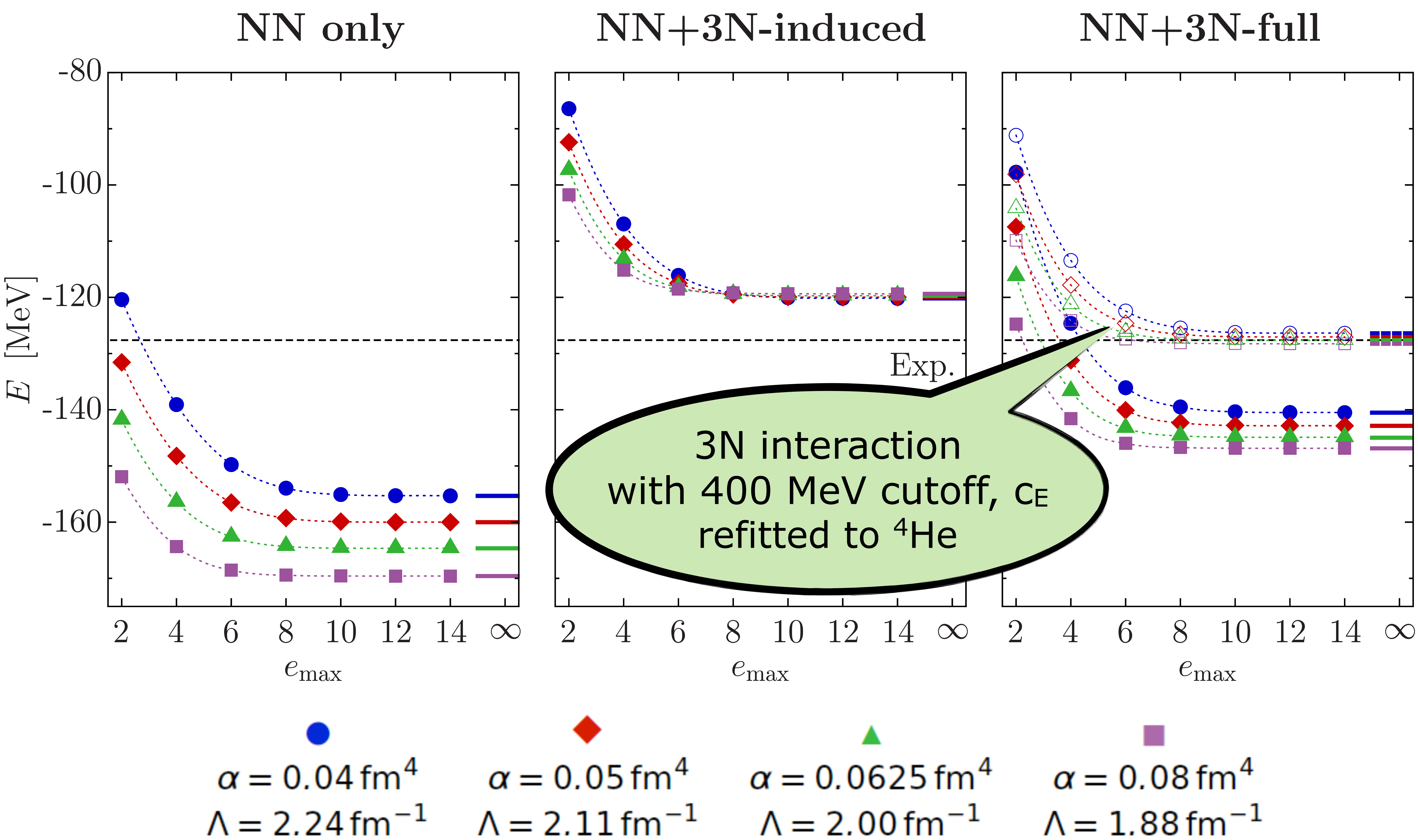
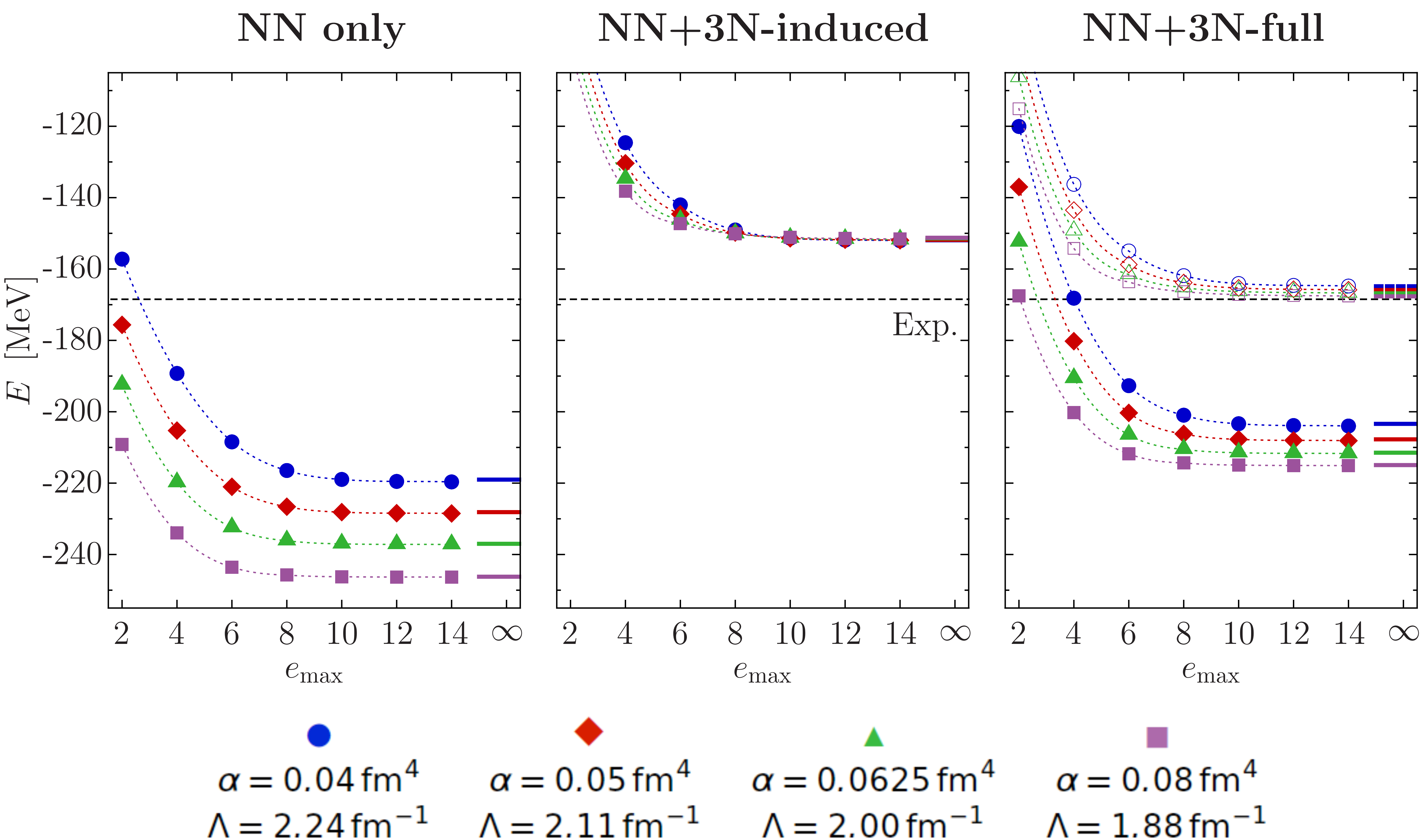
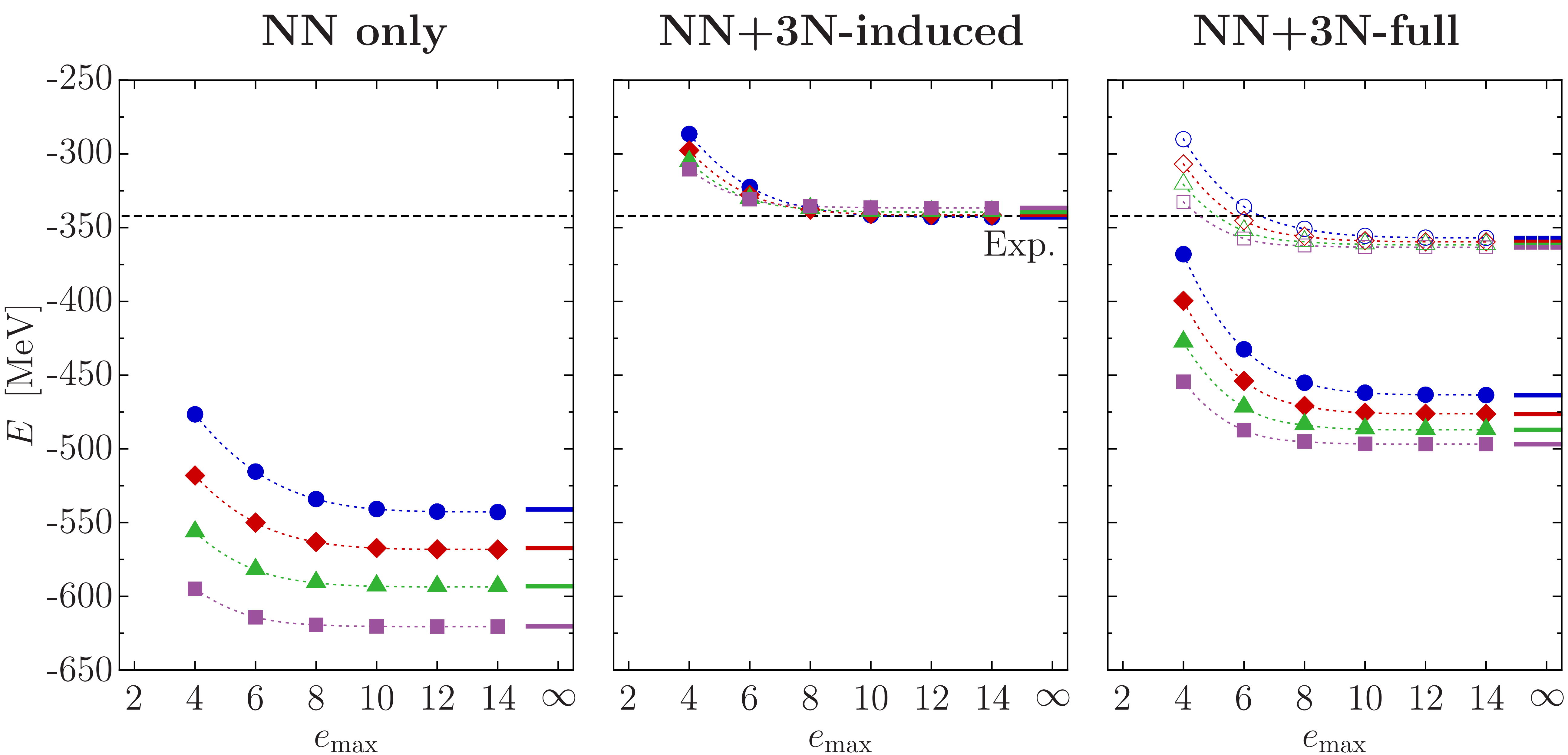


^{24}O: Coupled Cluster with $3N_{NO2B}$



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



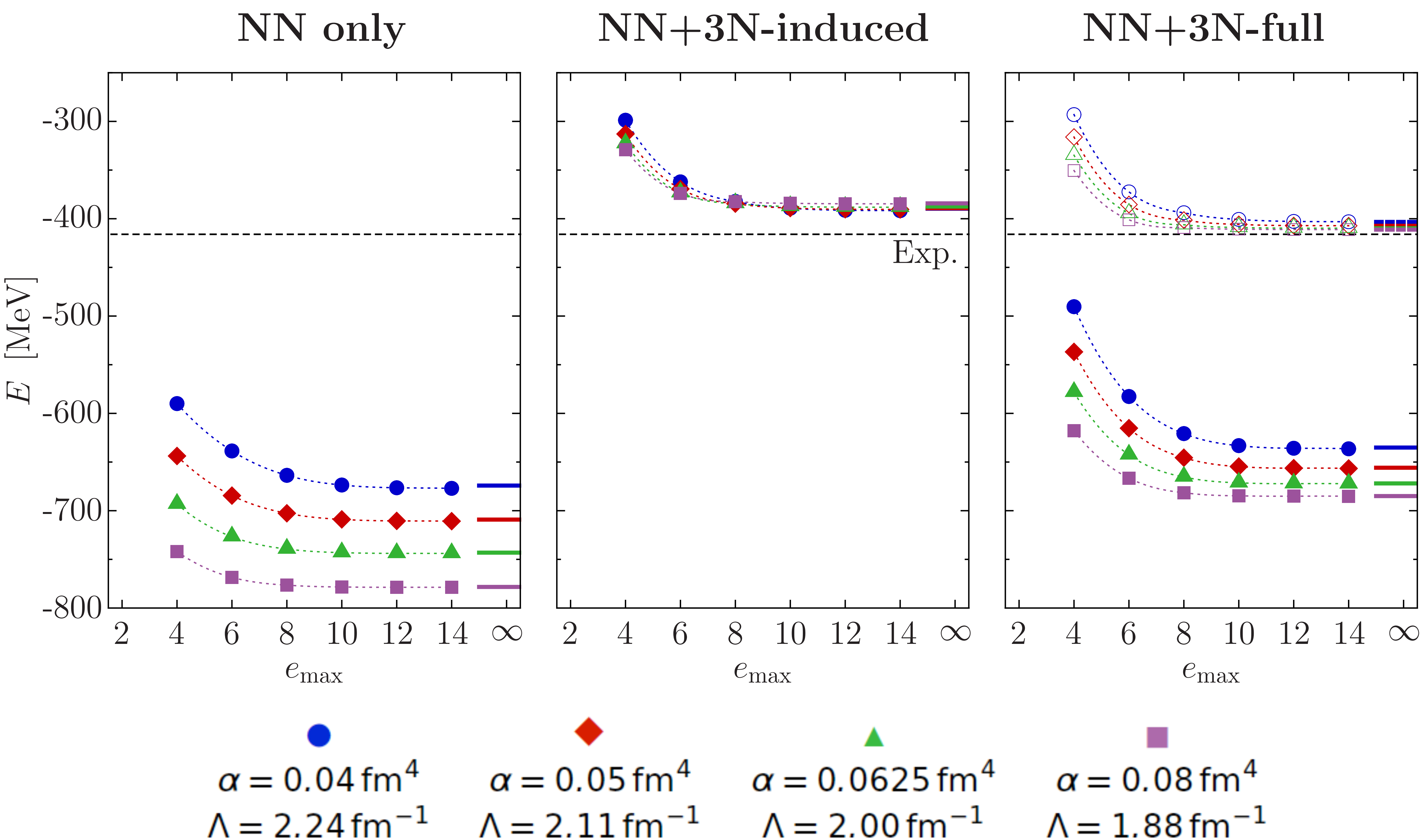
$\alpha = 0.04\,\text{fm}^4$ $\Lambda = 2.24\,\text{fm}^{-1}$

$\alpha = 0.05\,\text{fm}^4$ $\Lambda = 2.11\,\text{fm}^{-1}$

$\alpha = 0.0625\,\text{fm}^4$ $\Lambda = 2.00\,\text{fm}^{-1}$

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

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



CCSD with Explicit 3N Interactions (CCSD3B)

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

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

CCSD3B Equations

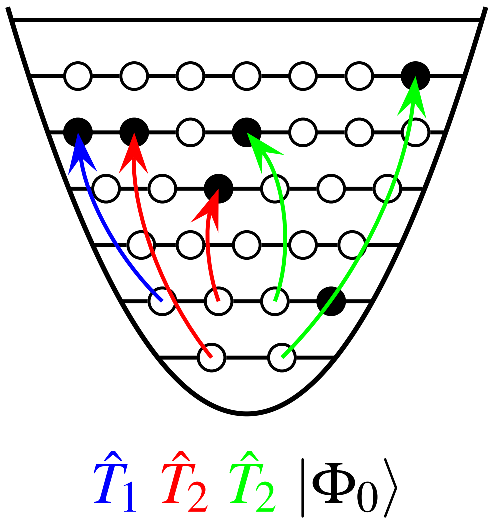
- the CCSD equations with explicit 3N read

$$\Delta E^{3B}_{CCSD} = \Delta E^{NO2B}_{CCSD} + \langle \Phi_0 | \hat{W}_{3B} (\hat{T}_1 \hat{T}_2 + \tfrac{1}{3!} \hat{T}_1^3) | \Phi_0 \rangle_C$$

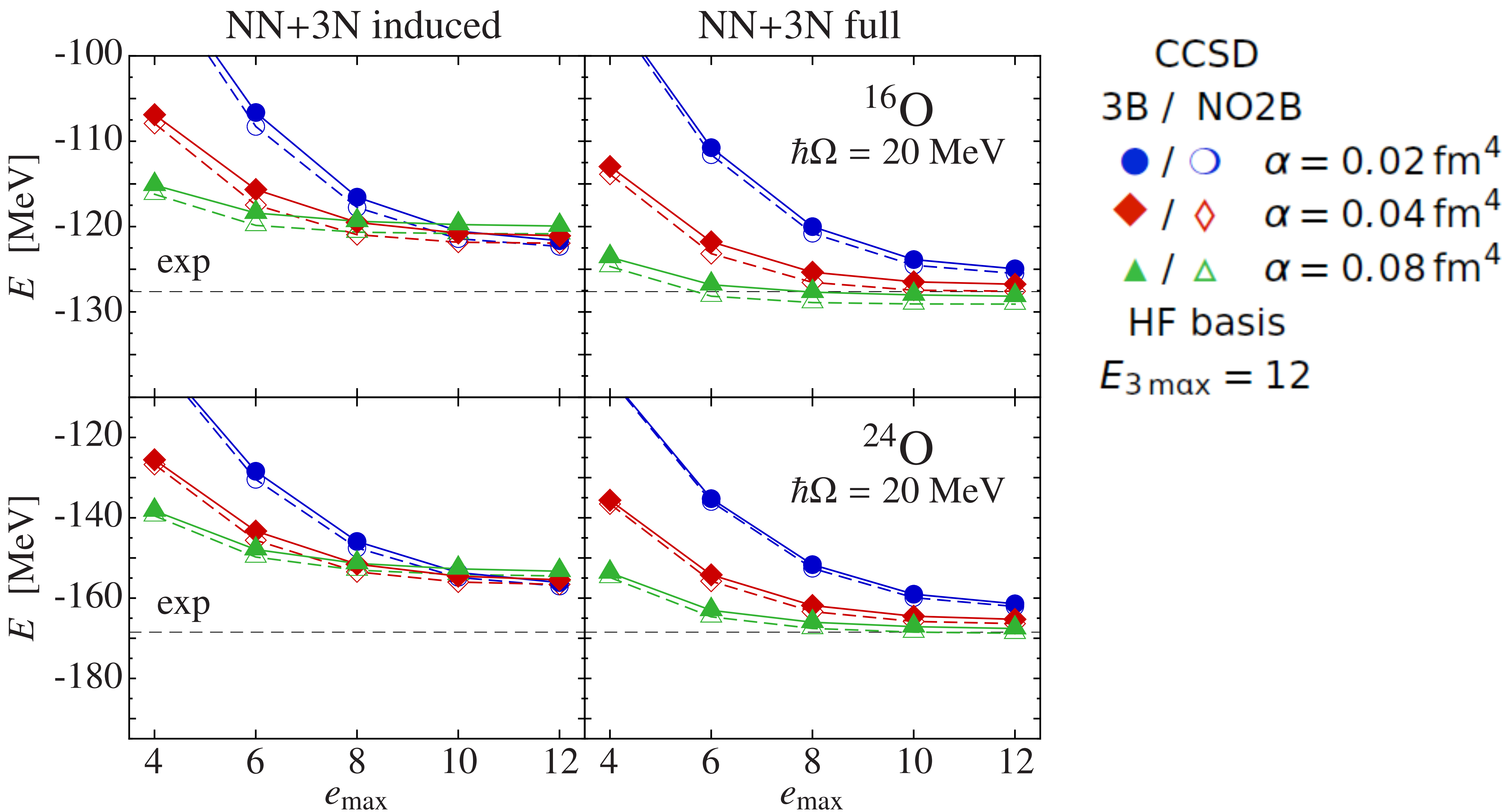
$$0 = T^{NO2B}_{1,CCSD} + \langle \Phi_i^a | \hat{W}_{3B} (\hat{T}_2 + \tfrac{1}{2} \hat{T}_1^2 + \hat{T}_1 \hat{T}_2 + \tfrac{1}{2} \hat{T}_2^2 + \tfrac{1}{3!} \hat{T}_1^3 + \tfrac{1}{2} \hat{T}_1^2 \hat{T}_2 + \tfrac{1}{4!} \hat{T}_1^4) | \Phi_0 \rangle_C$$

$$0 = T^{NO2B}_{2,CCSD} + \langle \Phi_{ij}^{ab} | \hat{W}_{3B} (\hat{T}_1 + \hat{T}_2 + \tfrac{1}{2} \hat{T}_1^2 + \hat{T}_1 \hat{T}_2 + \tfrac{1}{2} \hat{T}_2^2 + \tfrac{1}{3!} \hat{T}_1^3 + \tfrac{1}{2} \hat{T}_1^2 \hat{T}_2 + \tfrac{1}{2} \hat{T}_1 \hat{T}_2^2 + \tfrac{1}{4!} \hat{T}_1^4 + \tfrac{1}{5!} \hat{T}_1^5) | \Phi_0 \rangle_C$$

- all new contributions stem from $\hat{W}_{3B}$
- CCSD3B probes new **parts of the Hamiltonian** and new **excitation types**



CCSD with Explicit 3N Interaction



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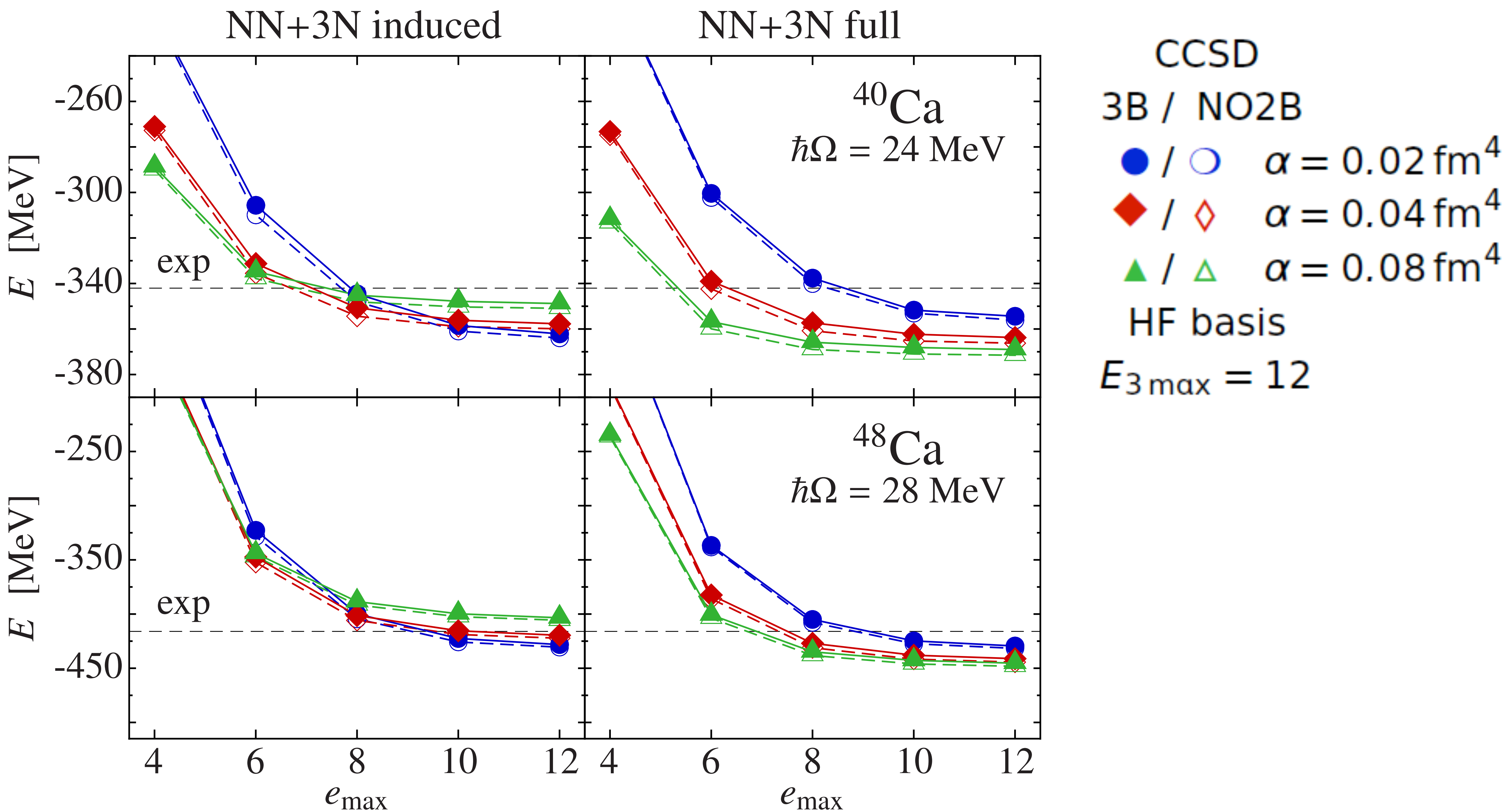

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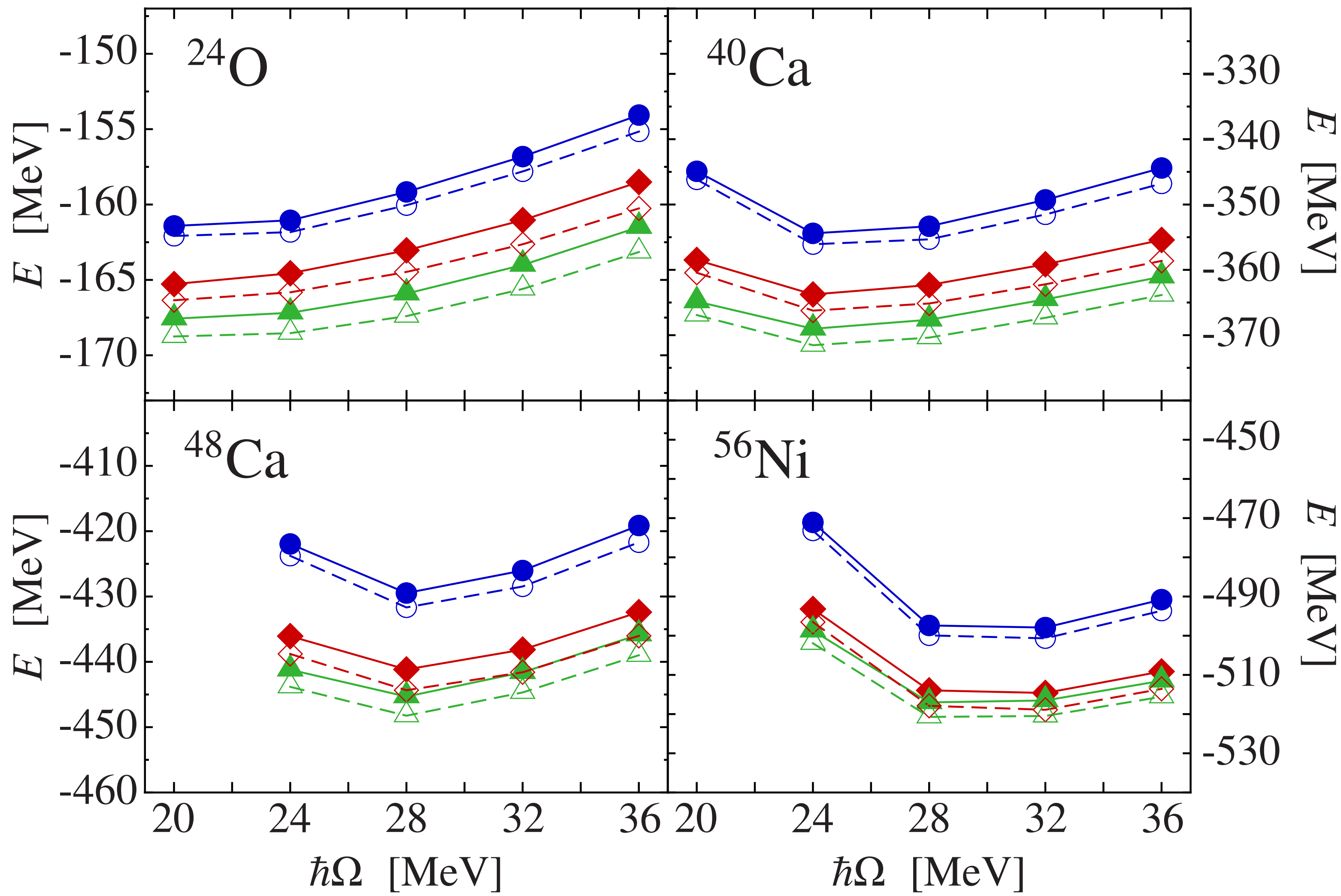
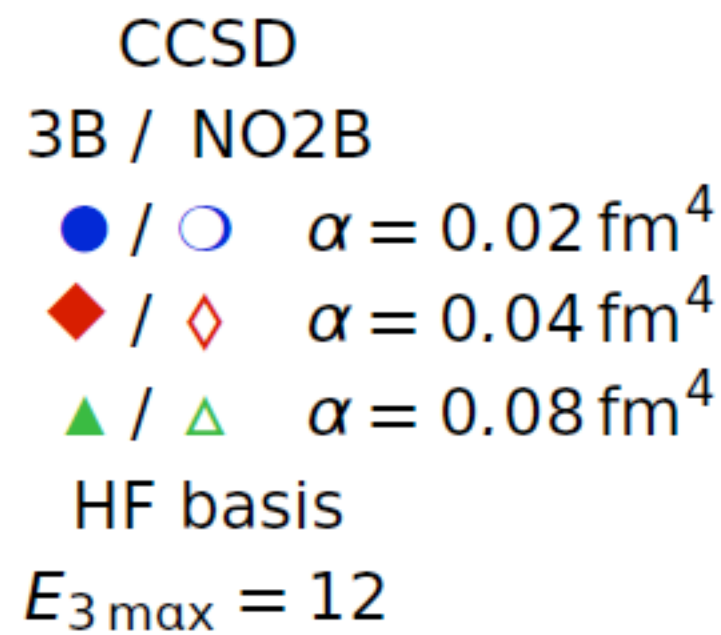
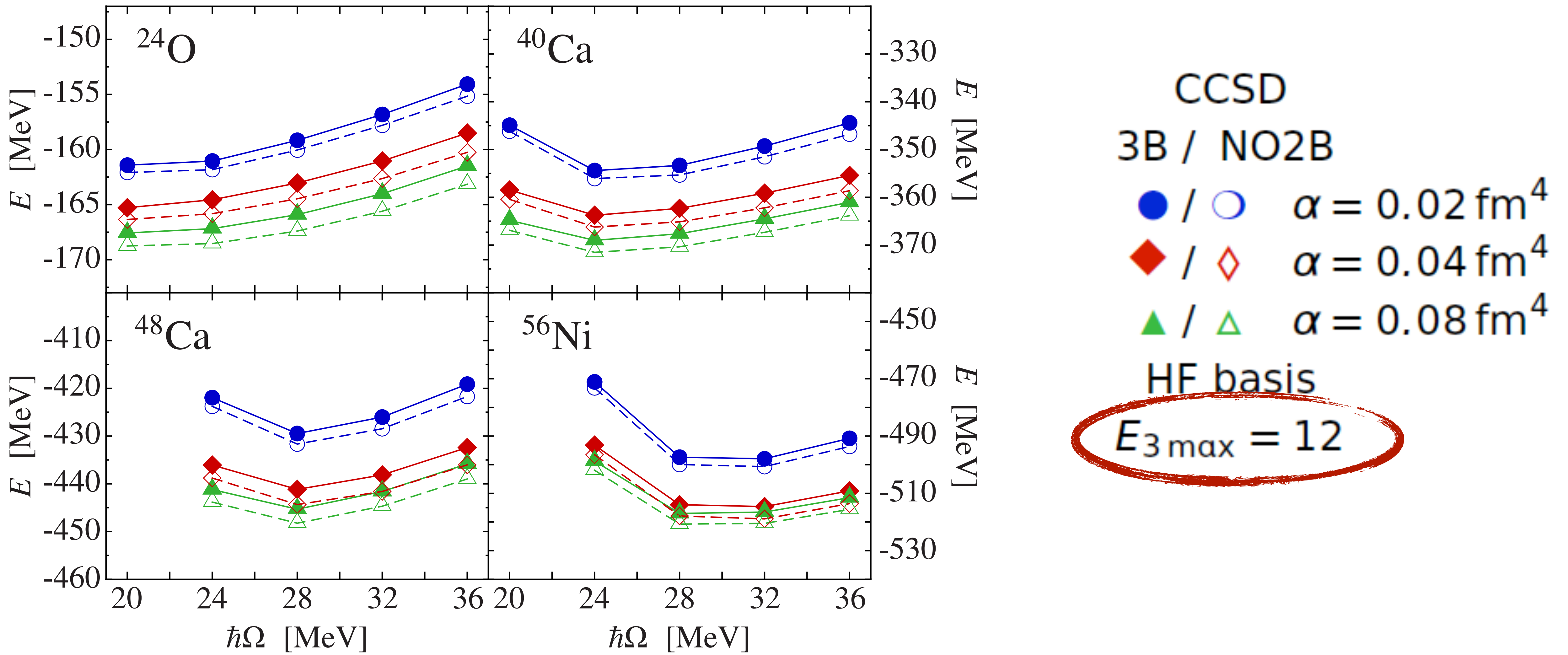




- **excellent agreement** between NO2B and explicit 3N (deviation < 1% for all nuclei considered)
- quality of NO2B **independent** of $e_{\text{max}}, \hbar\Omega, \alpha$
- **efficient and accurate** way to include 3N interactions

CCSD with Explicit 3N Interaction



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

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

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

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

$$e_p = 2n_p + l_p$$

- **current limits**:

$$E_{3\mathrm{max}} \leq \begin{cases} 12 & : \quad \mathrm{CC}, \qquad \text{explicit 3N} \\ 14, \ldots & : \quad \mathrm{NCSM}, \qquad \text{explicit 3N} \\ 14, \ldots & : \quad \mathrm{CC,NCSM} \quad \mathrm{NO2B} \end{cases}$$

storage

production

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E3max=14
Hamiltonian ≈
300 GB

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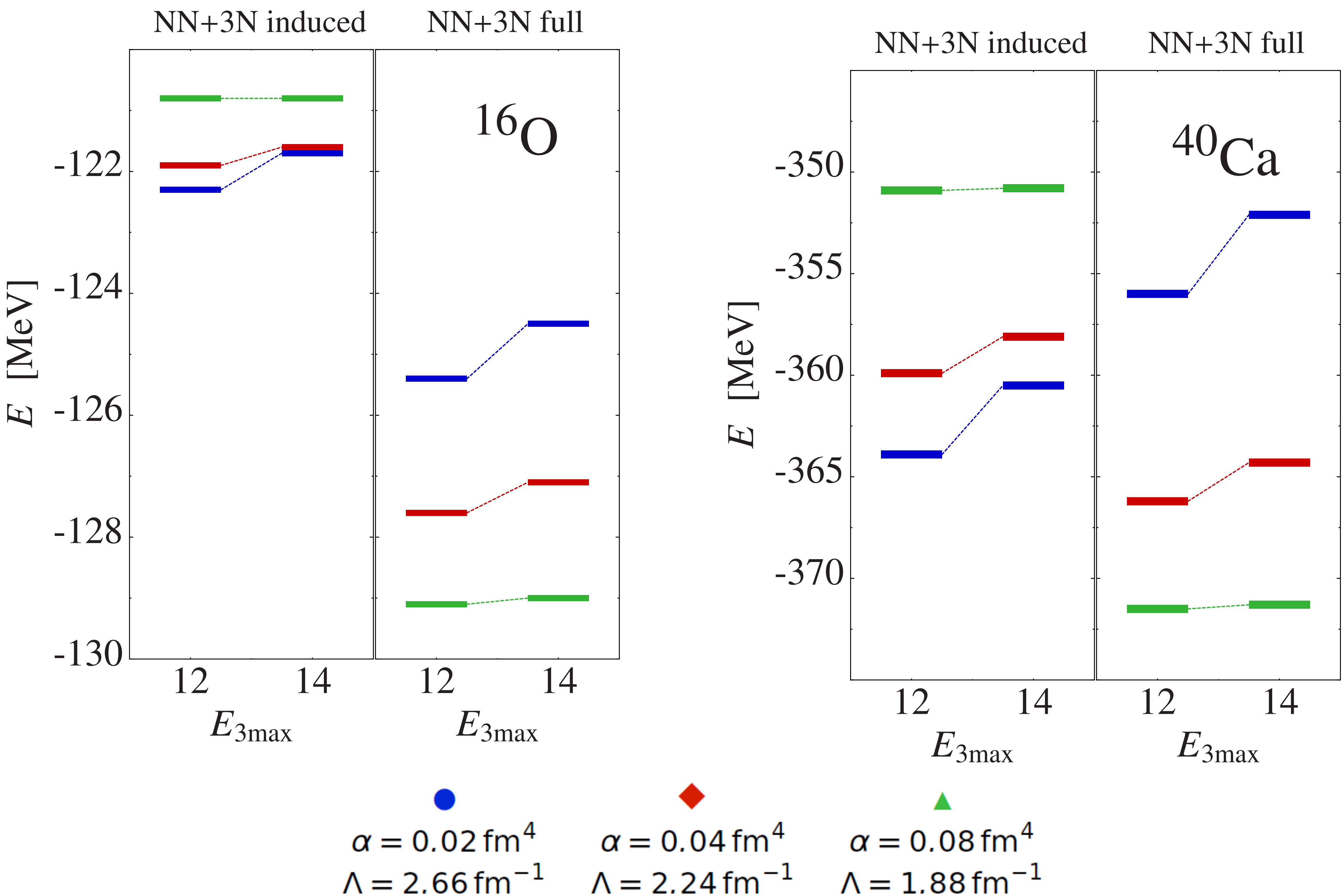
storage

production

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



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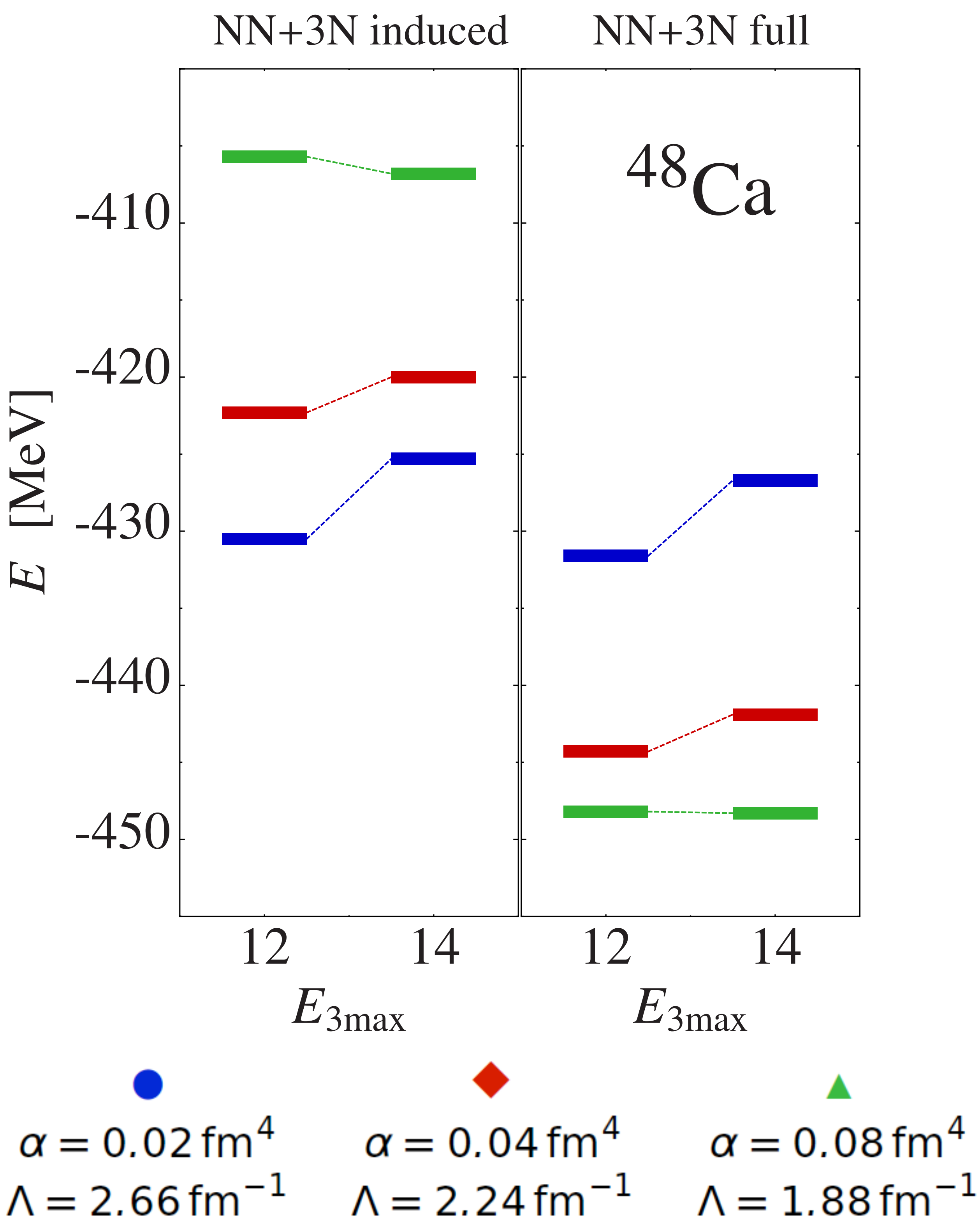

- E_{3max} not significant for **soft interactions** up to A≈60
- **harder interactions**: up to 2% change in g.s. energies for E_{3max} 12 → 14
- α-dependence for **NN+3N induced** gets **reduced** for larger E_{3max}
- α-dependence for **NN+3N full** gets **enhanced** for larger E_{3max}

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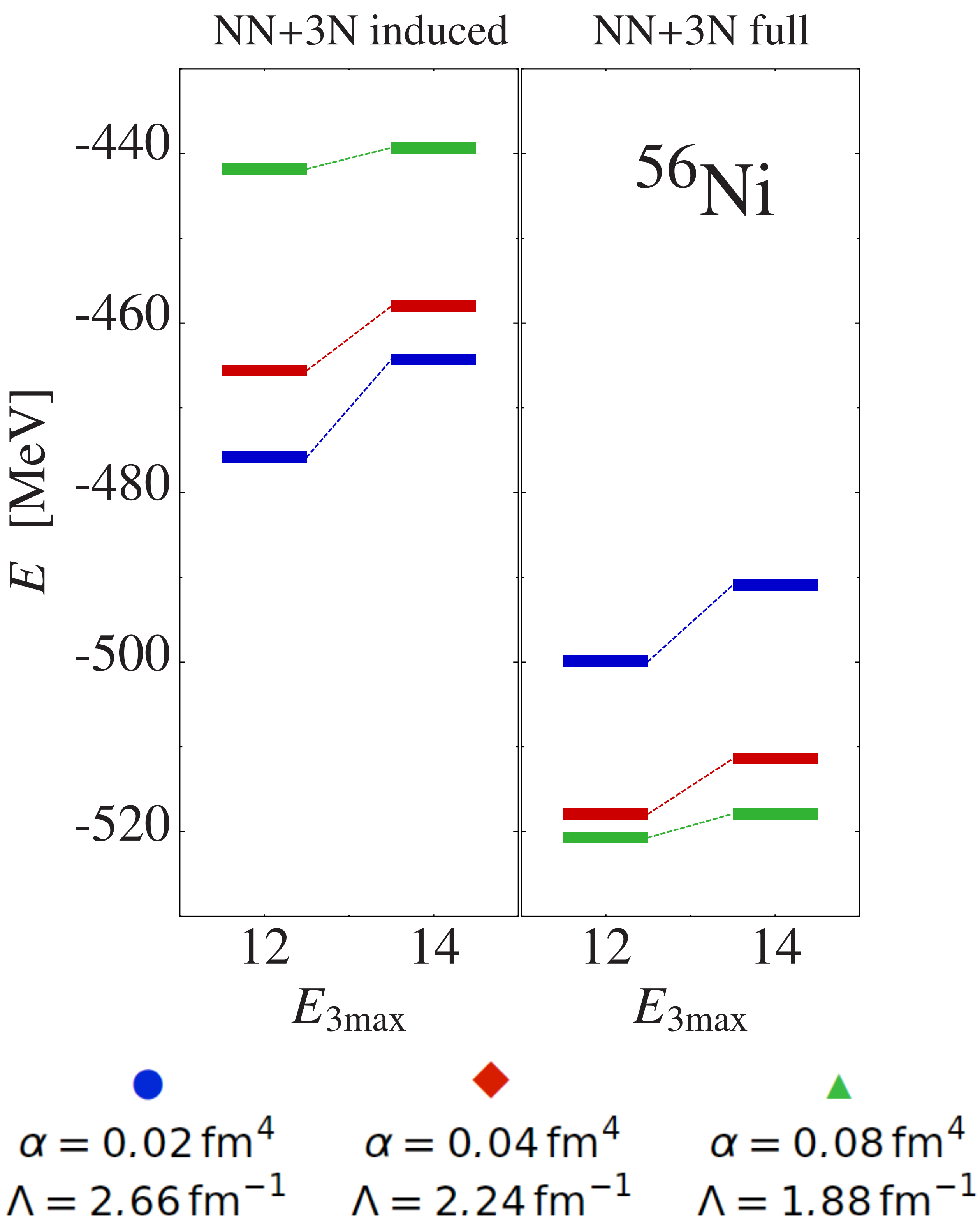

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current E_{3max} cuts do not allow to go beyond A≈60 even for soft interactions

ΛCCSD(T)

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

A.G. Taube, R. J. Bartlett, The Journal of Chemical Physics 128, 044111 (2008)

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

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)

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

- ΛCCSD(T) : denominator $\frac{1}{\epsilon^{abc}_{ijk}}$ **rotationally invariant**

  $\Rightarrow$ **spherical implementation** possible

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problematic for spherical formulation

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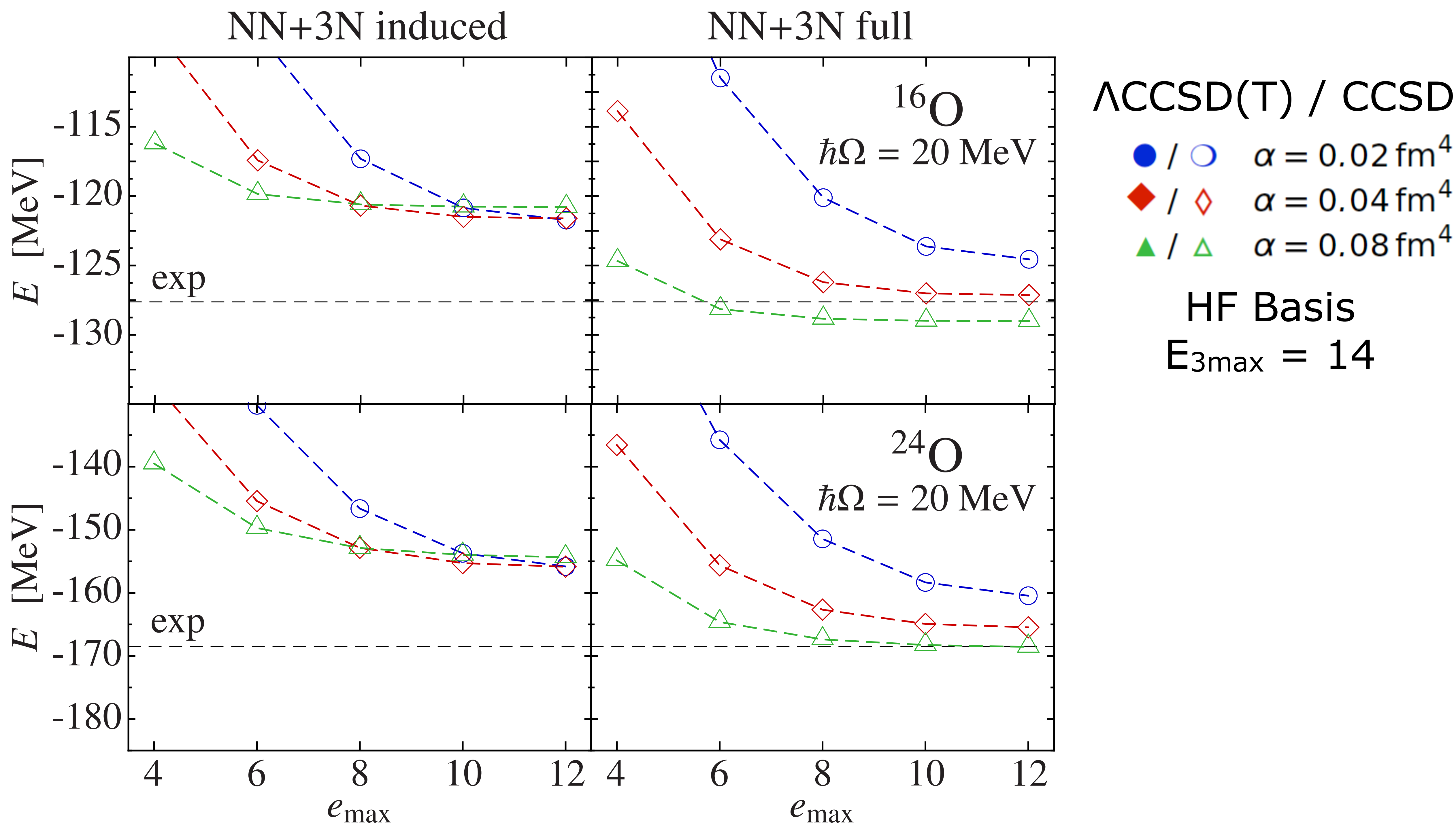
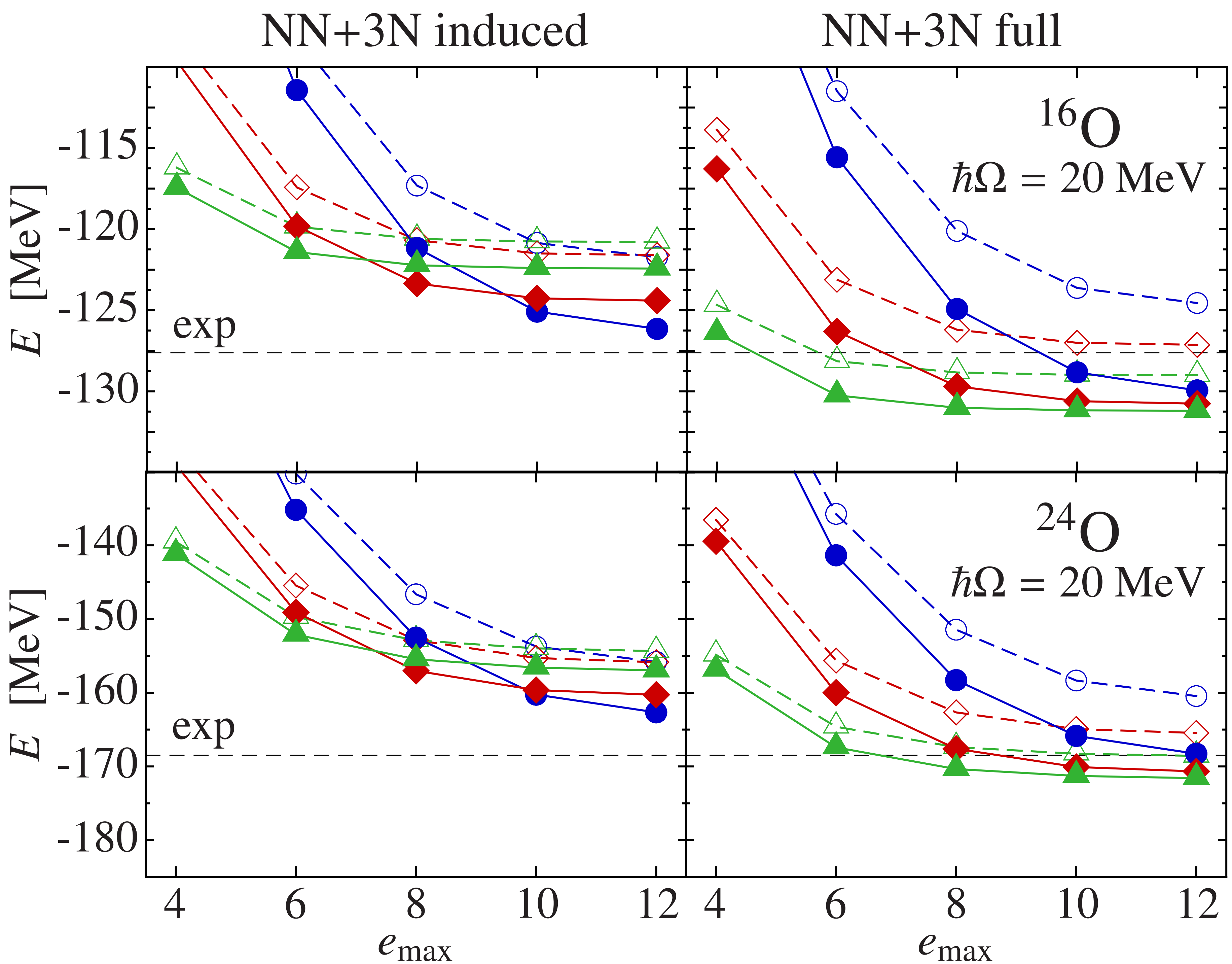
ΛCCSD(T)$_{NO2B}$


NN+3N induced
NN+3N full
^{16}O
ħΩ = 20 MeV
^{24}O
ħΩ = 20 MeV
exp
exp
E [MeV]
E [MeV]
-115
-120
-125
-130
-140
-150
-160
-170
-180
4 6 8 10 12
4 6 8 10 12
e_{max}
e_{max}
ΛCCSD(T) / CCSD
α = 0.02 fm^4
α = 0.04 fm^4
α = 0.08 fm^4
HF Basis
E_{3max} = 14

ΛCCSD(T)$_{NO2B}$



ΛCCSD(T) / CCSD

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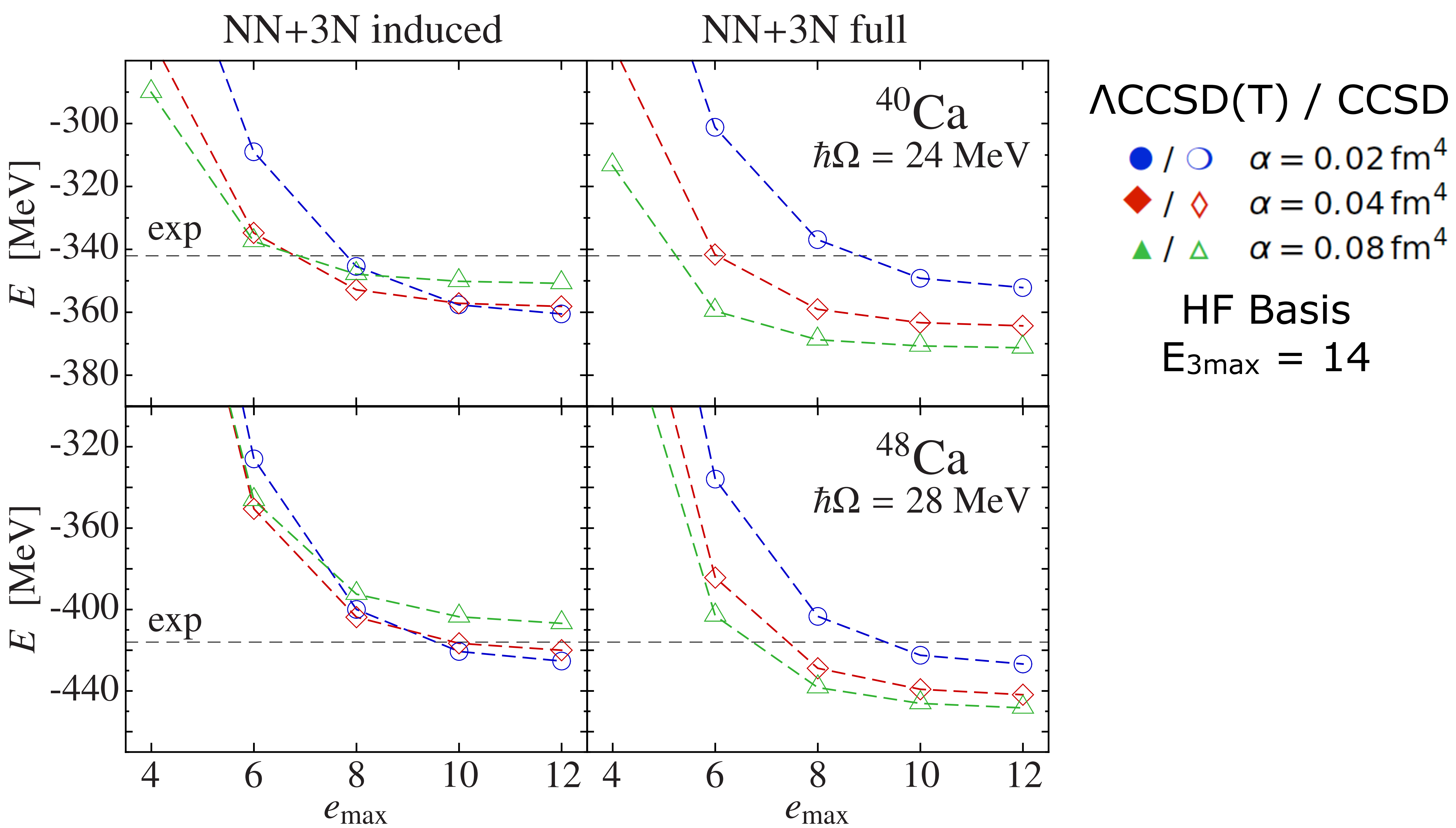
$\alpha = 0.04\,\text{fm}^4$

$\alpha = 0.08\,\text{fm}^4$

HF Basis

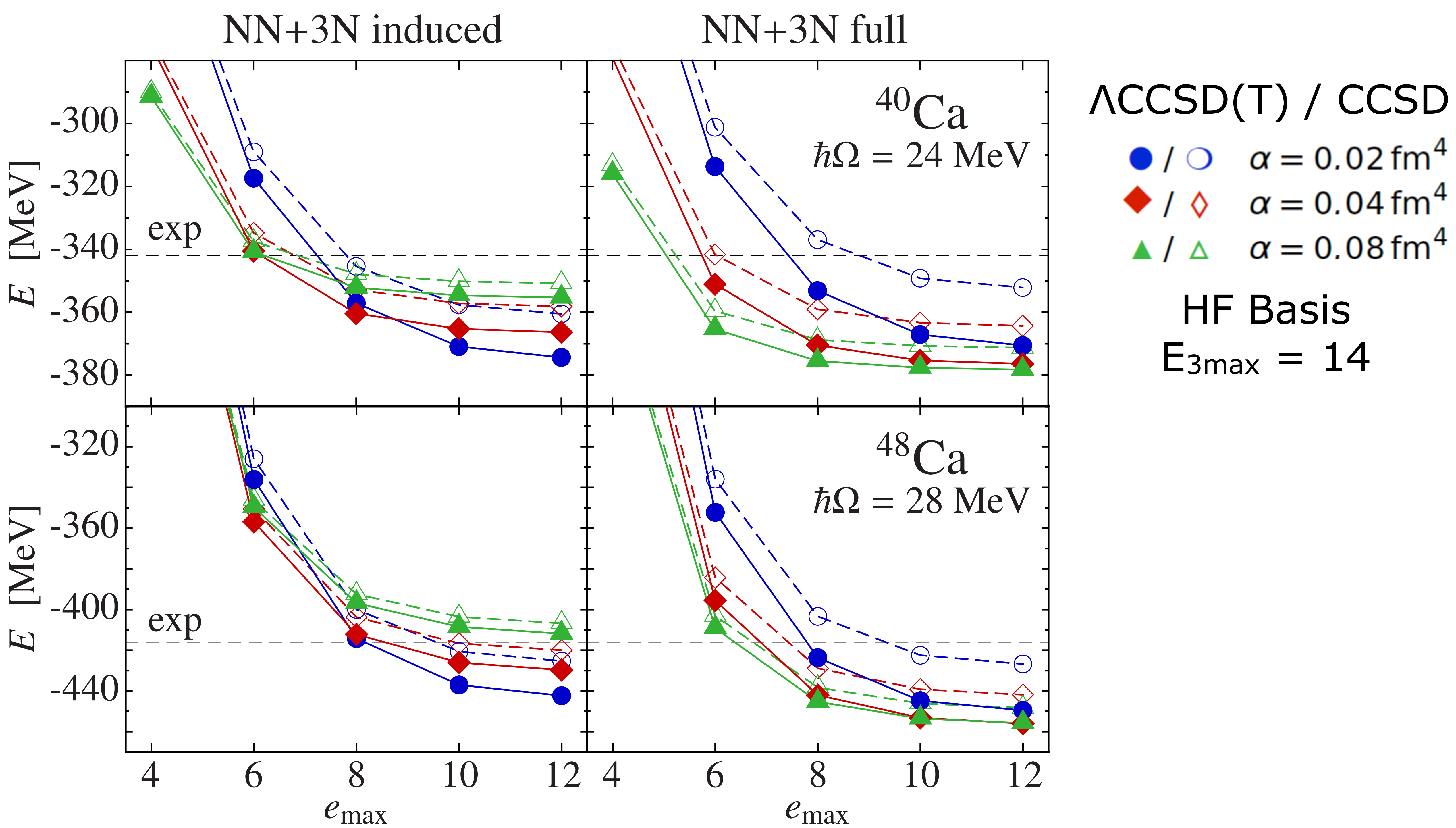
$E_{3max} = 14$

ΛCCSD(T)NO2B



NN+3N induced
NN+3N full
^{40}Ca
ħΩ = 24 MeV
^{48}Ca
ħΩ = 28 MeV
exp
exp
E [MeV]
E [MeV]
-300
-320
-340
-360
-380
-320
-360
-400
-440
4
6
8
10
12
4
6
8
10
12
e_{max}
e_{max}
ΛCCSD(T) / CCSD
α = 0.02 fm^4
α = 0.04 fm^4
α = 0.08 fm^4
HF Basis
E_{3max} = 14

ΛCCSD(T)$_{NO2B}$



NN+3N induced
NN+3N full
^{40}Ca
ħΩ = 24 MeV
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exp
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E [MeV]
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-300
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-340
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-320
-360
-400
-440
4
6
8
10
12
4
6
8
10
12
e_{max}
e_{max}
ΛCCSD(T) / CCSD
α = 0.02 fm^4
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HF Basis
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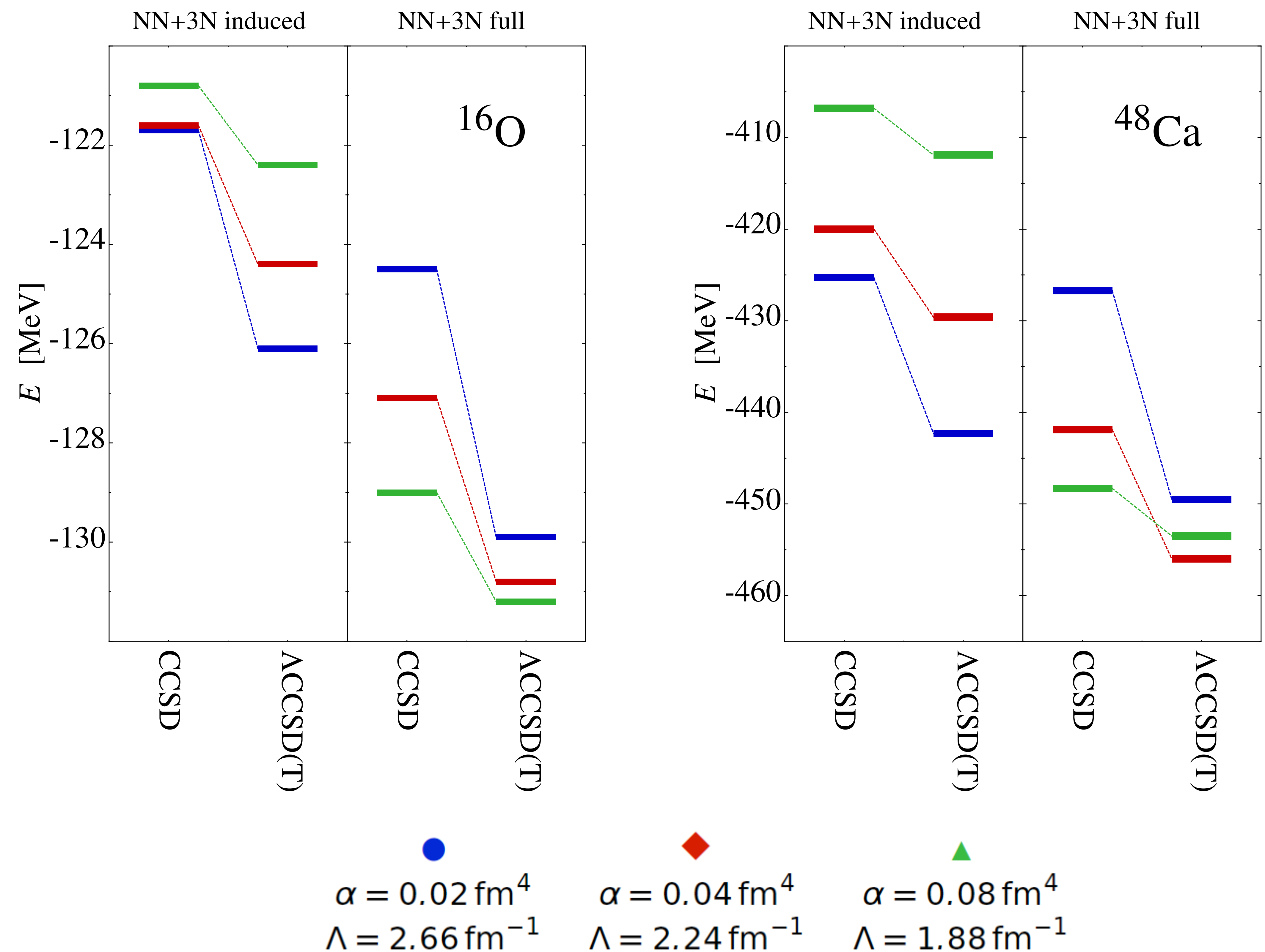
ΛCCSD(T)NO2B


NN+3N induced
NN+3N full
NN+3N induced
NN+3N full
^{16}O
^{48}Ca
E [MeV]
-122
-124
-126
-128
-130
-410
-420
-430
-440
-450
-460
CCSD
ΛCCSD(T)
$\alpha = 0.02\,\mathrm{fm}^4$
$\Lambda = 2.66\,\mathrm{fm}^{-1}$
$\alpha = 0.04\,\mathrm{fm}^4$
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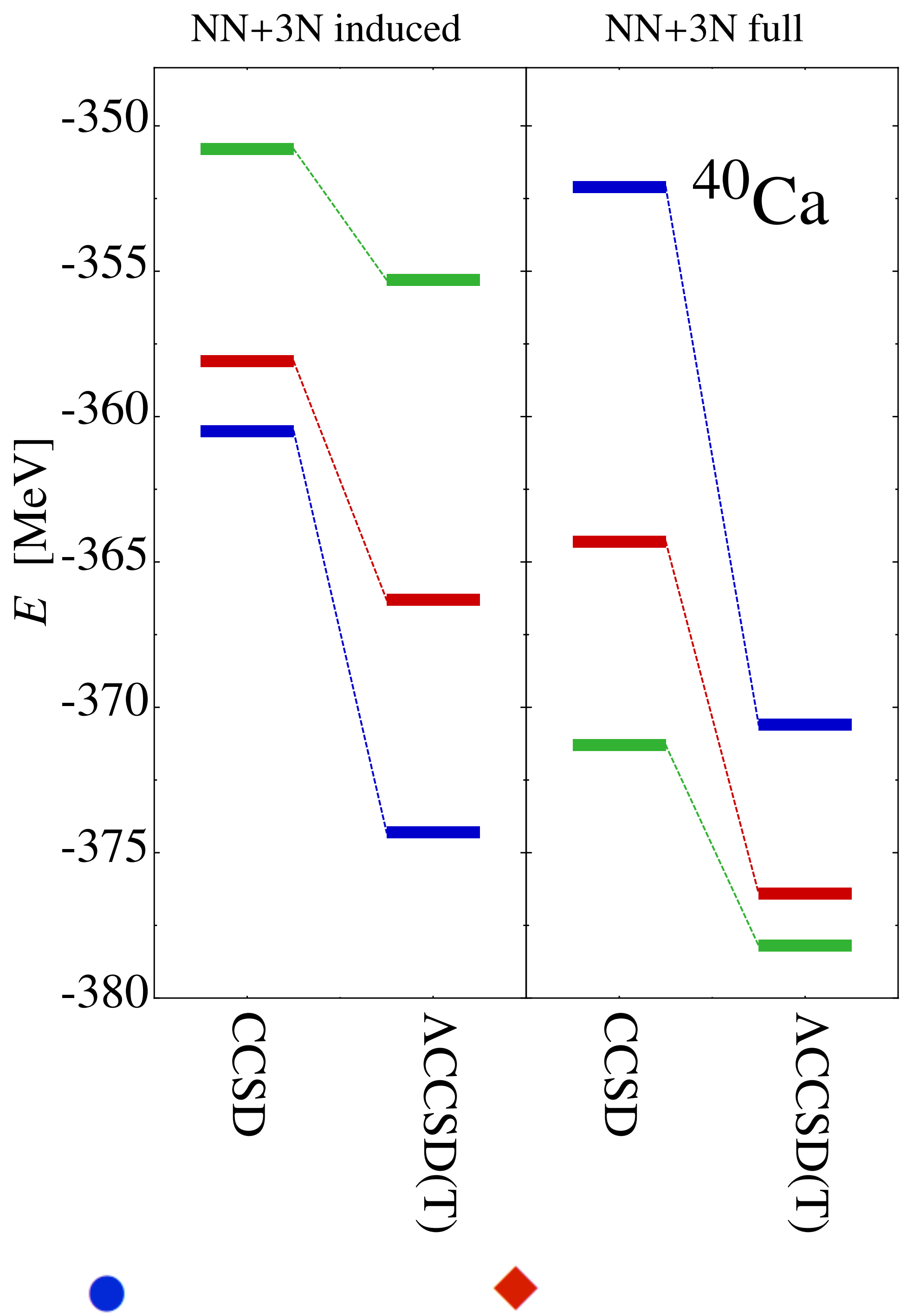
$\Lambda = 1.88\,\mathrm{fm}^{-1}$

CCSD$_{NO2B}$ vs. ΛCCSD(T)$_{NO2B}$



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

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

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

- inclusion of **triples excitations mandatory** (up to 6% more binding for heavier nuclei)
- cluster truncation works better for **softer interactions**
- results for harder interactions not necessarily closer to **exact bare result** than results for softer interactions
- $\Longrightarrow$ truncated CC calculations with **bare** 3N interaction suffer from cluster truncation and E_{3max} cut

ΛCCSD(T) with Explicit 3N Interactions (ΛCCSD(T)3B)

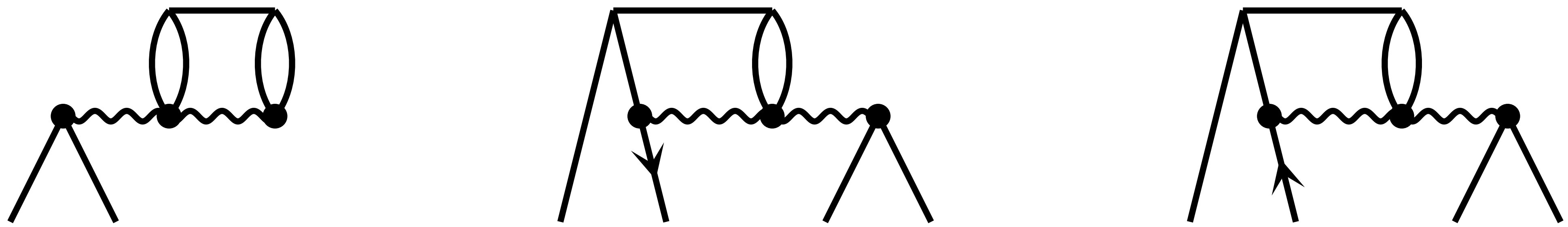
S. Binder, J. Langhammer, A. Calci, P. Piecuch, P. Navrátil, R. Roth --- in prep.

ΛCCSD(T)3B

- **effective Hamiltonian**

$$
\begin{aligned}
\hat{\mathcal{H}} &= e^{-\hat{T}}\ \hat{H}_N\ e^{\hat{T}} \\
&= \hat{\mathcal{H}}_{\text{NO2B}} + \hat{W}_{\text{3B}} + \sum_{n=1}^{6} \frac{1}{n!} \underbrace{\Big[\dots\Big[}_{n \text{ times}} \hat{W}_{\text{3B}}, \underbrace{\hat{T}\Big], \dots, \hat{T}\Big]}_{n \text{ times}} \\
&= \hat{\mathcal{H}}_{\text{NO2B}} + \text{ 116 relevant terms } + \dots
\end{aligned}
$$

- **ΛCCSD(T) runtime** dominated by Λ equations through



ΛCCSD(T)3B

- ΛCCSD(T)3B energy correction

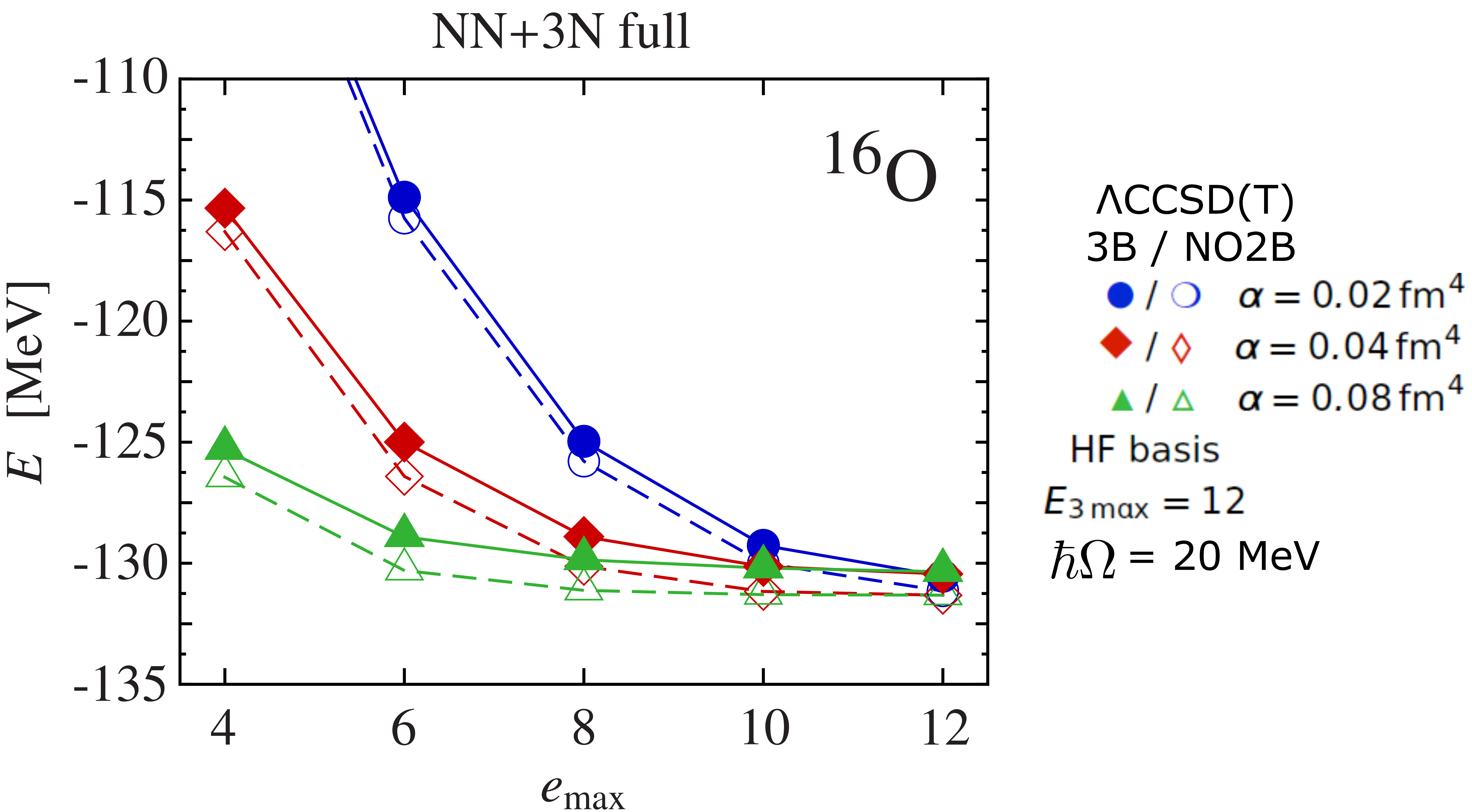
$$\Delta E_{\Lambda\mathrm{CCSD}(T)} = \frac{1}{(3!)^2} \sum_{\substack{abc\\ijk}} \tilde{\lambda}^{ijk}_{abc} \frac{1}{\epsilon^{abc}_{ijk}} \tilde{t}^{abc}_{ijk}$$

- contributions from residual 3N interaction to $\tilde{t}^{abc}_{ijk}, \tilde{\lambda}^{ijk}_{abc}$ **manageable**

$$\tilde{\lambda}^{ijk}_{abc} = \tilde{\lambda}^{ijk}_{abc}[\mathrm{NO2B}] - \hat{P}_{ab/c} \sum_{l} w^{ijk}_{abl}\, \lambda^{l}_{c} + \hat{P}_{ij/k} \sum_{d} w^{ijd}_{abc}\, \lambda^{k}_{d}$$
$$+\tfrac{1}{2}\, \hat{P}_{ij/k} \sum_{de} w^{dek}_{abc}\, \lambda^{ij}_{de} + \tfrac{1}{2}\, \hat{P}_{ab/c} \sum_{lm} w^{ijk}_{lmc}\, \lambda^{lm}_{ab} + \hat{P}^{ab/c}_{ij/k} \sum_{dl} w^{ijd}_{abl}\, \lambda^{kl}_{cd}$$

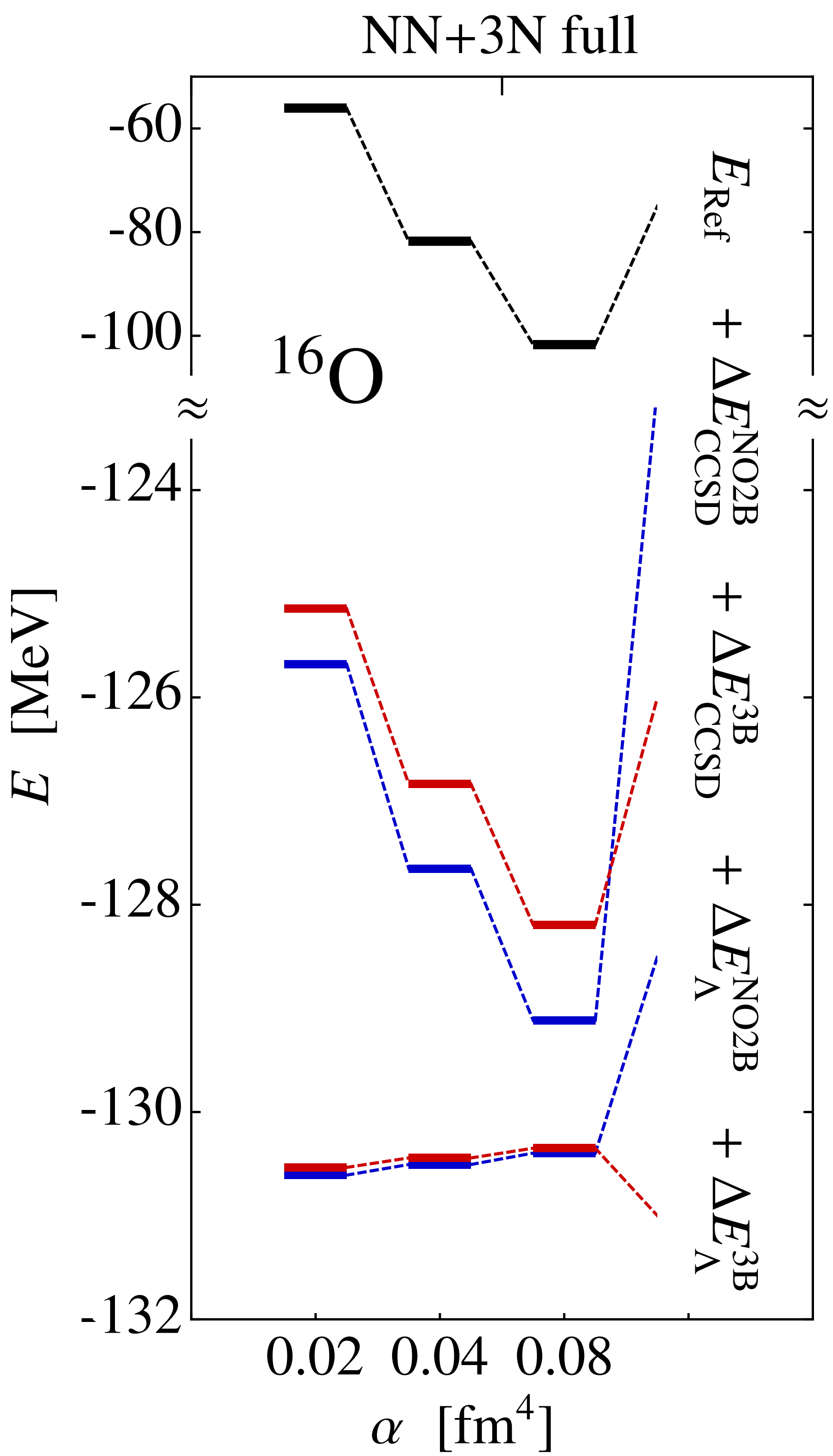
$$\tilde{t}^{abc}_{ijk} = \tilde{t}^{abc}_{ijk}[\mathrm{NO2B}] - \hat{P}_{ab/c} \sum_{l} w^{abl}_{ijk}\, t^{c}_{l} + \hat{P}_{ij/k} \sum_{d} w^{abc}_{ijd}\, t^{d}_{k}$$
$$+\tfrac{1}{2}\, \hat{P}_{ij/k} \sum_{de} w^{abc}_{dek}\, t^{de}_{ij} + \tfrac{1}{2}\, \hat{P}_{ab/c} \sum_{lm} w^{lmc}_{ijk}\, t^{ab}_{lm} + \hat{P}^{ab/c}_{ij/k} \sum_{dl} w^{abl}_{ijd}\, t^{cd}_{kl}$$

ΛCCSD(T)3B



NN+3N full
-110
-115
-120
-125
-130
-135
E [MeV]
4
6
8
10
12
e_{max}
^{16}O
ΛCCSD(T)
3B / NO2B
$\alpha = 0.02\,\mathrm{fm}^4$
$\alpha = 0.04\,\mathrm{fm}^4$
$\alpha = 0.08\,\mathrm{fm}^4$
HF basis
$E_{3\,max} = 12$
$\hbar\Omega$ = 20 MeV

ΛCCSD(T)3B



- NO2B shows **excellent agreement** also for ΛCCSD(T)
- ^{16}O: residual 3N contribute **0.5-0.7%** to total binding energy $E_{\Lambda\text{CCSD(T)3B}}$
- $E_{\Lambda\text{CCSD(T)}} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle + \Delta E_{\text{CCSD}} + \Delta E_{\Lambda\text{CCSD(T)}}$

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

- residual 3N (α=0.08 fm^4) contribute
  - **0.00 MeV** or **0.0 %** to $\langle \Phi_0 | \hat{H} | \Phi_0 \rangle$
  - **0.70 MeV** or **2.7 %** to ΔE_{CCSD}
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- significant contribution of residual 3N **only for ΔE_{CCSD}**
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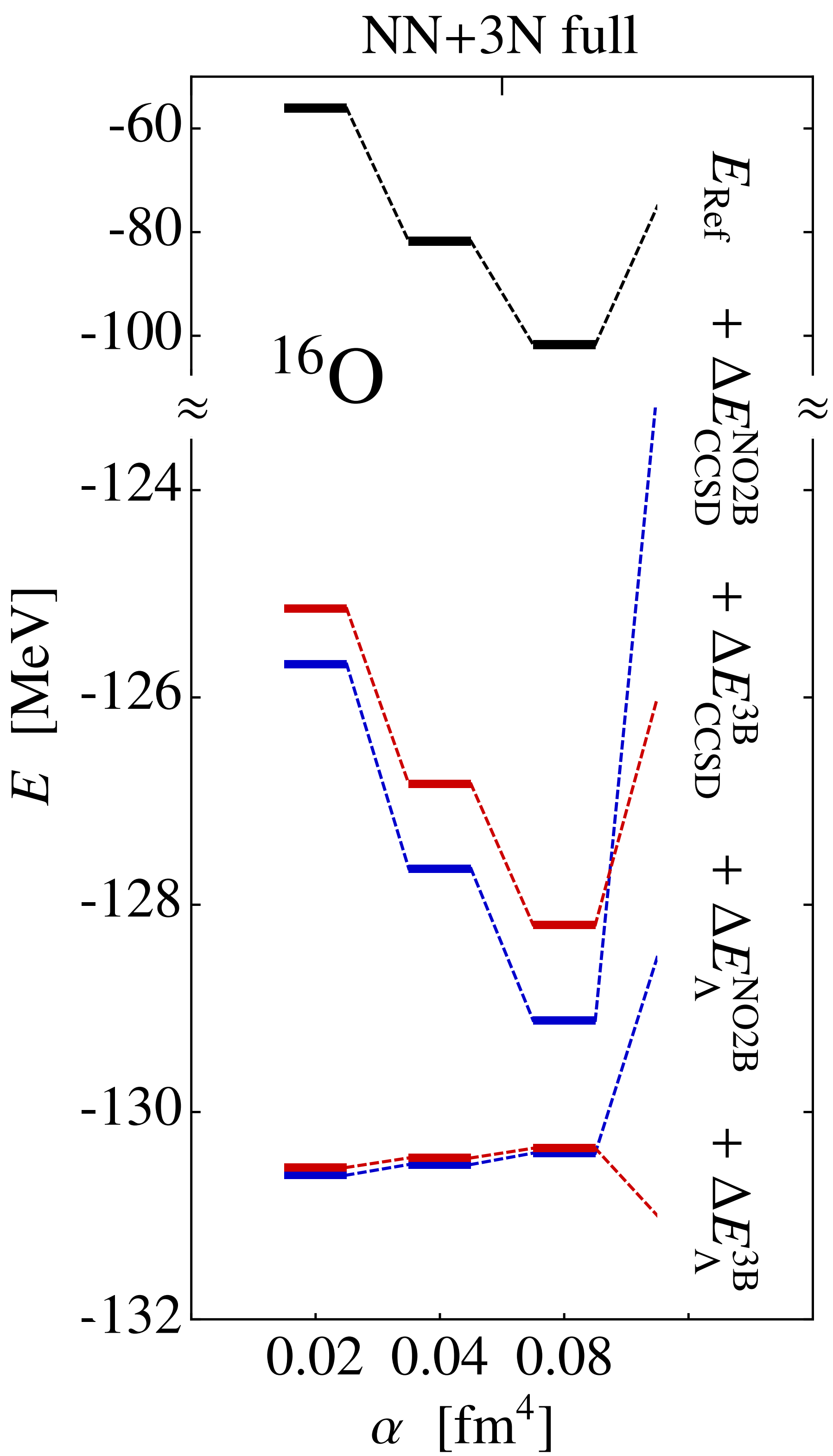
ΛCCSD(T)3B



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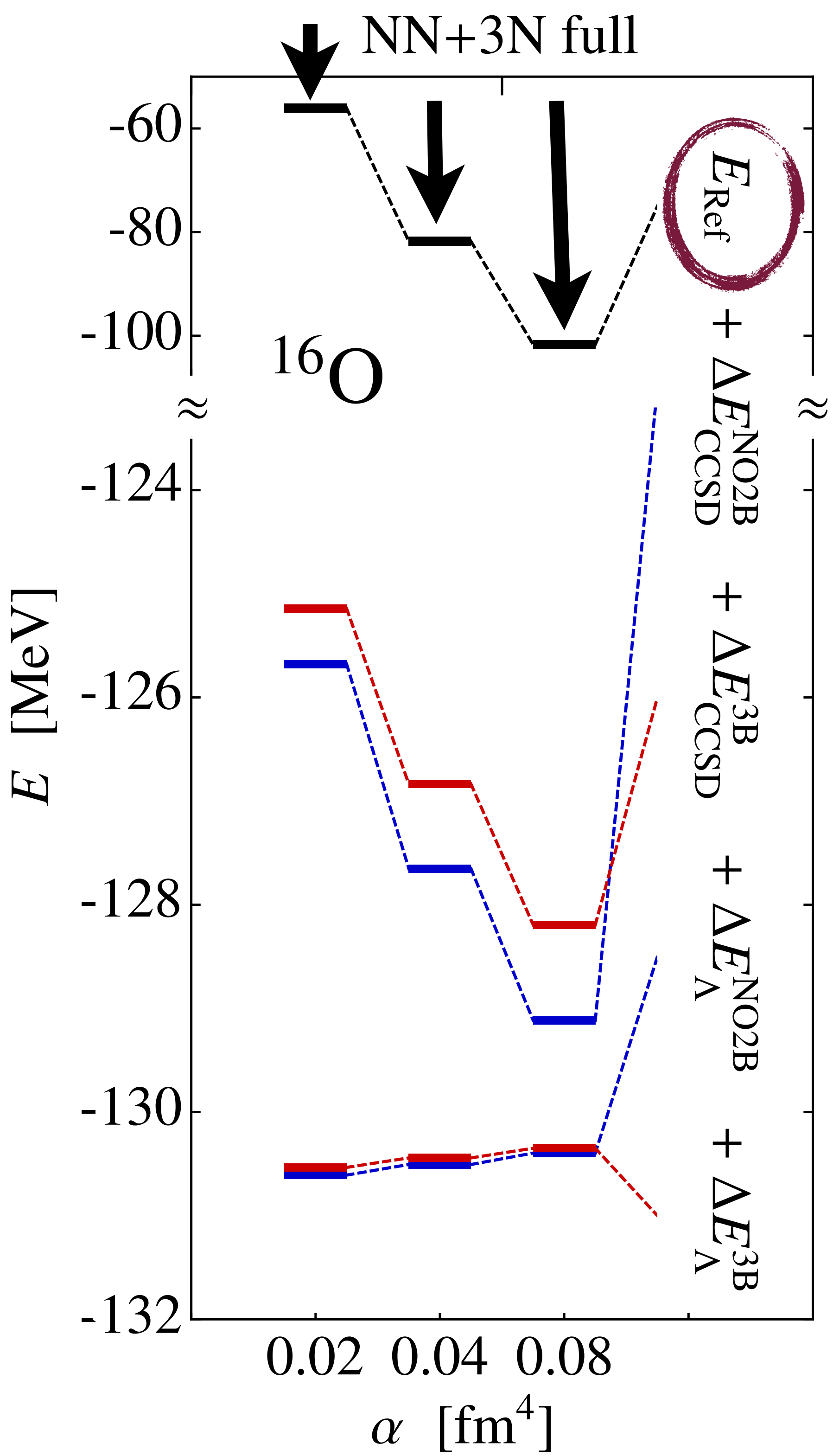
ΛCCSD(T)3B



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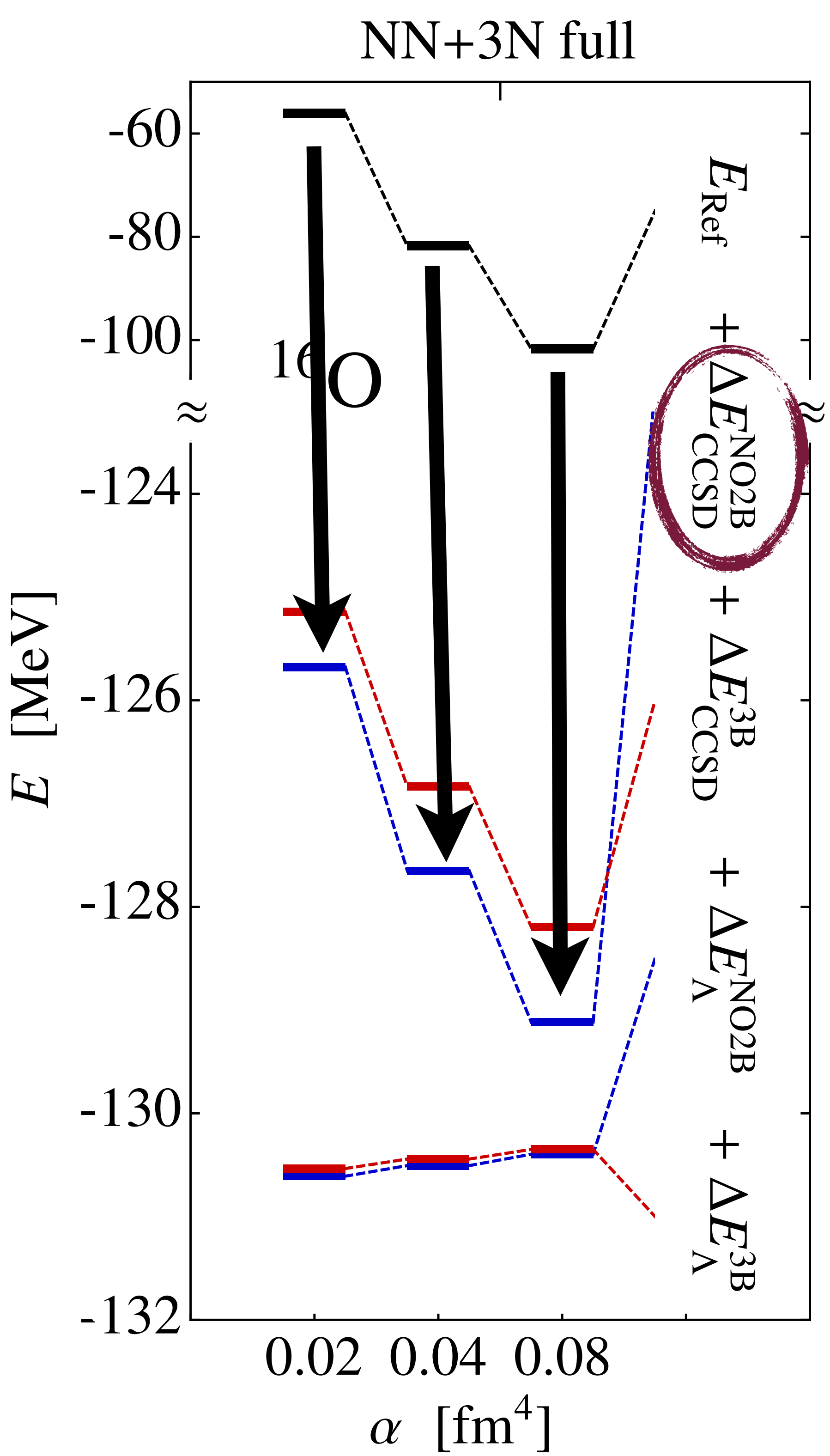
ΛCCSD(T)3B



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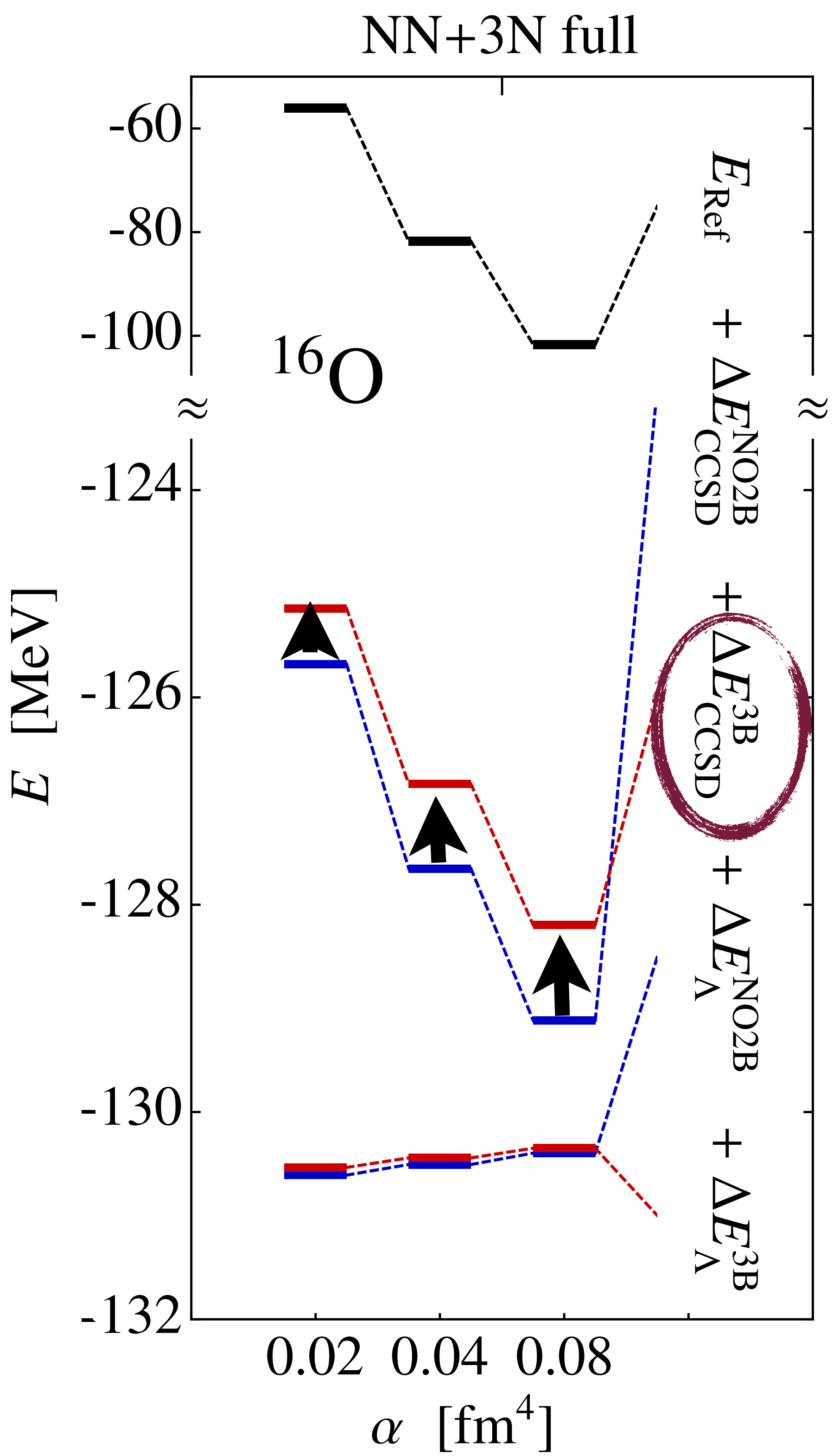
ΛCCSD(T)3B



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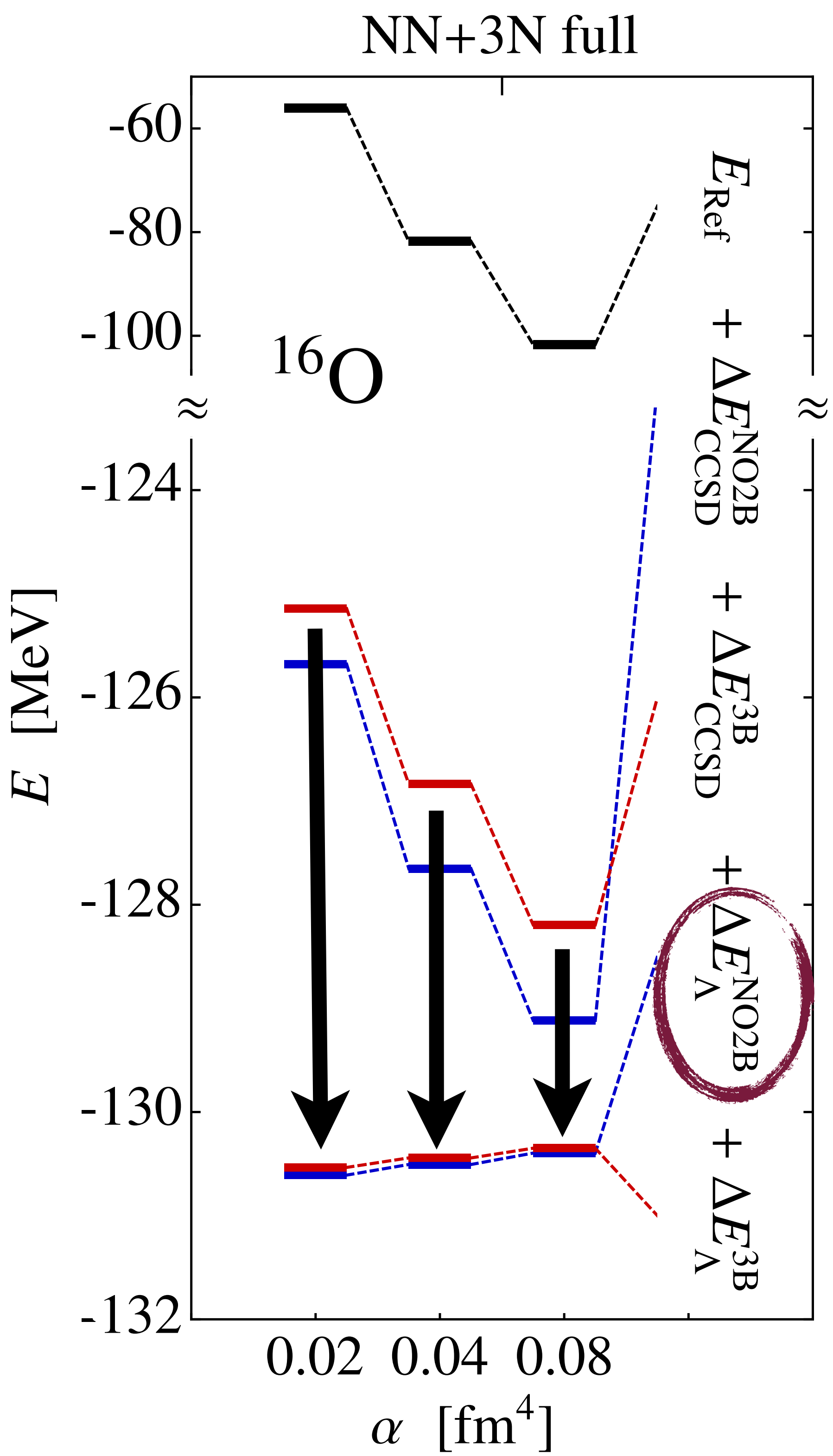
ΛCCSD(T)3B



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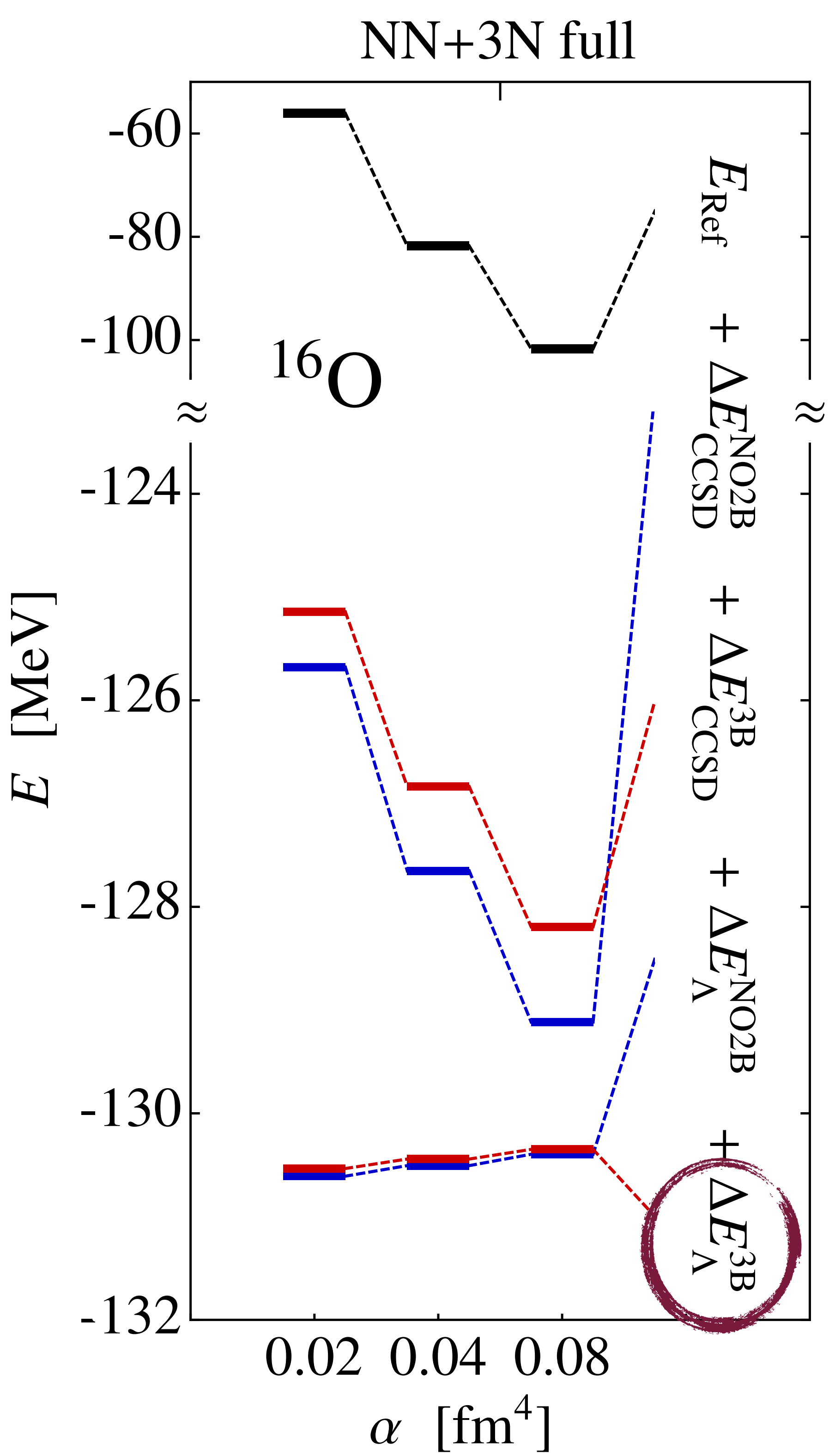

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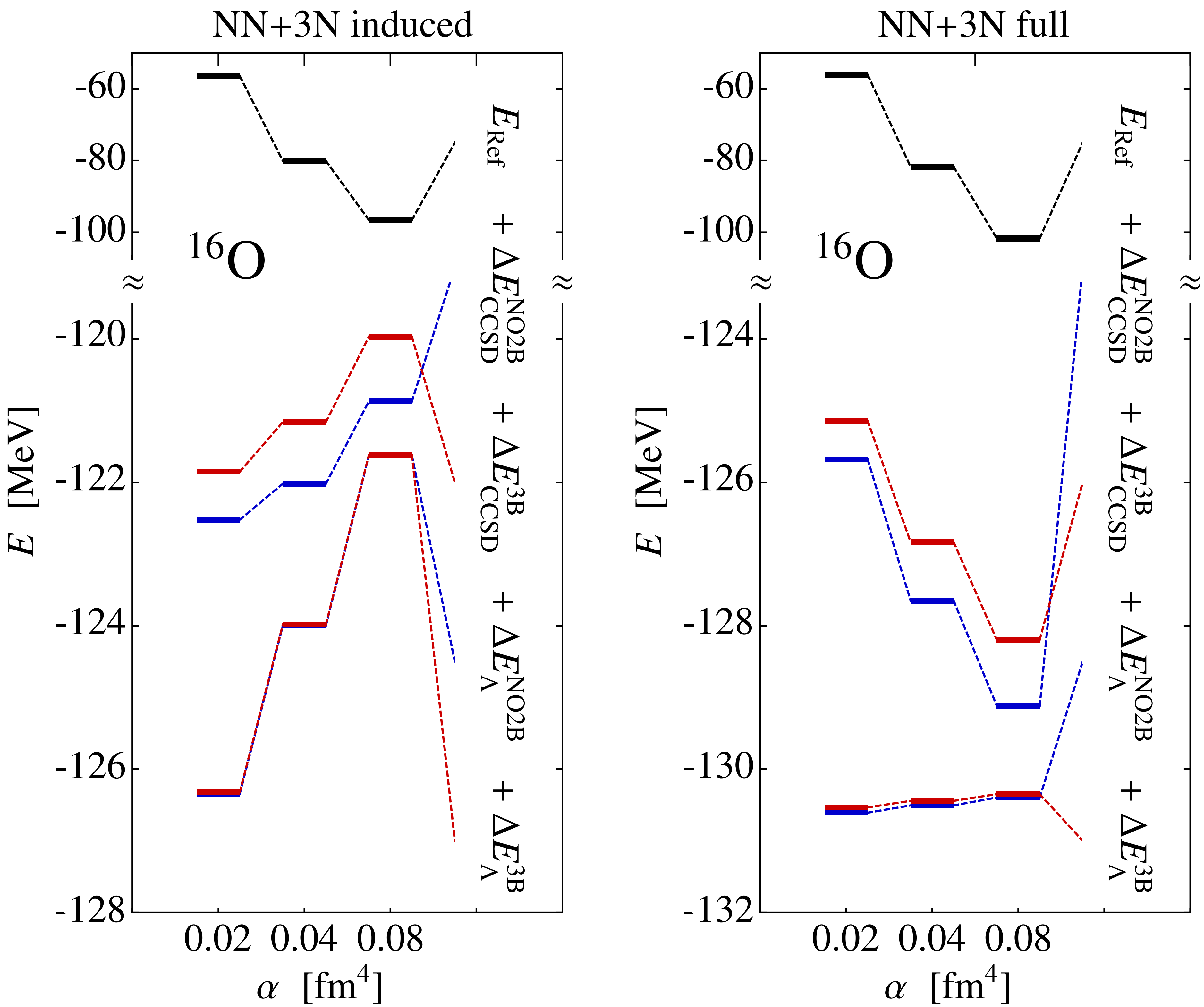
ΛCCSD(T)3B



ΛCCSD(T)3B

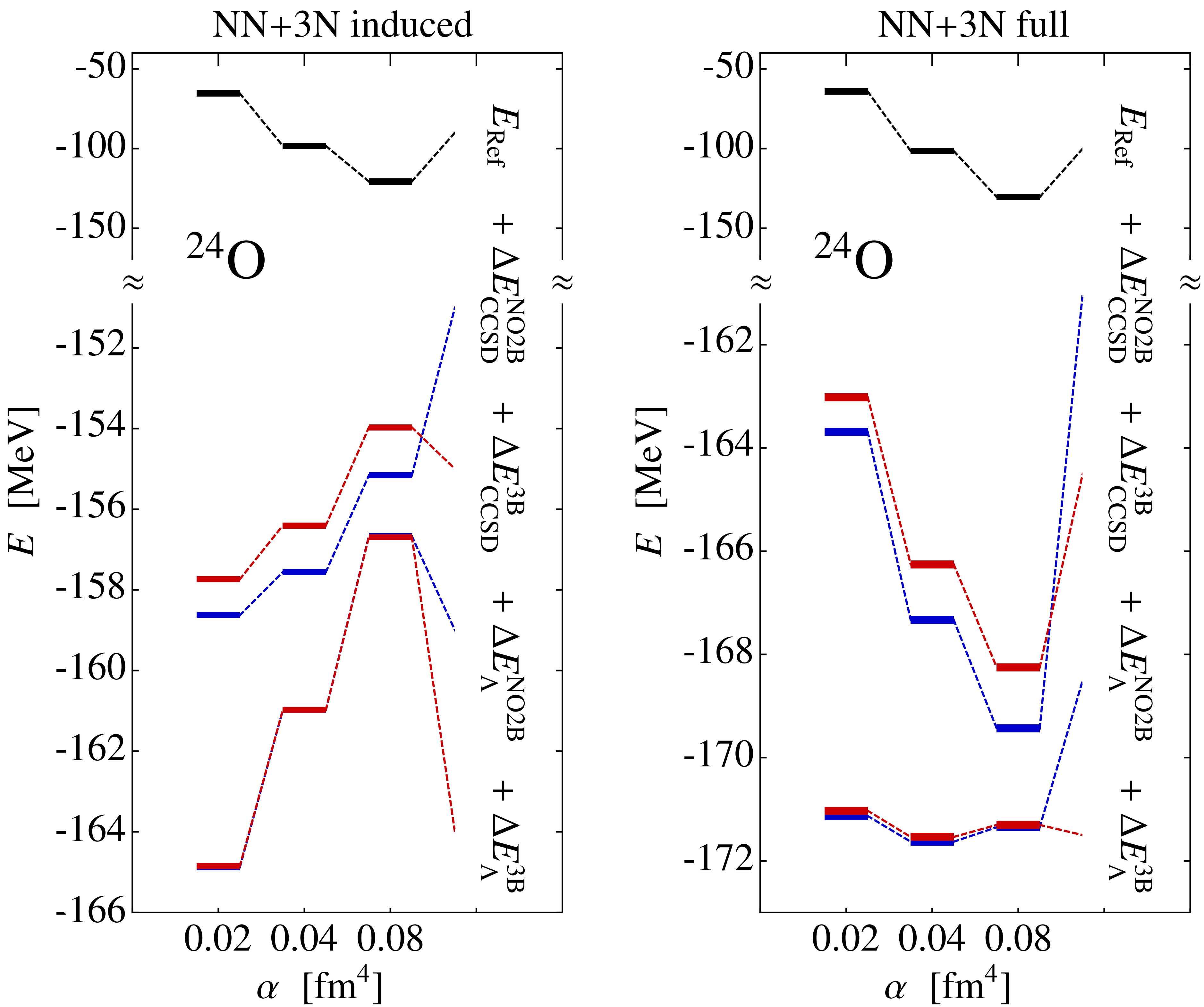
HF basis

e_{max} = 12

E_{3max} = 12

$\hbar\Omega$ = 20 MeV

ΛCCSD(T)3B



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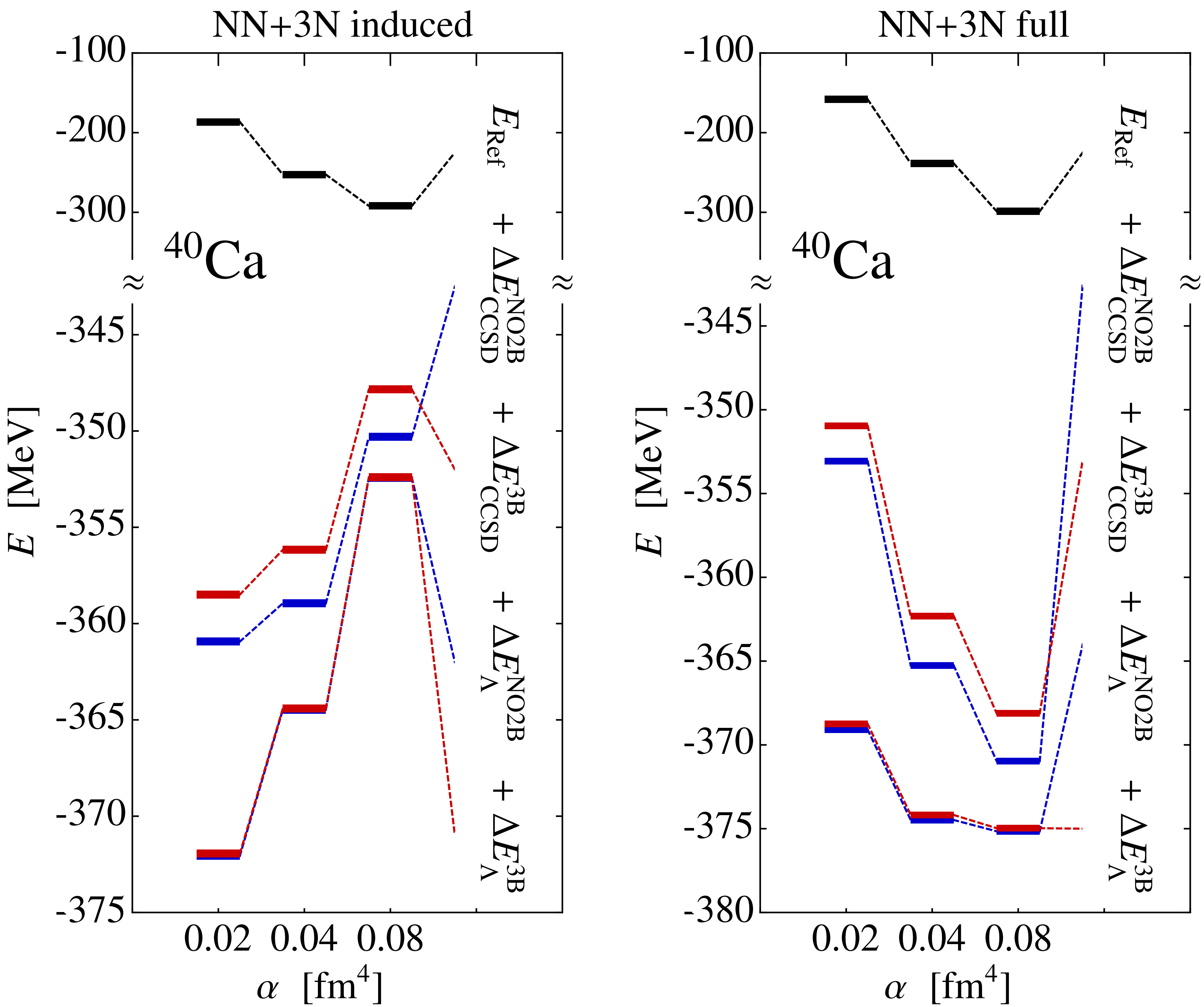
ΛCCSD(T)3B



ΛCCSD(T)3B

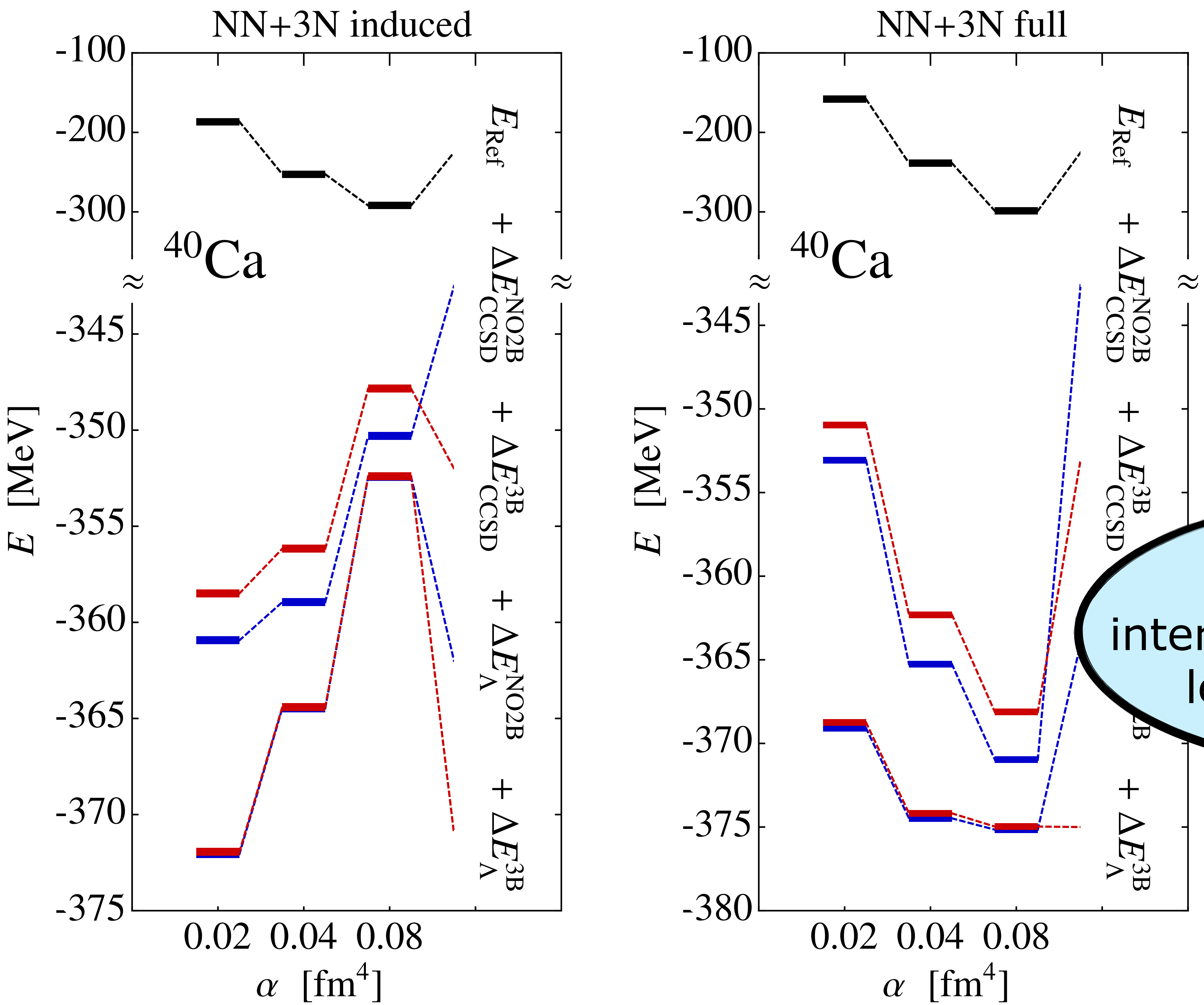
HF basis

e_{max} = 10

E_{3max} = 12

$\hbar\Omega$ = 24 MeV

ΛCCSD(T)3B

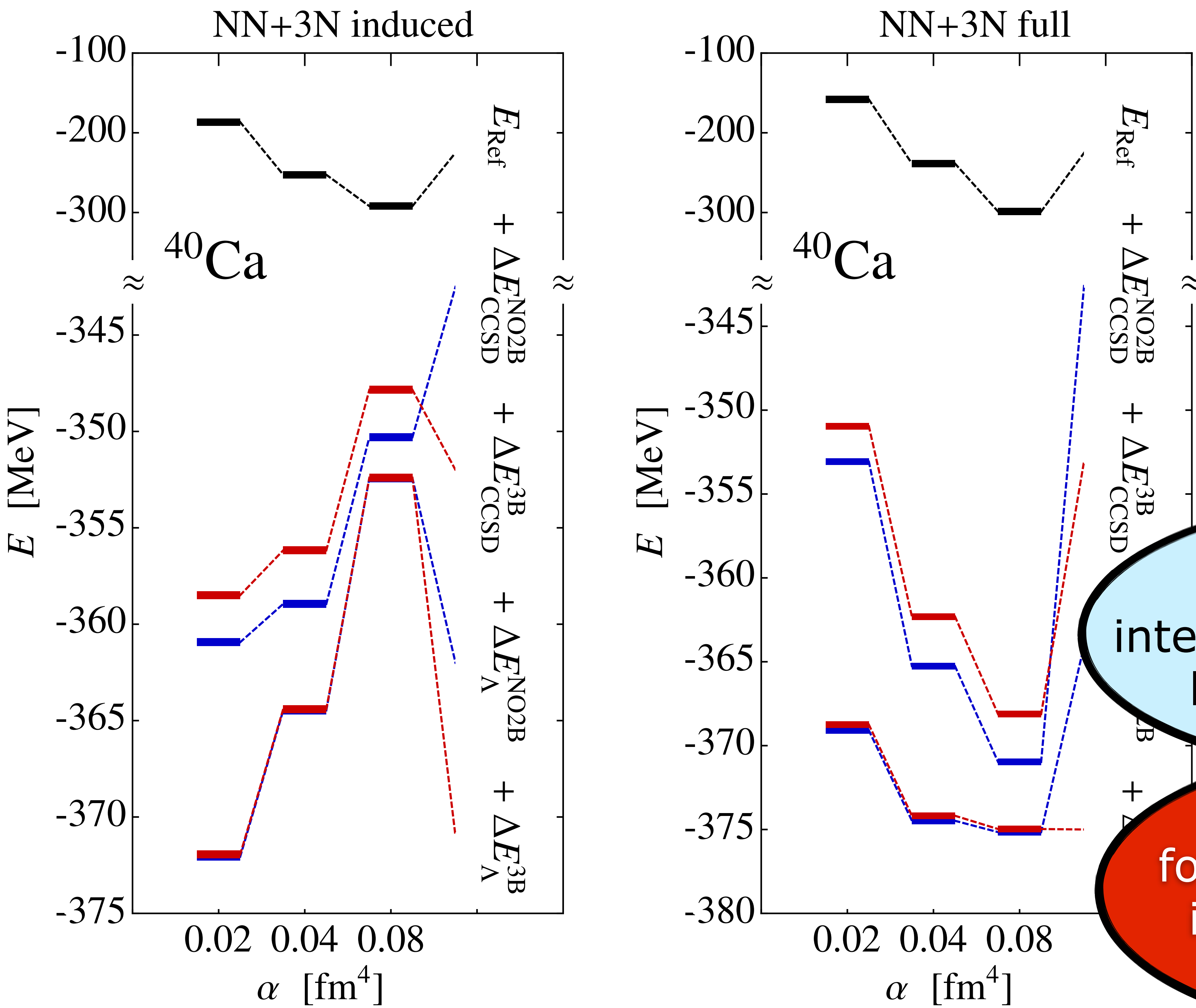


ΛCCSD(T)3B

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

residual 3N interaction at ΛCCSD(T) level insignificant

ΛCCSD(T)3B



ΛCCSD(T)3B

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

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BUT: for softer interactions important at CCSD level

Epilogue

- **thanks to my group & collaborators**
  - A. Calci, E. Gebrerufael, P. Isserstedt, H. Krutsch, J. Langhammer, S. Reinhard, R. Roth, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth

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  TRIUMF, Canada
- P. Piecuch
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- J. Vary, P. Maris
  Iowa State University, USA
- H. Hergert, K. Hebeler
  The Ohio State University, USA
- C. Forssén
  Chalmers University, Sweden
- H. Feldmeier, T. Neff
  GSI Helmholtzzentrum
- P. Papakonstantinou
  IPN Orsay, France

Computing Time

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NERSC

CSC Center for Scientific Computing Frankfurt

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

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Thanks for your attention!

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