Coupled-Cluster Calculations of Medium-Mass Nuclei

Sven Binder

INSTITUT FÜR KERNPHYSIK

TECHNISCHE UNIVERSITÄT DARMSTADT

From QCD to Nuclear Structure

Nuclear Structure

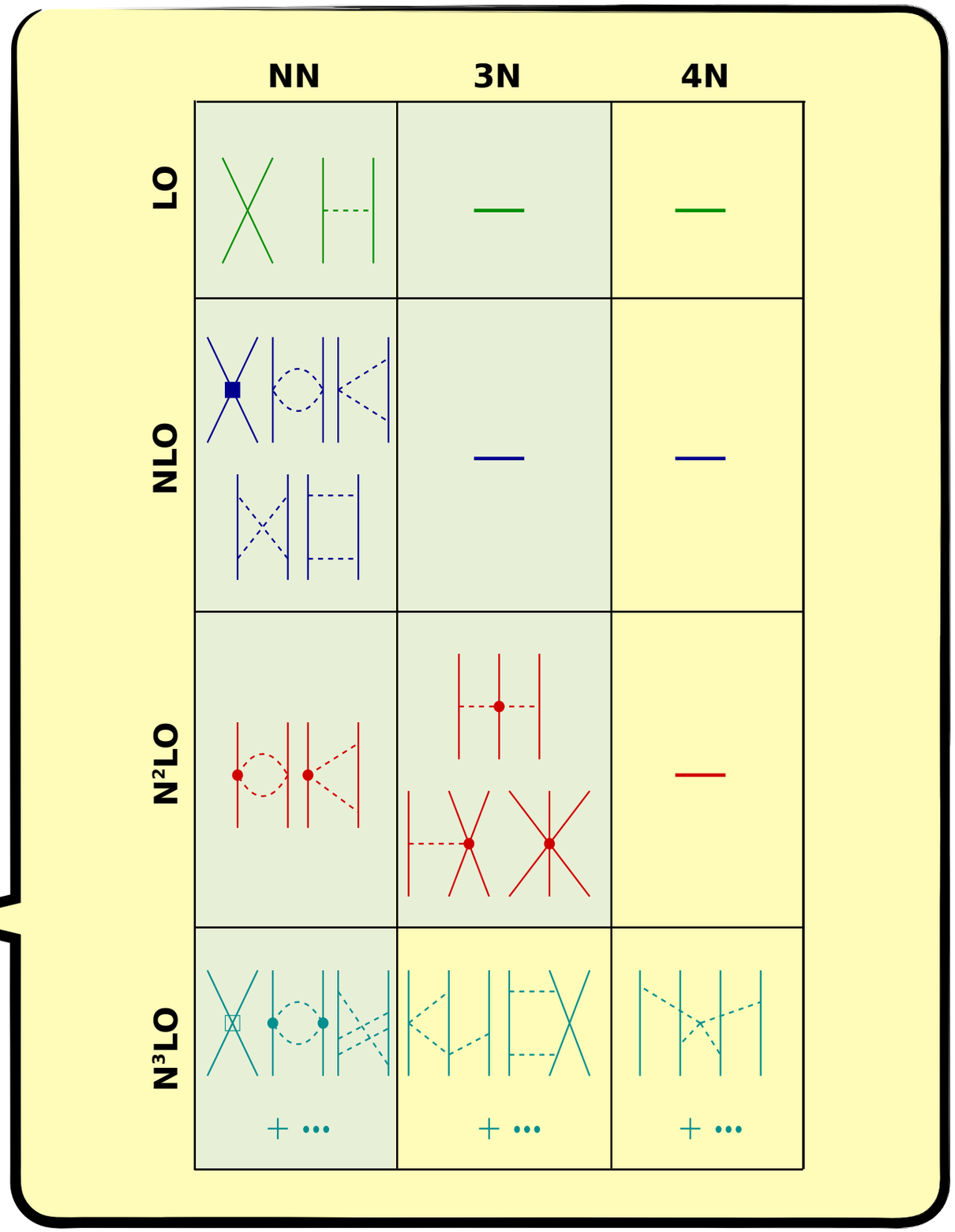
Low-Energy QCD

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

NN+3N interaction from Chiral EFT

Low-Energy QCD

adapt Hamiltonian to truncated low-energy model spaces

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

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

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

Calculations in A-Body Space

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

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

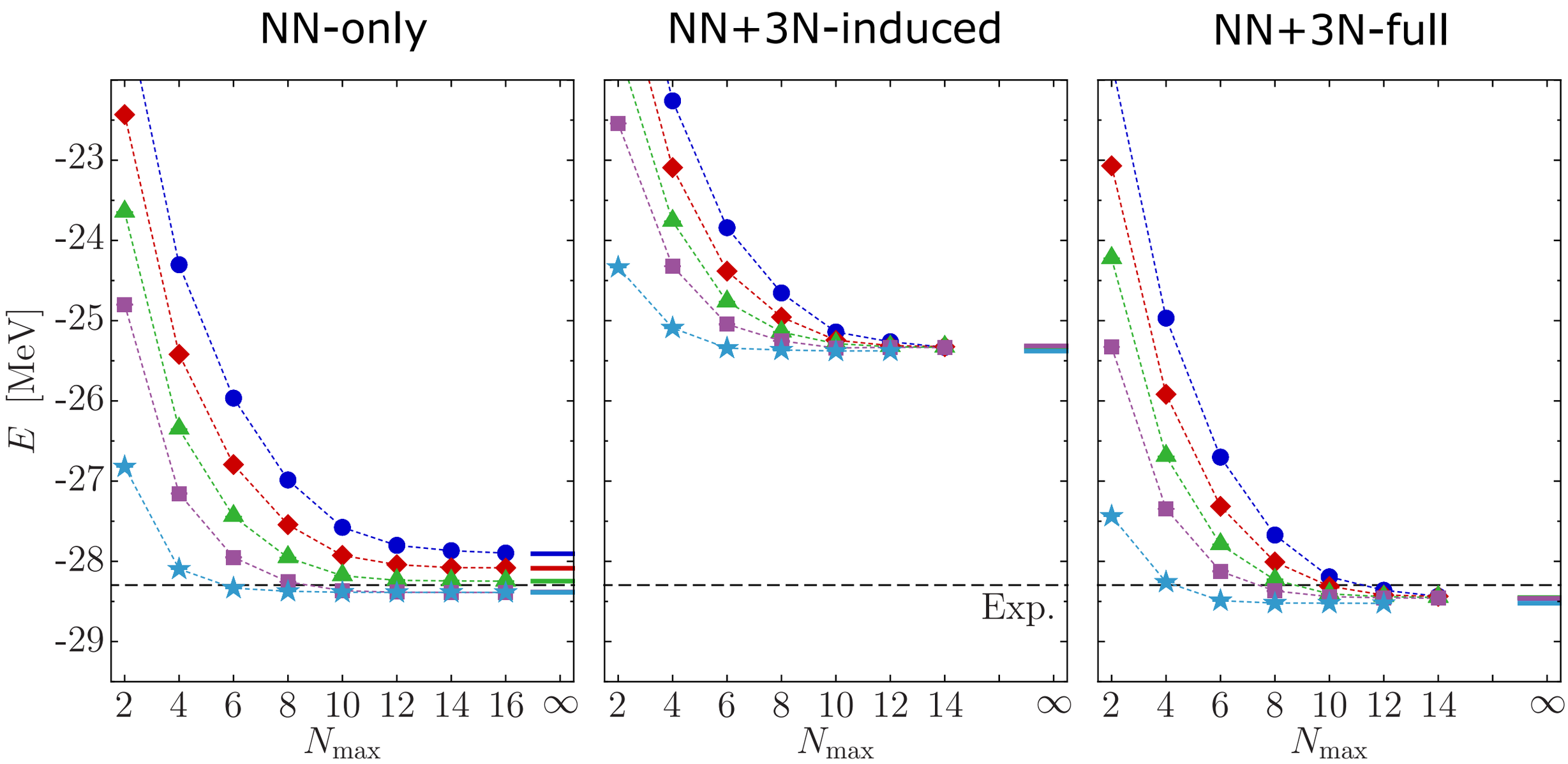
- truncation of cluster series inevitable → invariance of energy eigenvalues (α-variation)

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

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

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



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

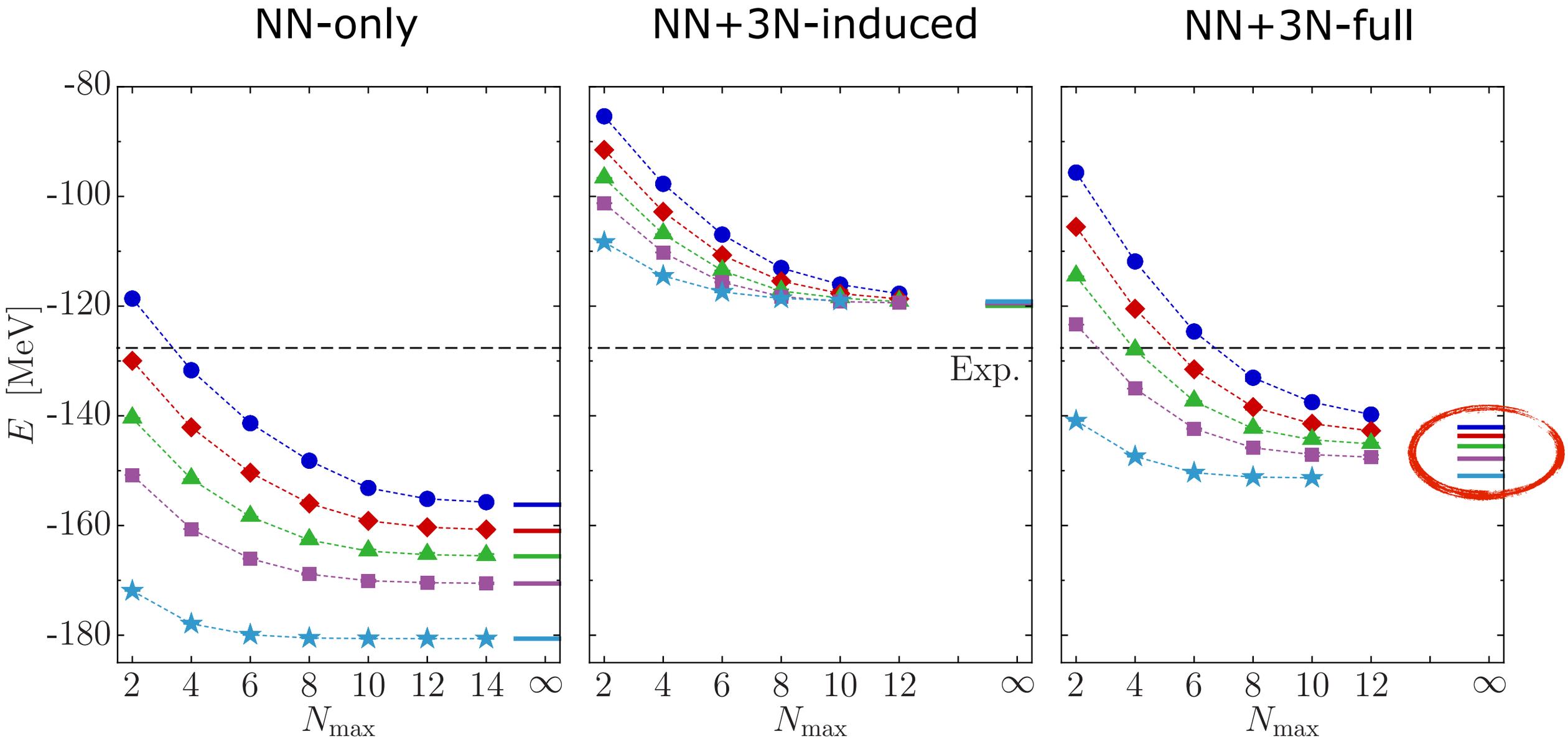
$\alpha = 0.05\,\mathrm{fm}^4$ $\Lambda = 2.11\,\mathrm{fm}^{-1}$

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

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

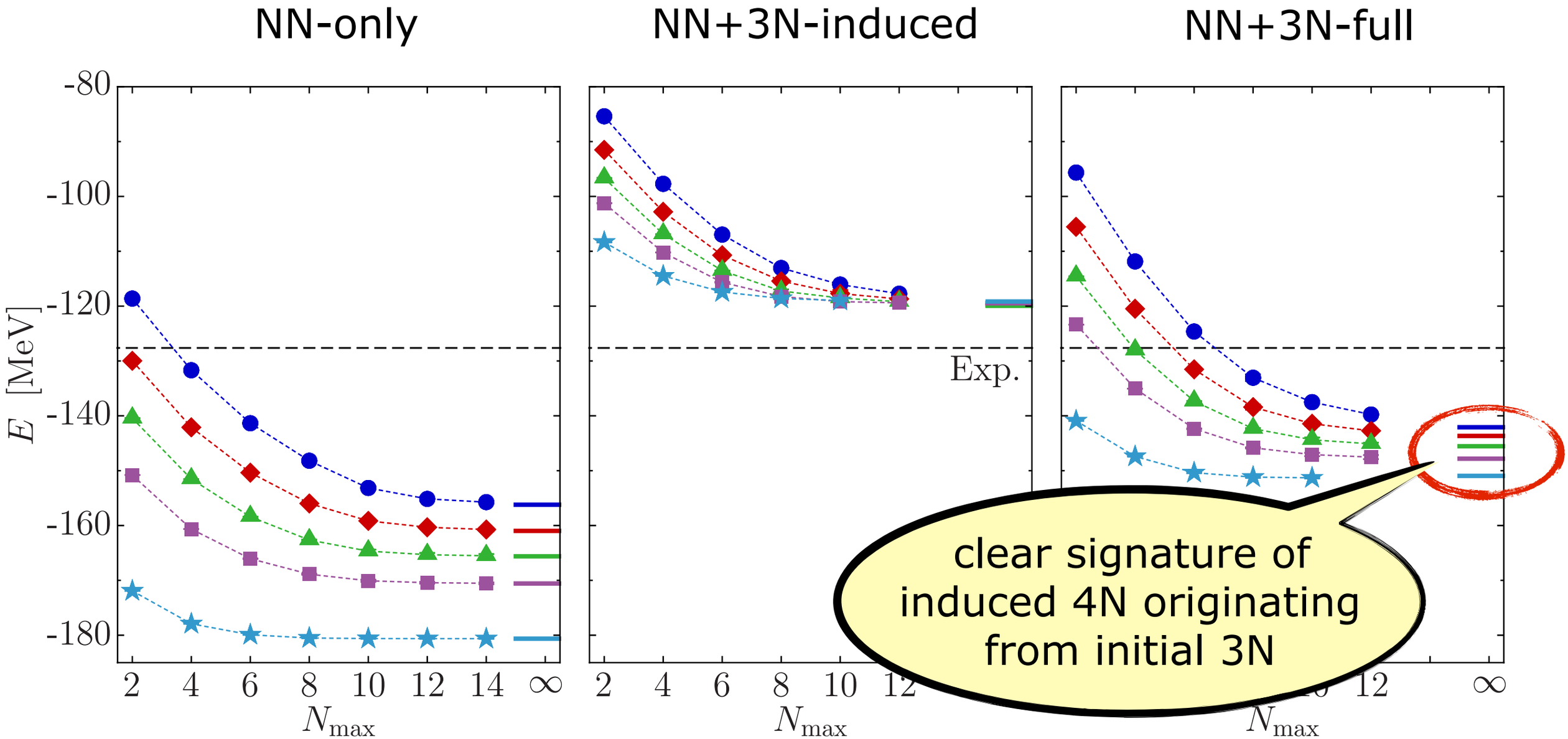
$\alpha = 0.16\,\mathrm{fm}^4$ $\Lambda = 1.58\,\mathrm{fm}^{-1}$

^{16}O: IT-NCSM Ground-State Energies



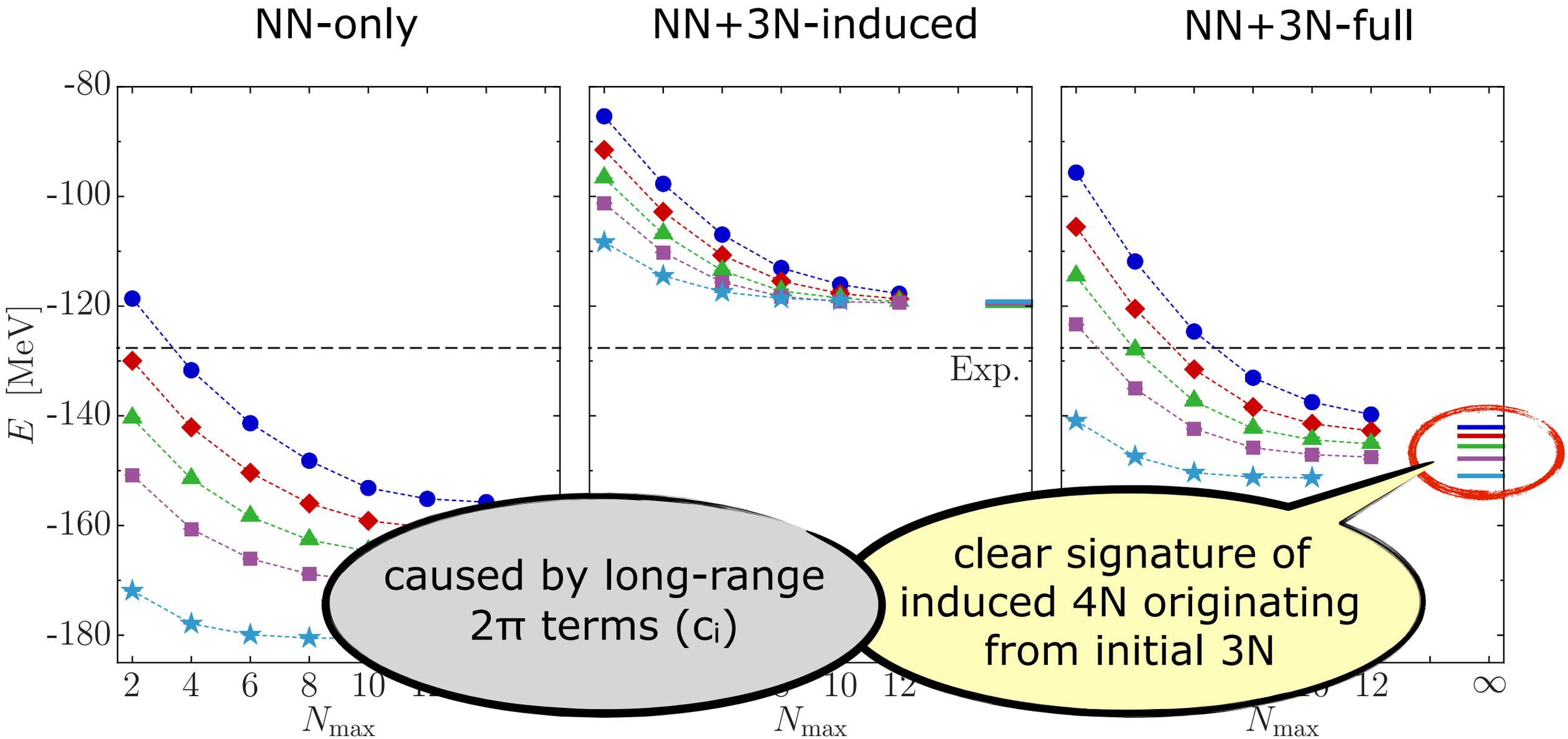
$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.05\,\mathrm{fm}^4$	$\alpha = 0.0625\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$	$\alpha = 0.16\,\mathrm{fm}^4$
$\Lambda = 2.24\,\mathrm{fm}^{-1}$	$\Lambda = 2.11\,\mathrm{fm}^{-1}$	$\Lambda = 2.00\,\mathrm{fm}^{-1}$	$\Lambda = 1.88\,\mathrm{fm}^{-1}$	$\Lambda = 1.58\,\mathrm{fm}^{-1}$

^{16}O: IT-NCSM Ground-State Energies



$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.05\,\mathrm{fm}^4$	$\alpha = 0.0625\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$	$\alpha = 0.16\,\mathrm{fm}^4$
$\Lambda = 2.24\,\mathrm{fm}^{-1}$	$\Lambda = 2.11\,\mathrm{fm}^{-1}$	$\Lambda = 2.00\,\mathrm{fm}^{-1}$	$\Lambda = 1.88\,\mathrm{fm}^{-1}$	$\Lambda = 1.58\,\mathrm{fm}^{-1}$

^{16}O: IT-NCSM Ground-State Energies



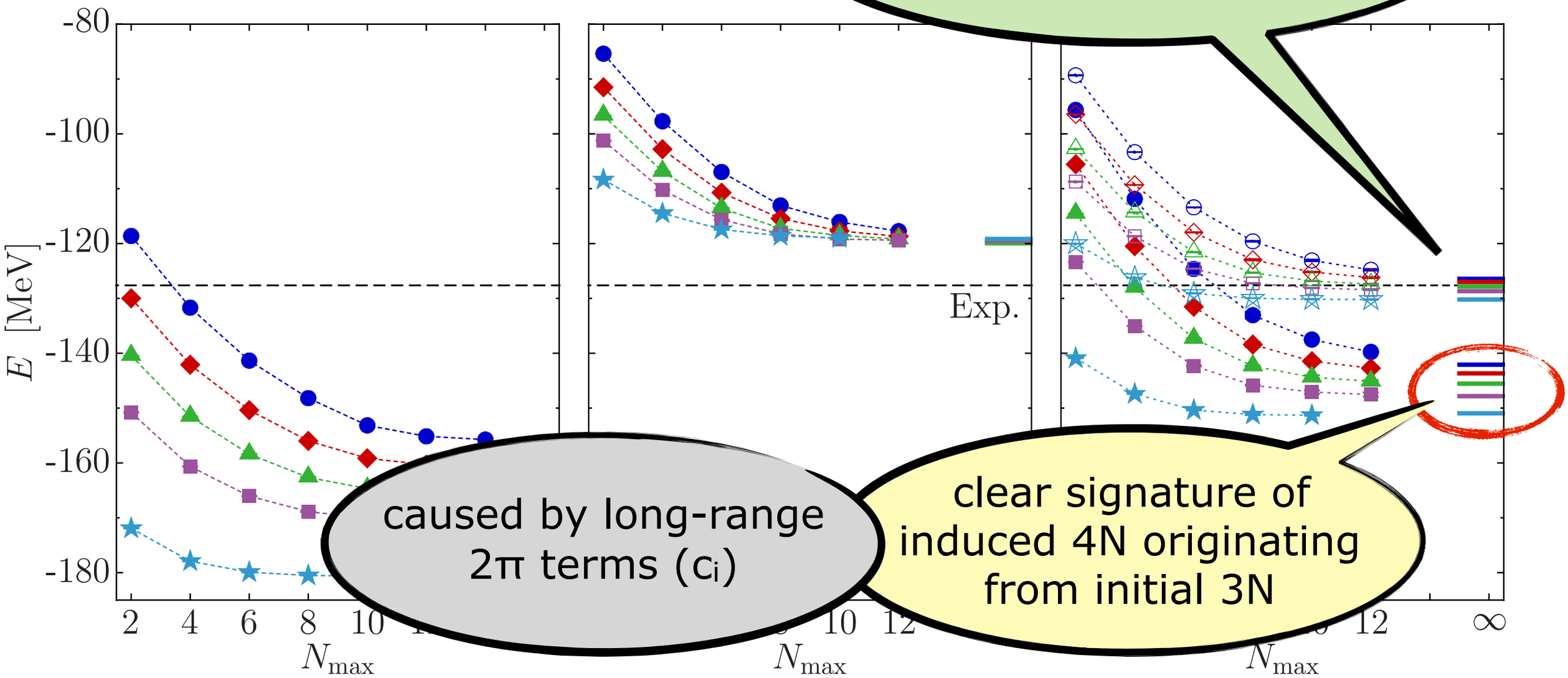
$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.05\,\mathrm{fm}^4$	$\alpha = 0.0625\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$	$\alpha = 0.16\,\mathrm{fm}^4$
$\Lambda = 2.24\,\mathrm{fm}^{-1}$	$\Lambda = 2.11\,\mathrm{fm}^{-1}$	$\Lambda = 2.00\,\mathrm{fm}^{-1}$	$\Lambda = 1.88\,\mathrm{fm}^{-1}$	$\Lambda = 1.58\,\mathrm{fm}^{-1}$

^{16}O: IT–NCSM Ground-S

3N interaction with 400 MeV cutoff, c_E fitted to ^{4}He ground state

NN-only

NN+3N



caused by long-range 2π terms (c_i)

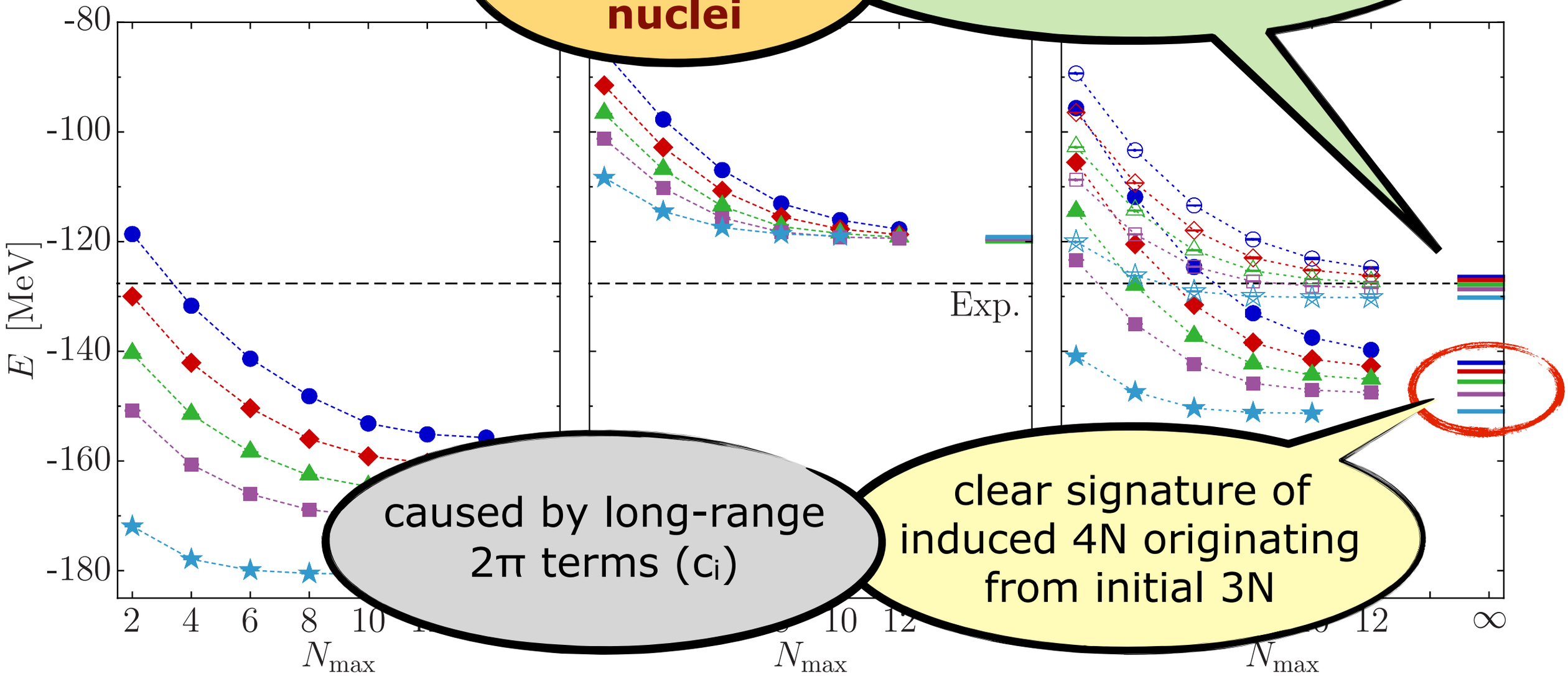
clear signature of induced 4N originating from initial 3N

●	◆	▲	■	★
$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.05\,\mathrm{fm}^4$	$\alpha = 0.0625\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$	$\alpha = 0.16\,\mathrm{fm}^4$
$\Lambda = 2.24\,\mathrm{fm}^{-1}$	$\Lambda = 2.11\,\mathrm{fm}^{-1}$	$\Lambda = 2.00\,\mathrm{fm}^{-1}$	$\Lambda = 1.88\,\mathrm{fm}^{-1}$	$\Lambda = 1.58\,\mathrm{fm}^{-1}$

^{16}O: IT–NCSM Ground-S

choice for **medium-mass nuclei**

3N interaction with 400 MeV cutoff, c_E fitted to ^{4}He ground state



caused by long-range 2π terms (c_i)

clear signature of induced 4N originating from initial 3N

●	◆	▲	■	★
$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.05\,\mathrm{fm}^4$	$\alpha = 0.0625\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$	$\alpha = 0.16\,\mathrm{fm}^4$
$\Lambda = 2.24\,\mathrm{fm}^{-1}$	$\Lambda = 2.11\,\mathrm{fm}^{-1}$	$\Lambda = 2.00\,\mathrm{fm}^{-1}$	$\Lambda = 1.88\,\mathrm{fm}^{-1}$	$\Lambda = 1.58\,\mathrm{fm}^{-1}$

Uncertainty Summary

- **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 $W^{3\mathrm{B}}$

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)

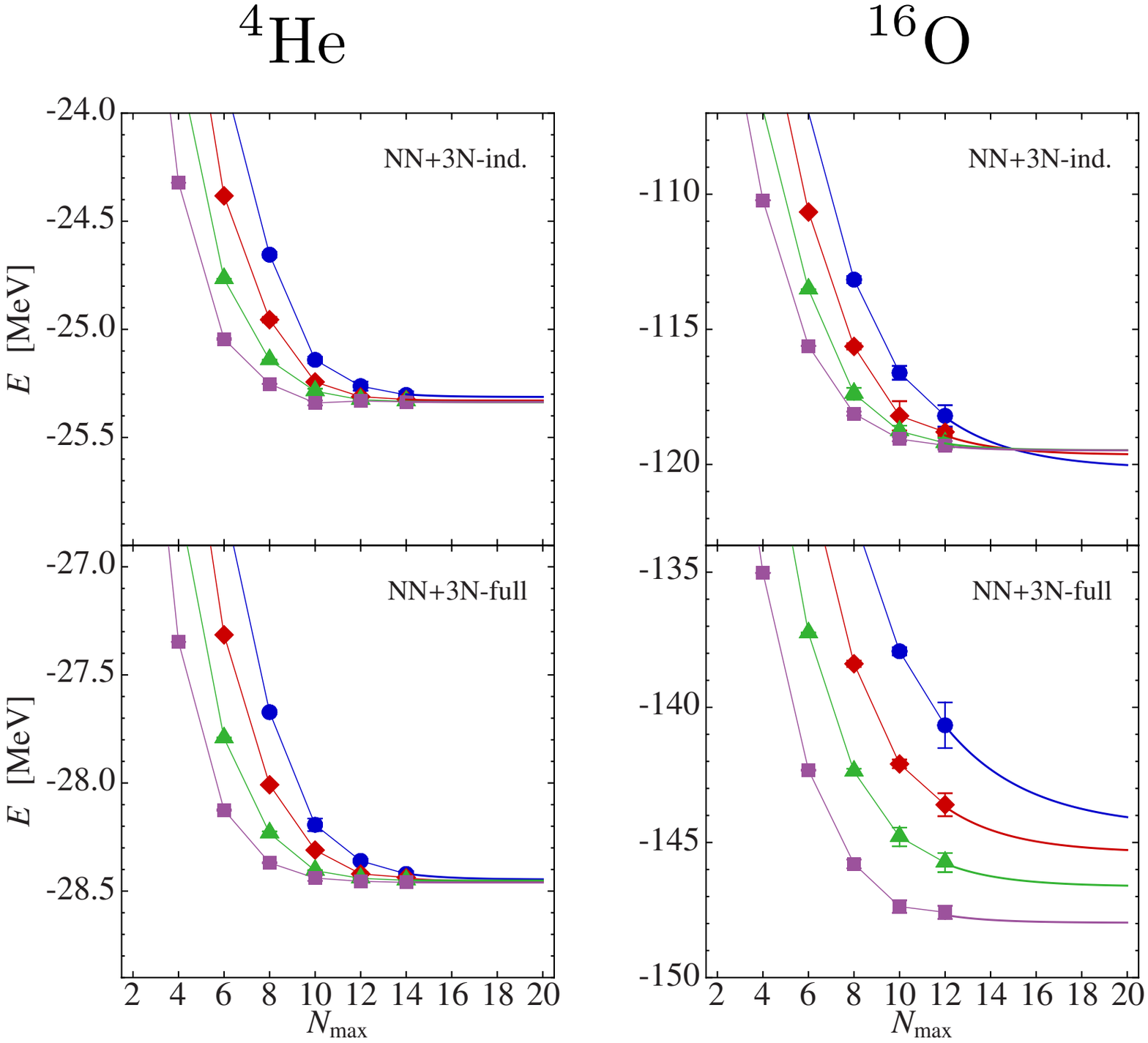
$$\hat{V}_{3\mathrm{N}} = \sum V^{3\mathrm{N}}_{\circ\circ\circ\circ\circ\circ} \, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

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

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

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

Benchmark of Normal-Ordered 3N

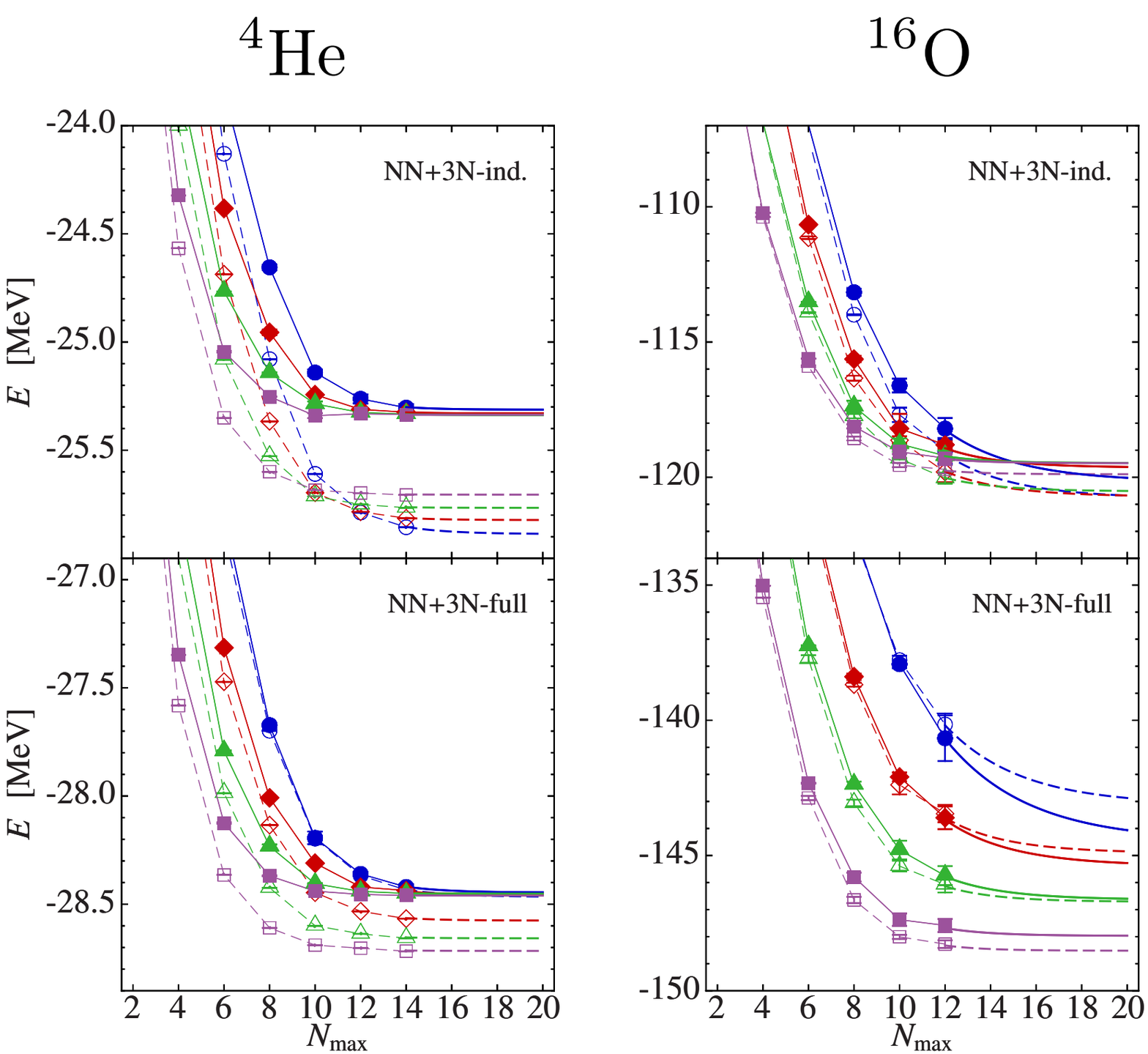


- compare IT-NCSM results with explicit 3N to normal-ordered 3N truncated at the 2B level (NO2B)
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O

● / ○ $\alpha = 0.04$ fm^4
◆ / ◇ $\alpha = 0.05$ fm^4
▲ / △ $\alpha = 0.0625$ fm^4
■ / □ $\alpha = 0.08$ fm^4

$\hbar\Omega = 20$ MeV

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

● / ○ $\alpha = 0.04$ fm^4
◆ / ◇ $\alpha = 0.05$ fm^4
▲ / △ $\alpha = 0.0625$ fm^4
■ / □ $\alpha = 0.08$ fm^4

$\hbar\Omega = 20$ MeV

Uncertainty Summary

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

- **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

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk\ldots \\ abc\ldots}} t_{ijk\ldots}^{abc\ldots} \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \ldots \hat{a}_k \hat{a}_j \hat{a}_i\}$$

- **similarity-transformed** Schroedinger equation

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

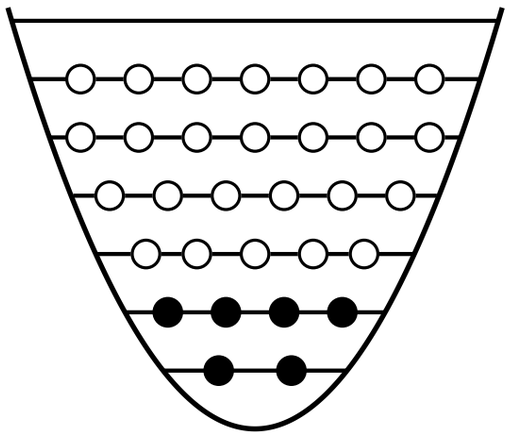
- $\hat{\mathcal{H}}$: non-Hermitian **effective Hamiltonian**

CCSD

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

CCSD

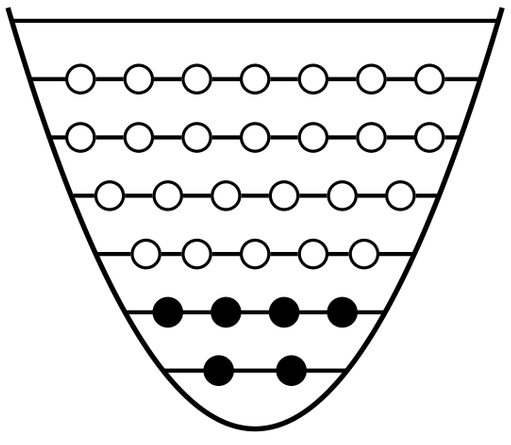
- **CCSD**: truncate $\hat{T}$ at the **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



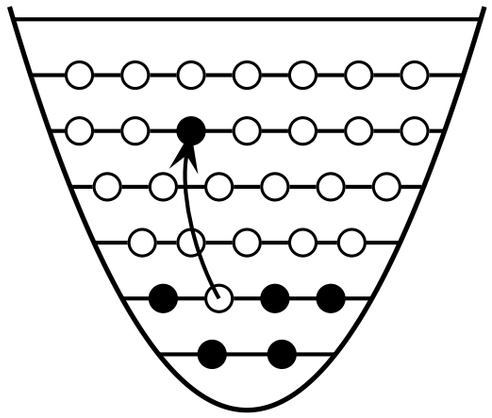
$|\Phi_0\rangle$

CCSD

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



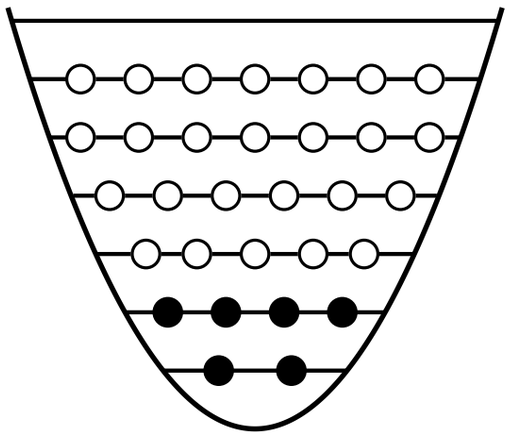
$|\Phi_0\rangle$



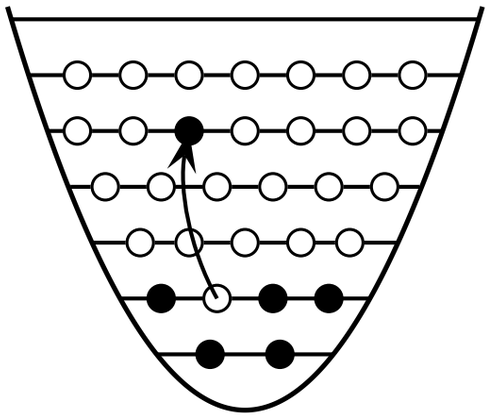
$\hat{T}_1 \, |\Phi_0\rangle$

CCSD

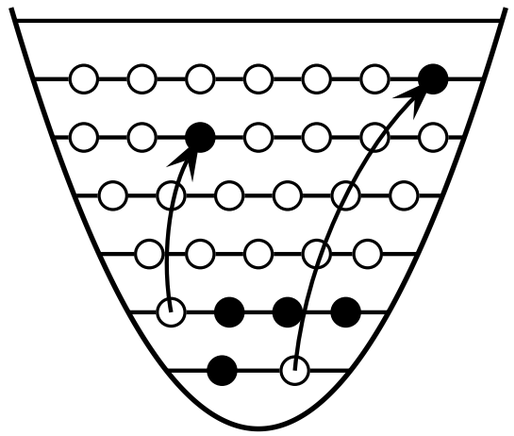
- **CCSD**: truncate $\hat{T}$ at the **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



$|\Phi_0\rangle$



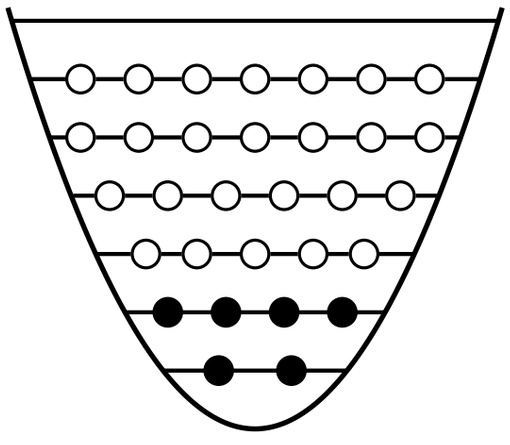
$\hat{T}_1 \, |\Phi_0\rangle$



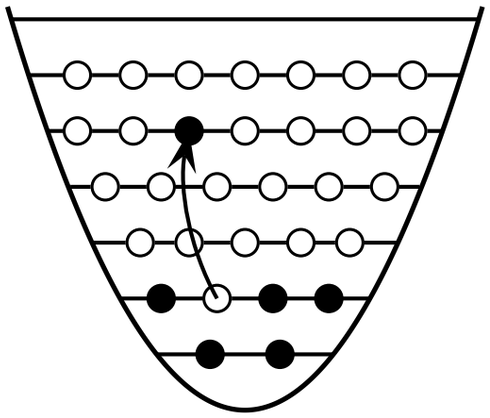
$\hat{T}_2 \, |\Phi_0\rangle$

CCSD

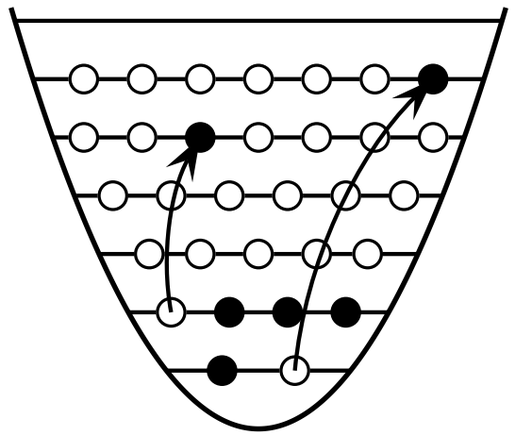
- **CCSD**: truncate $\hat{T}$ at the **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



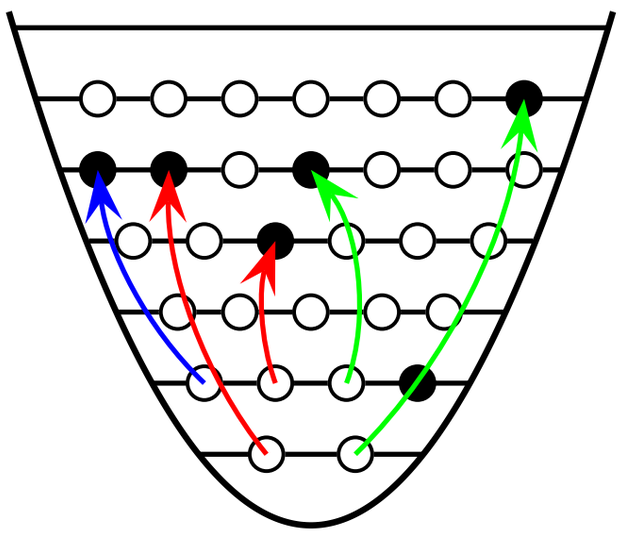
$|\Phi_0\rangle$



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



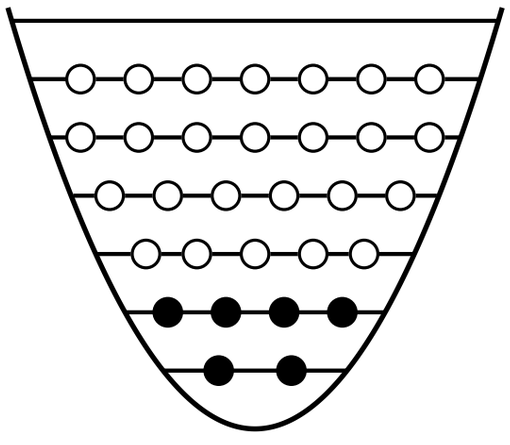
$\hat{T}_2 \, |\Phi_0\rangle$



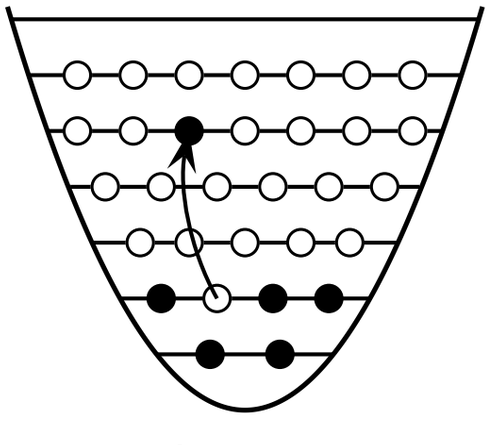
$\hat{T}_1 \, \hat{T}_2 \, \hat{T}_2 \, |\Phi_0\rangle$

CCSD

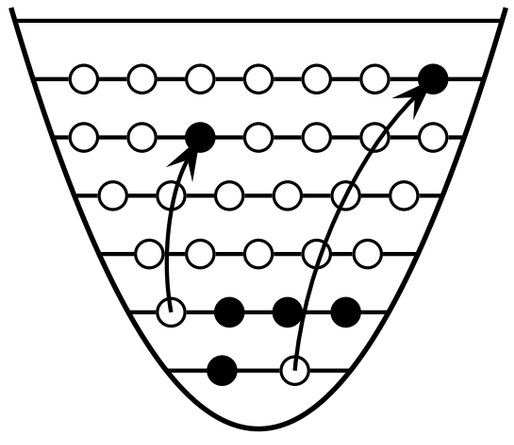
- **CCSD**: truncate $\hat{T}$ at the **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



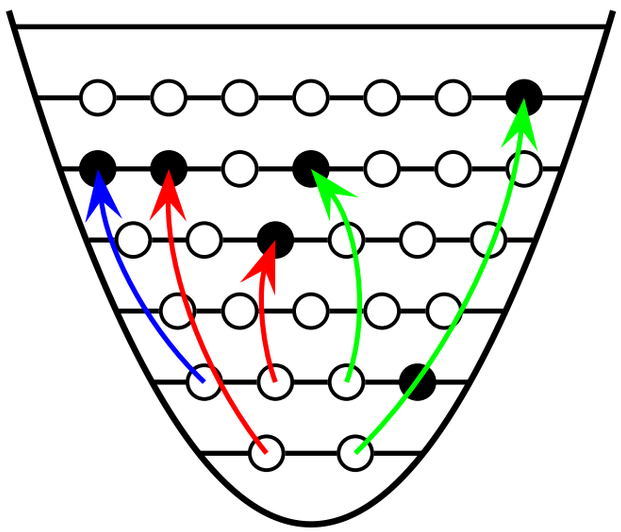
$|\Phi_0\rangle$



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



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



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

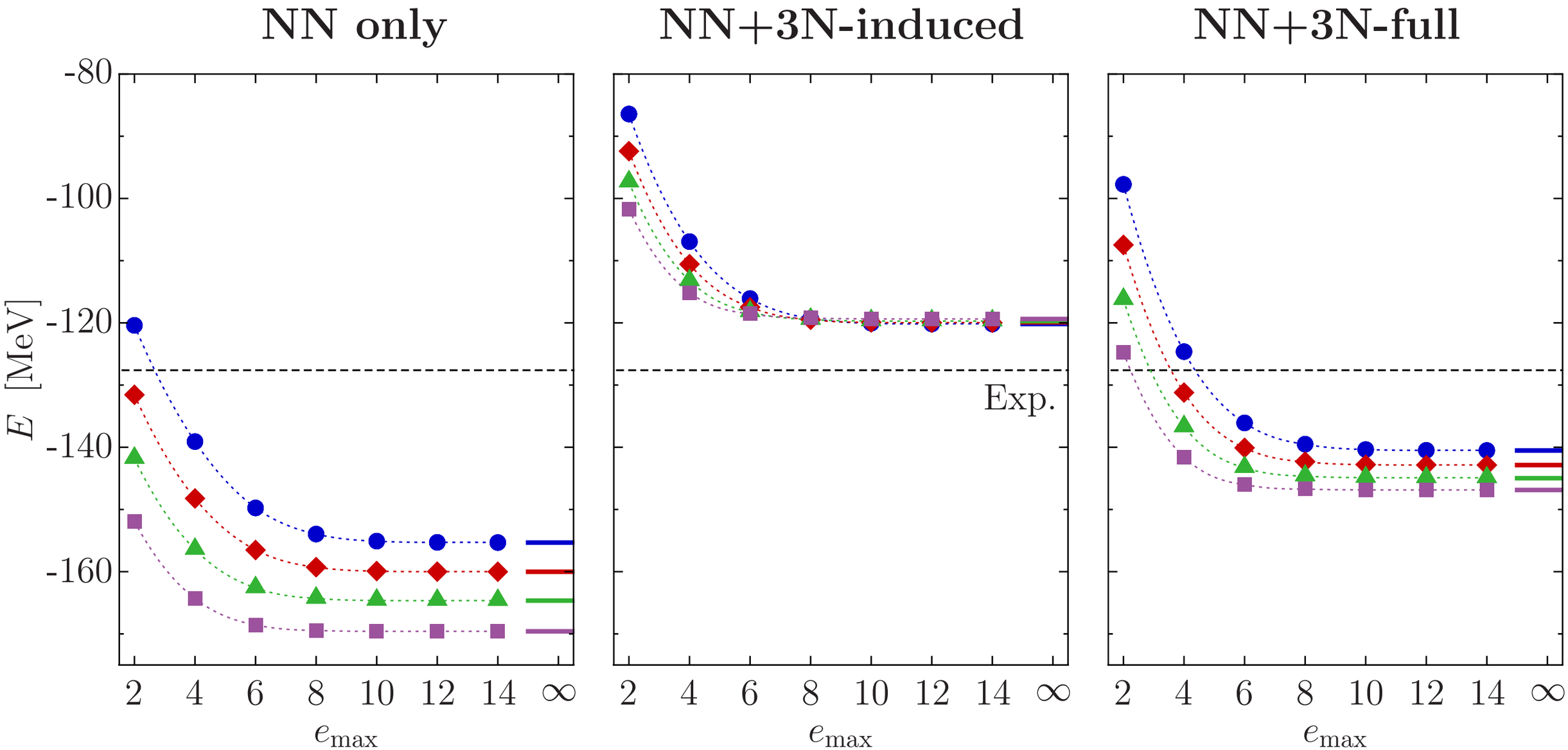
- CCSD equations

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

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

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

^{16}O: CCSD with 3N$_{NO2B}$



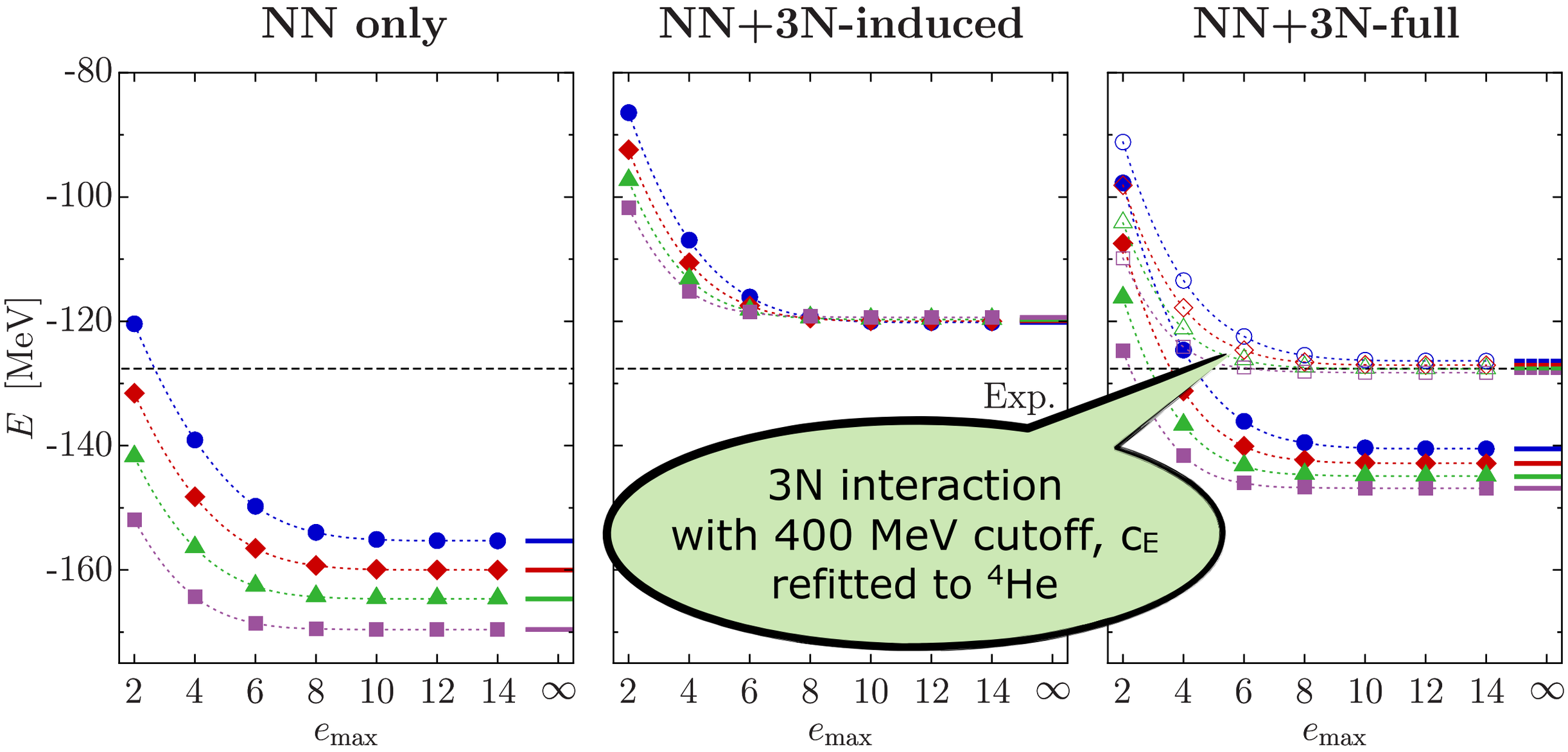
$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

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

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

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

^{16}O: CCSD with 3N$_{NO2B}$



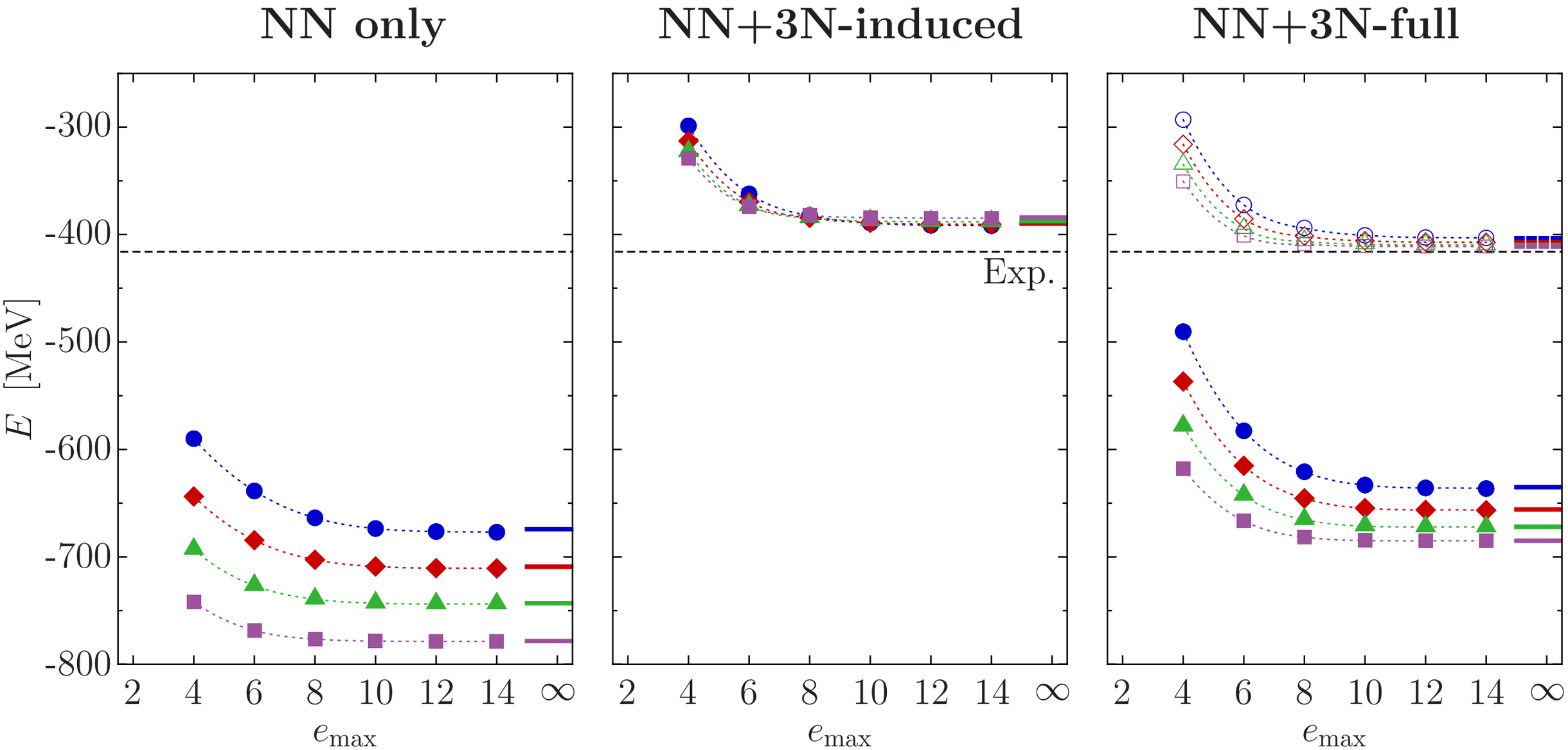
$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

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

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

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

^{48}Ca: CCSD with 3N$_{NO2B}$



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

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

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

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

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)

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

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

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

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

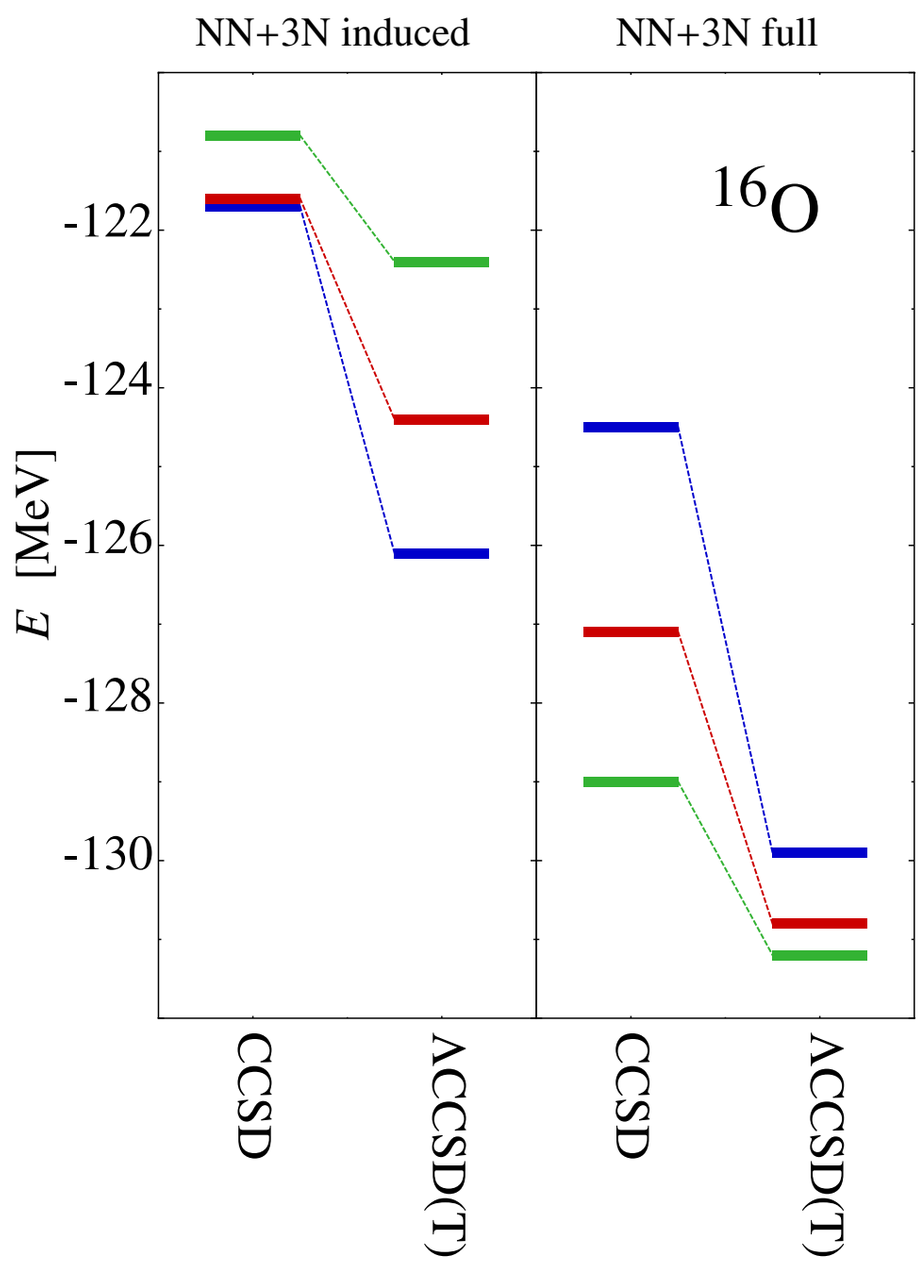
indicator of **convergence** of cluster expansion

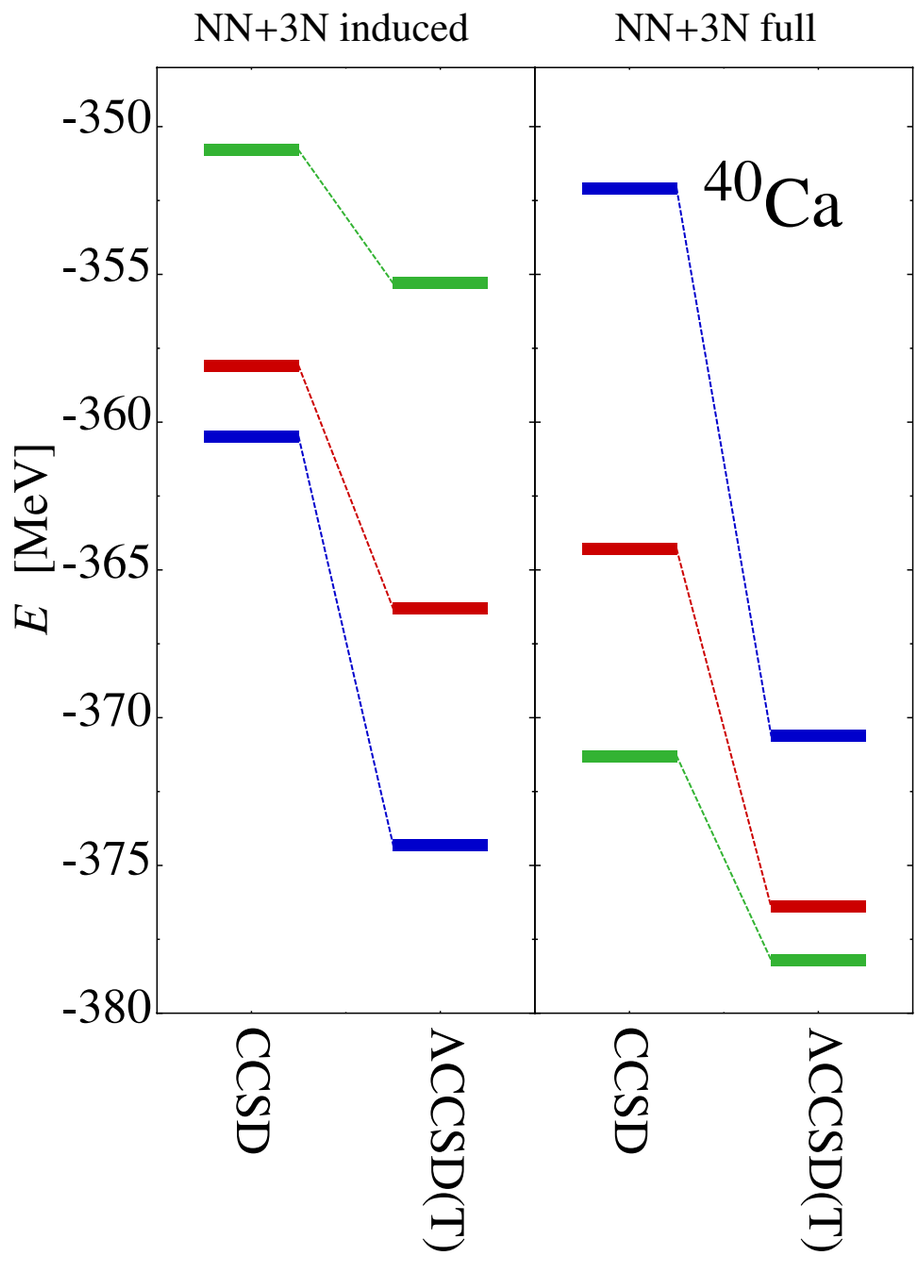
due to **triple excitations** (non-iterative)

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

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

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



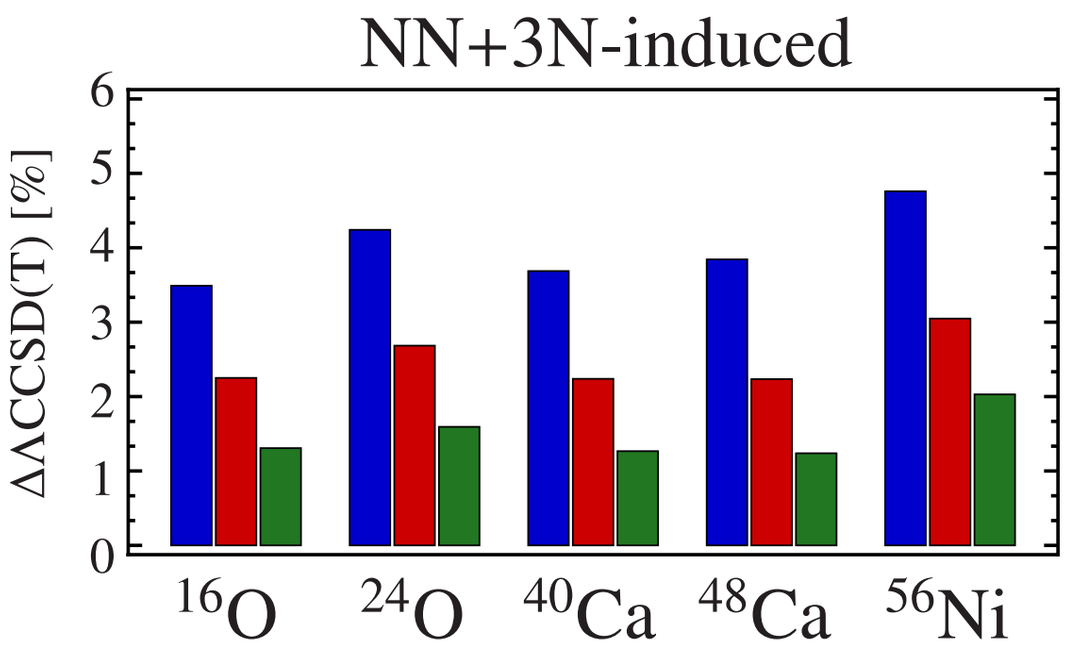


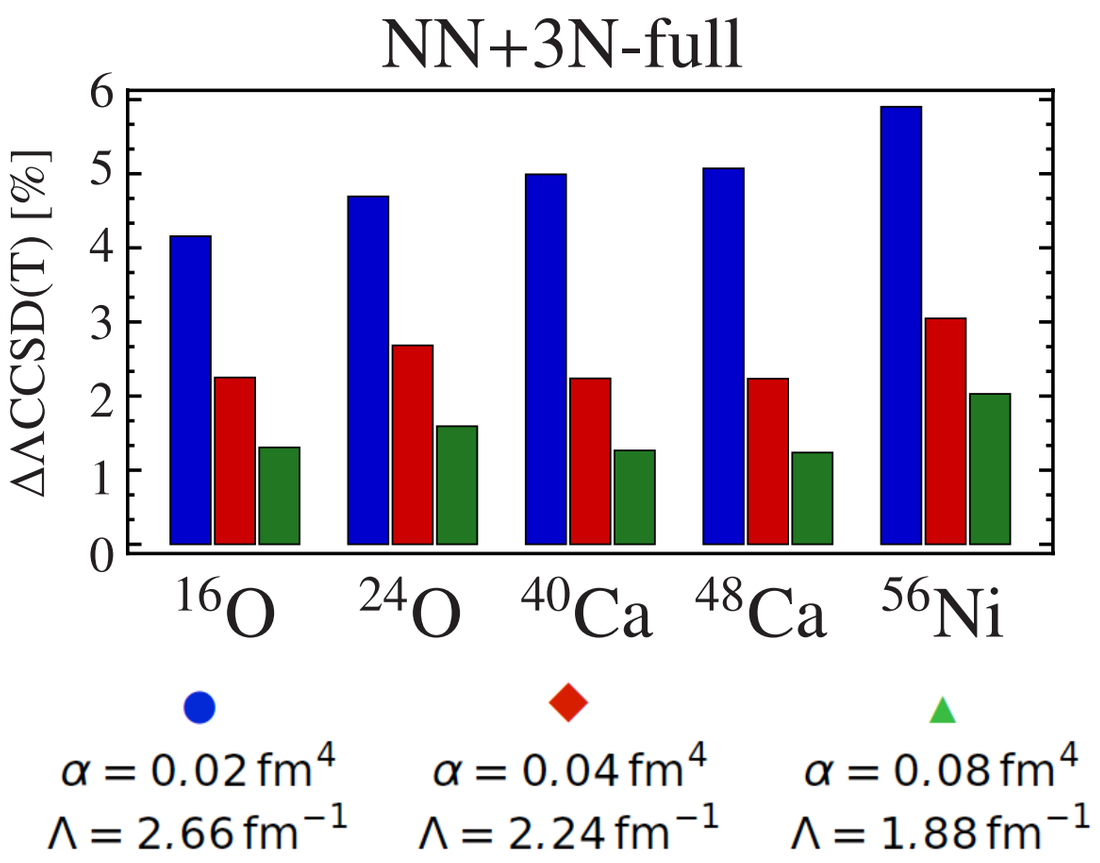
● $\alpha = 0.02\,\mathrm{fm}^4$ $\Lambda = 2.66\,\mathrm{fm}^{-1}$

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

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

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





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**

⇒ **hard interactions**:

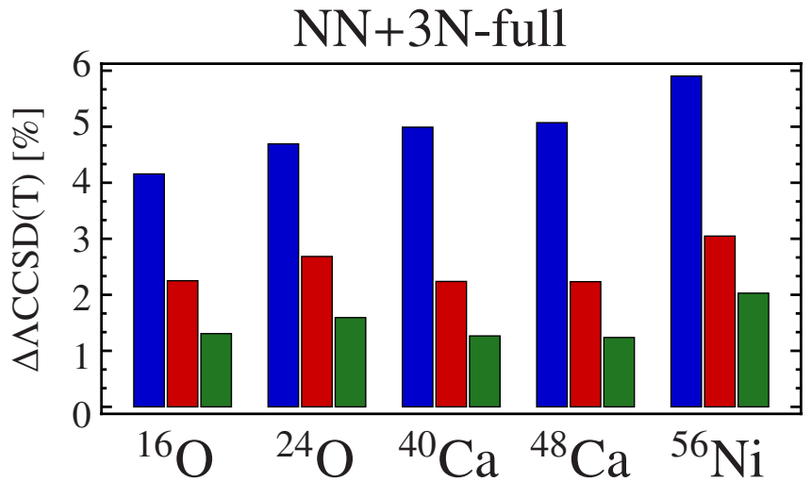
CCSD wavefunction sufficient?

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

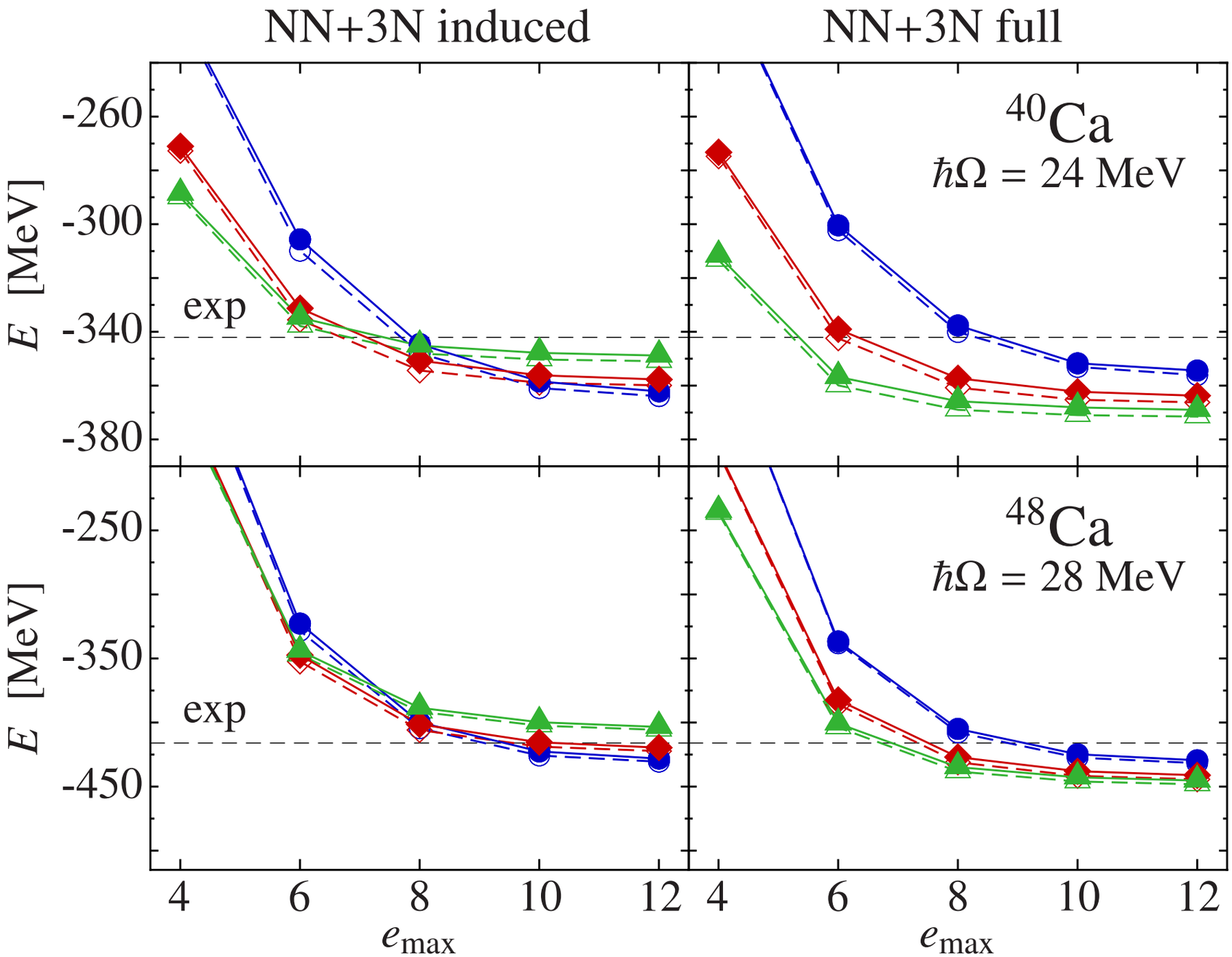


Coupled-Cluster with Explicit 3N Interactions

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)

CCSD with Explicit 3N Interaction



CCSD

3B / NO2B

● / ○ $\alpha = 0.02\,\mathrm{fm}^4$

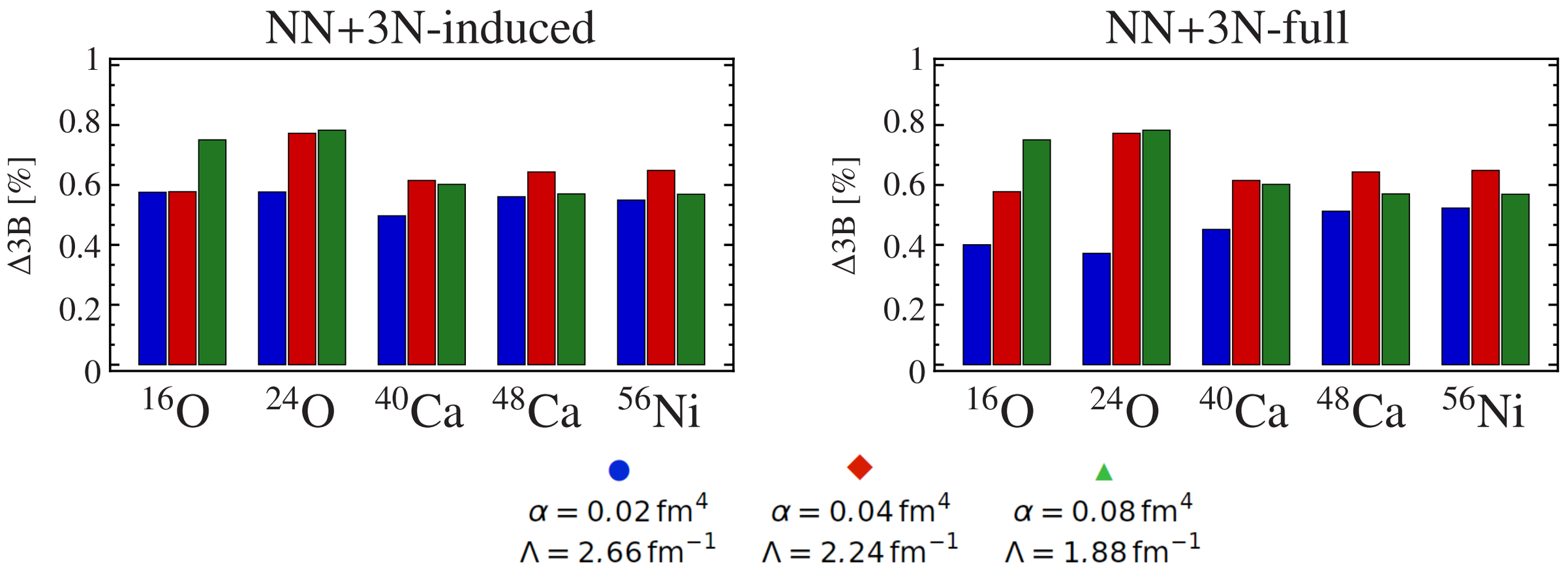
◆ / ◇ $\alpha = 0.04\,\mathrm{fm}^4$

▲ / △ $\alpha = 0.08\,\mathrm{fm}^4$

HF basis

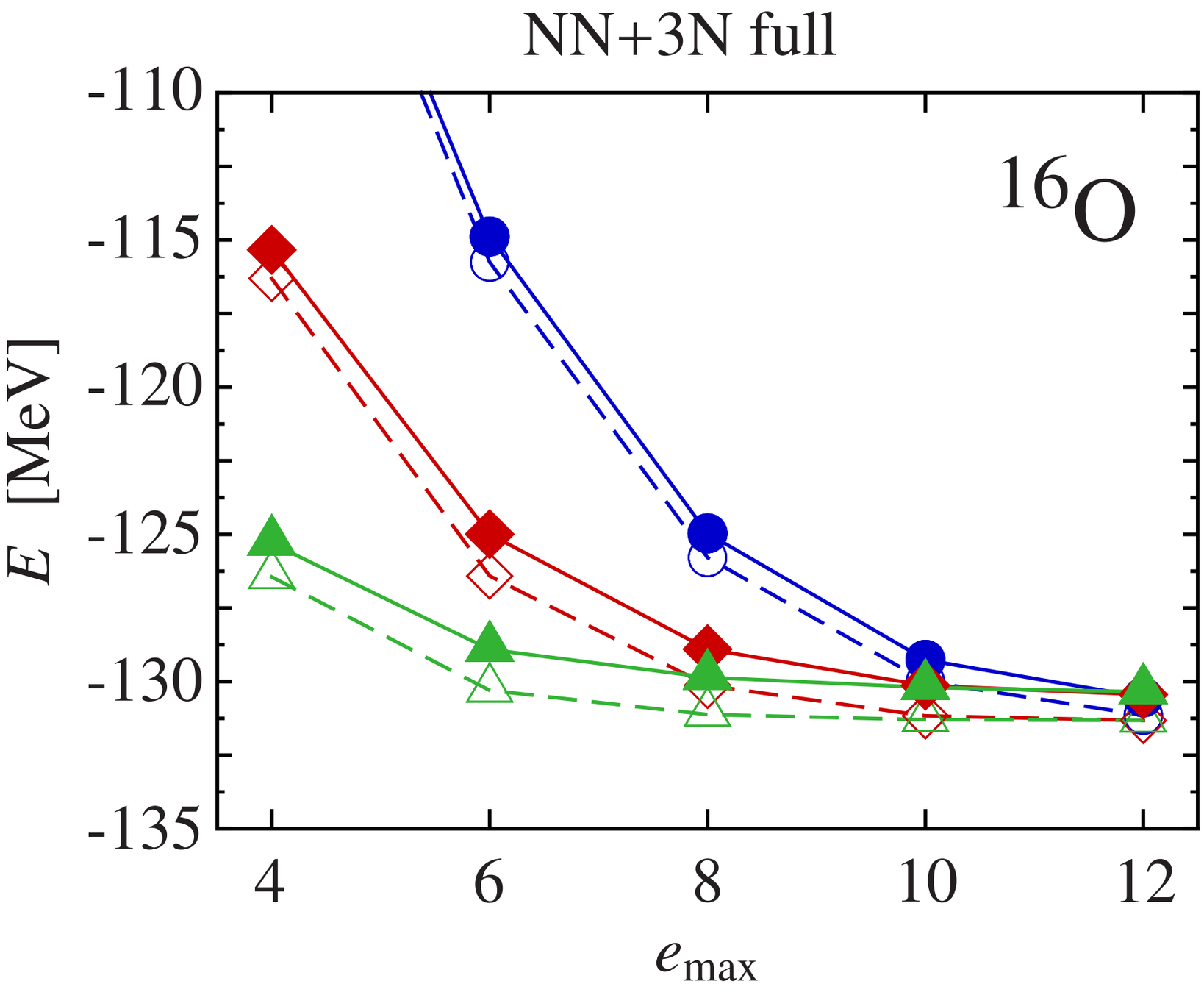
$E_{3\,max} = 12$

CCSD with Explicit 3N Interaction



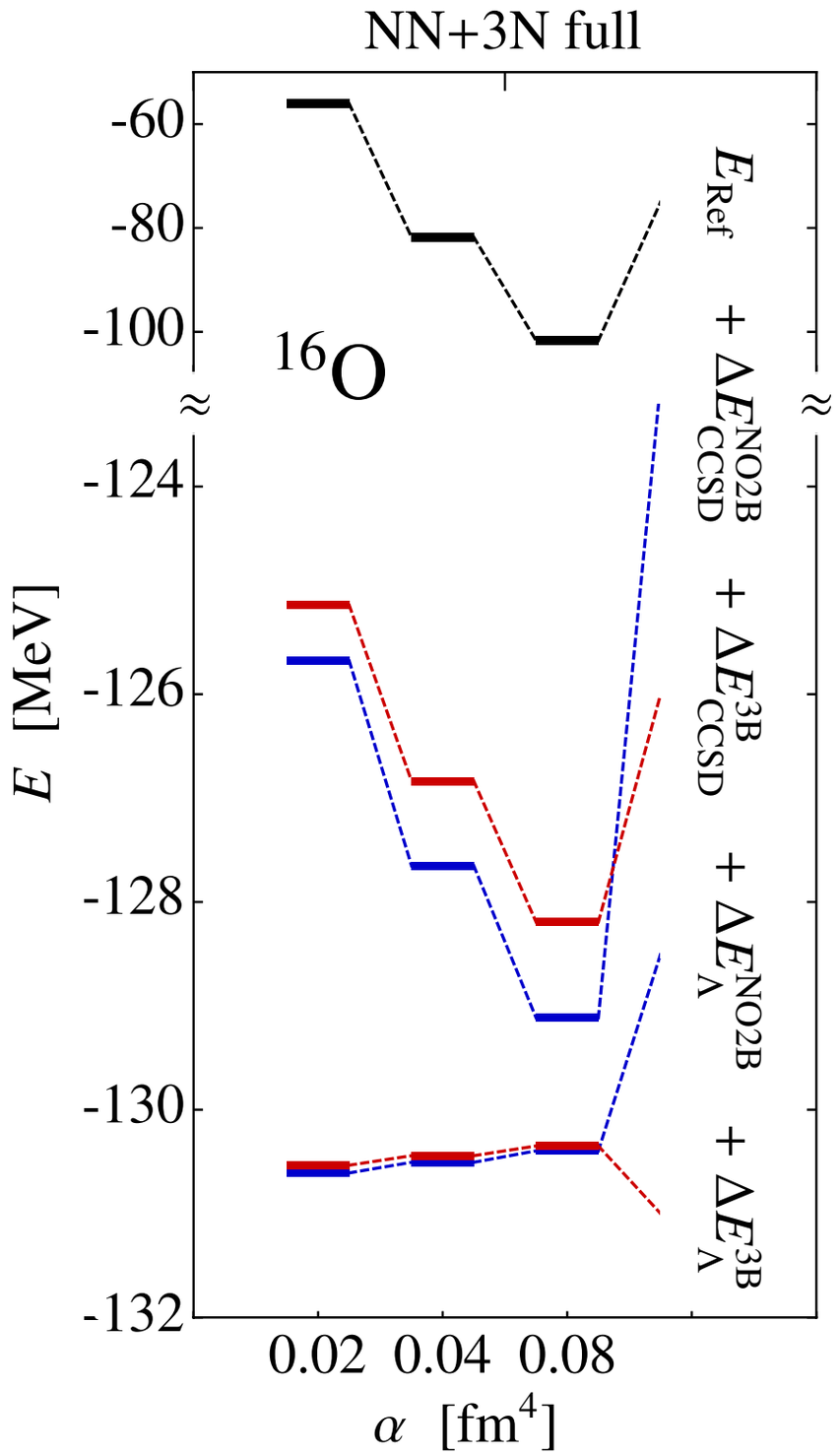
- **excellent agreement** between NO2B and explicit 3N (deviation < 1% for all nuclei considered)
- quality of NO2B **independent** of $e_{\max}, \hbar\Omega, \alpha$
- **efficient and accurate** way to include 3N interactions

ΛCCSD(T) with Explicit 3N Interaction



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) with Explicit 3N Interaction



- NO2B shows **excellent agreement** also for ΛCCSD(T)

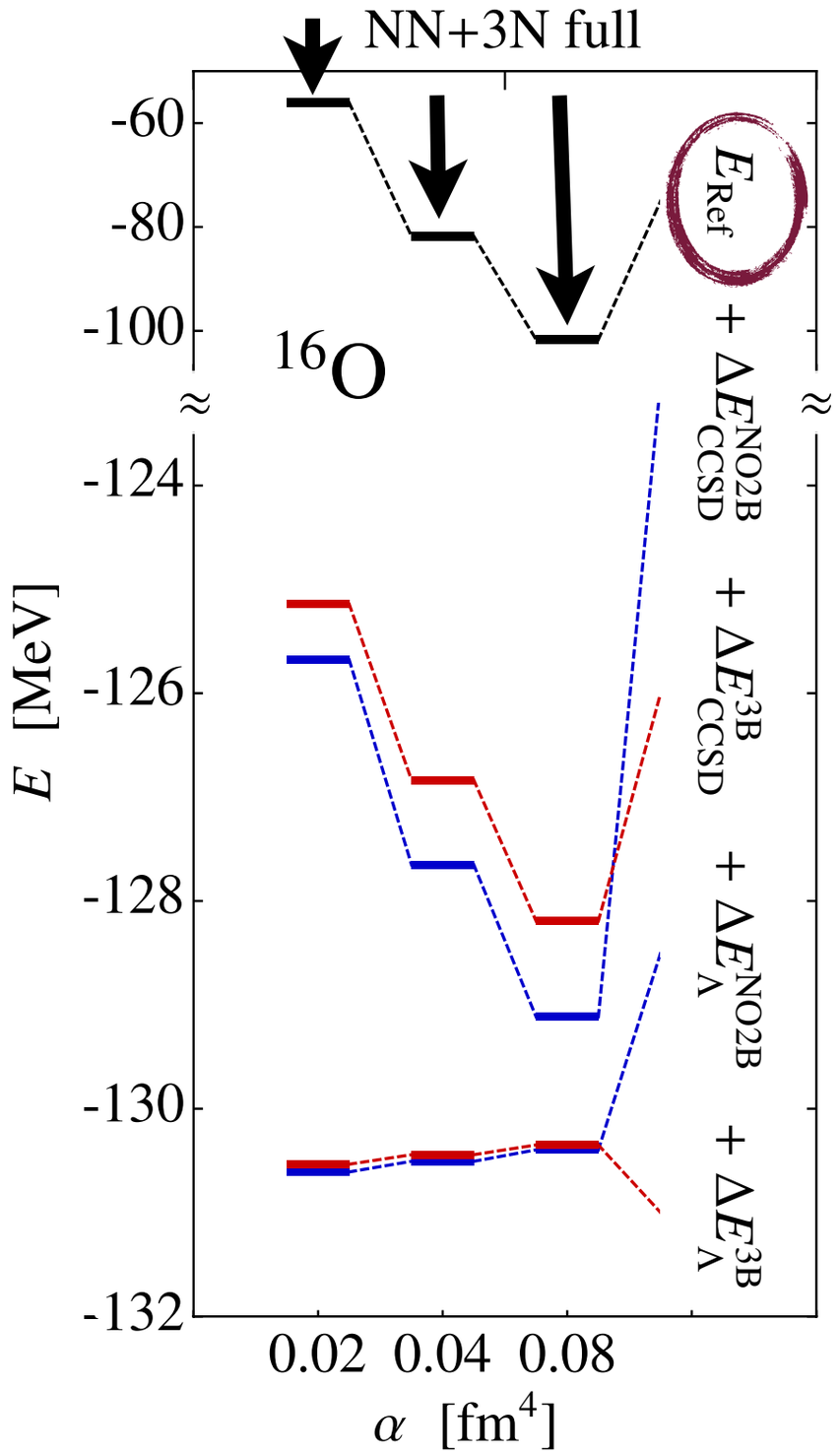
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

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

- 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



- NO2B shows **excellent agreement** also for ΛCCSD(T)

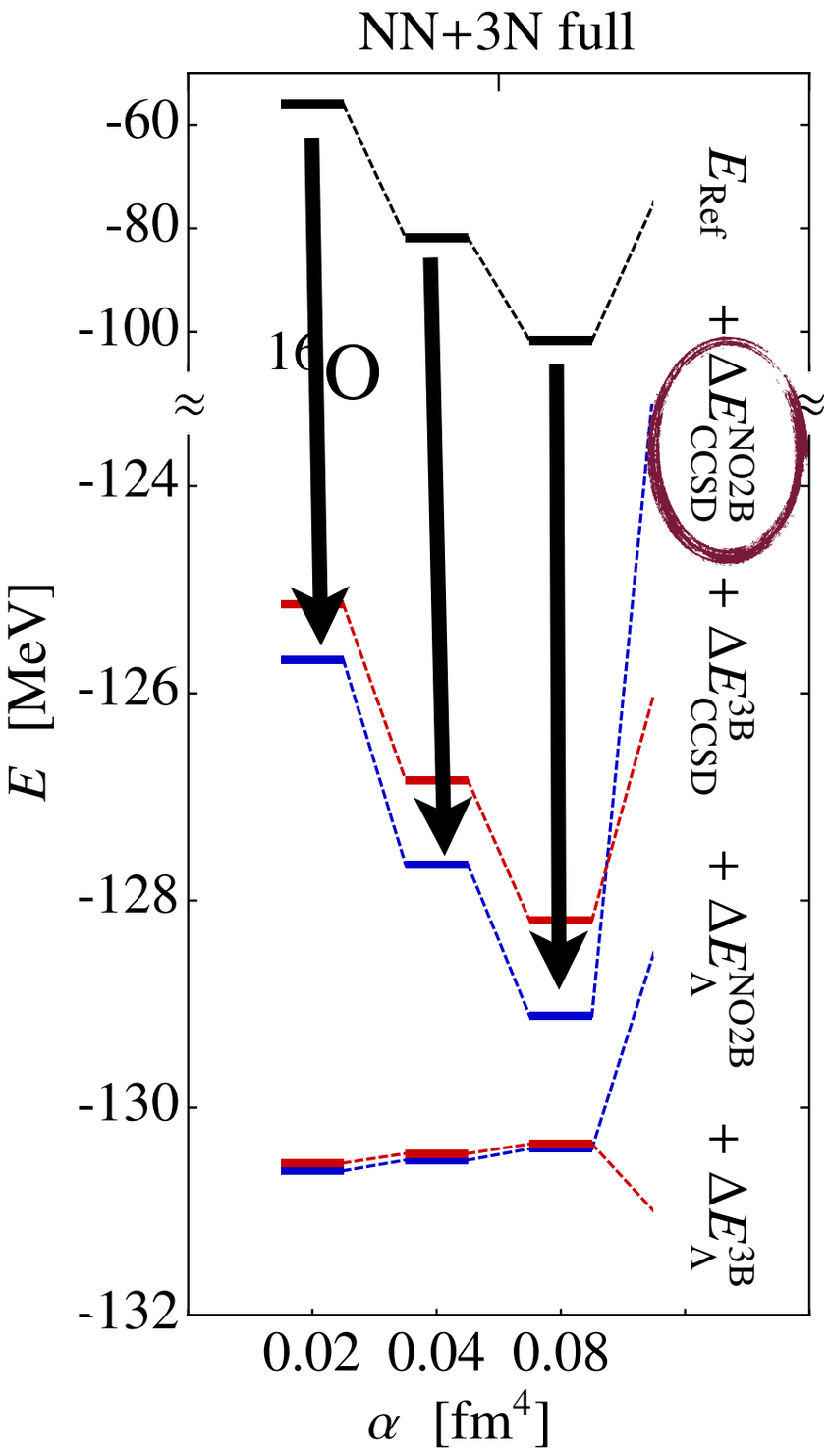
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

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

- 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



- NO2B shows **excellent agreement** also for ΛCCSD(T)

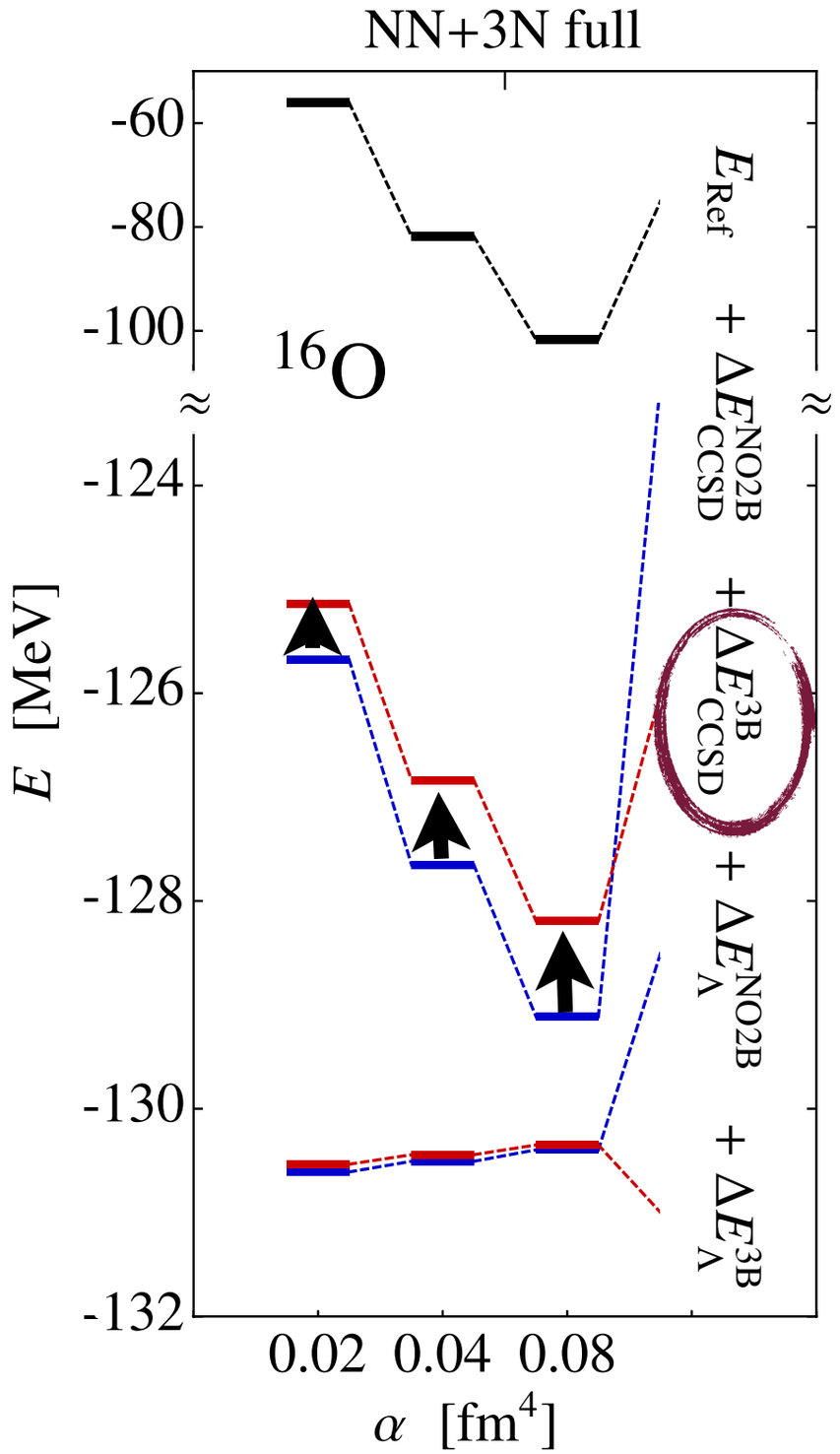
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

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

- 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



- NO2B shows **excellent agreement** also for ΛCCSD(T)

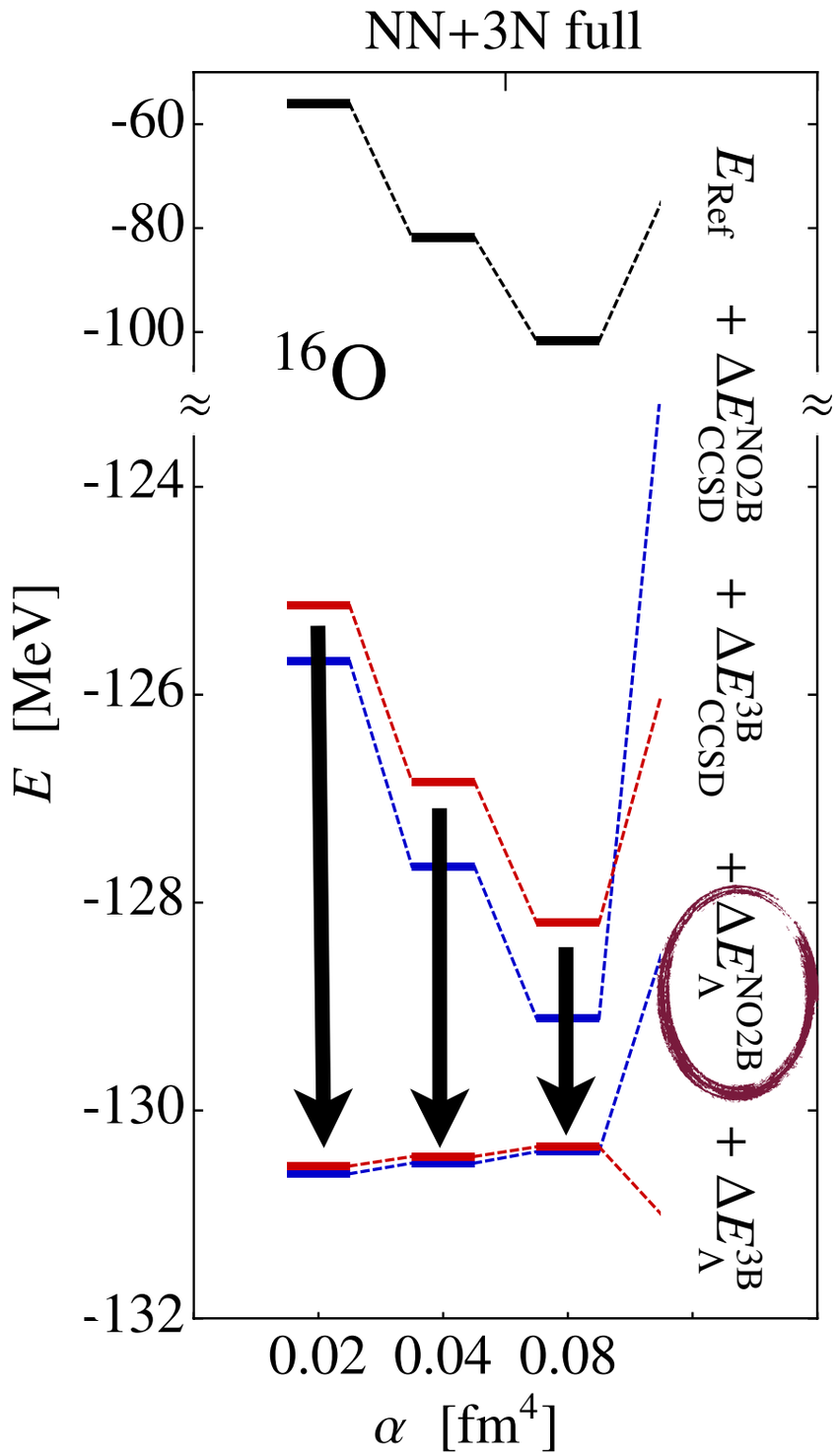
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

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

- 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



- NO2B shows **excellent agreement** also for ΛCCSD(T)

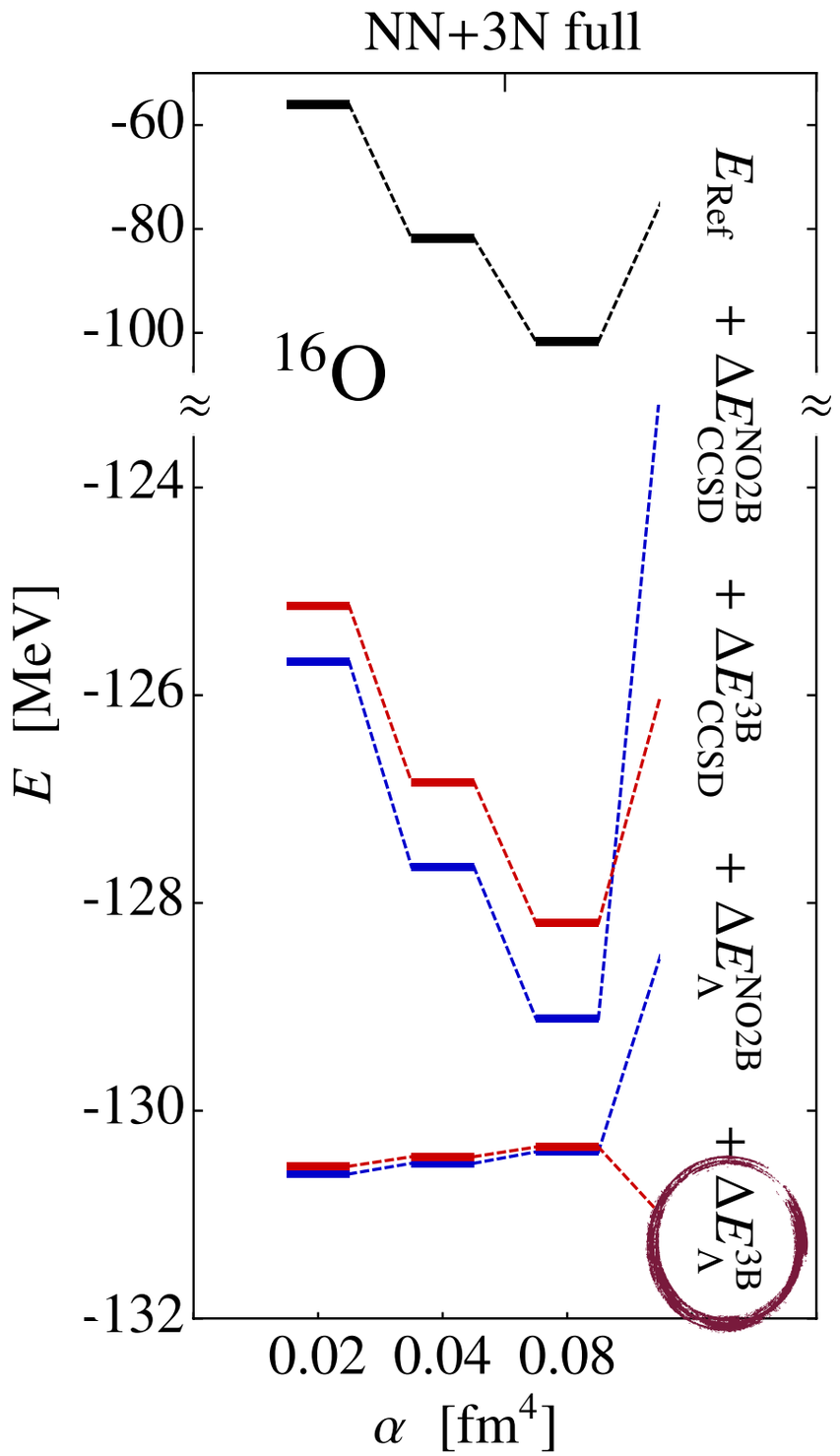
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

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

- 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



- NO2B shows **excellent agreement** also for ΛCCSD(T)

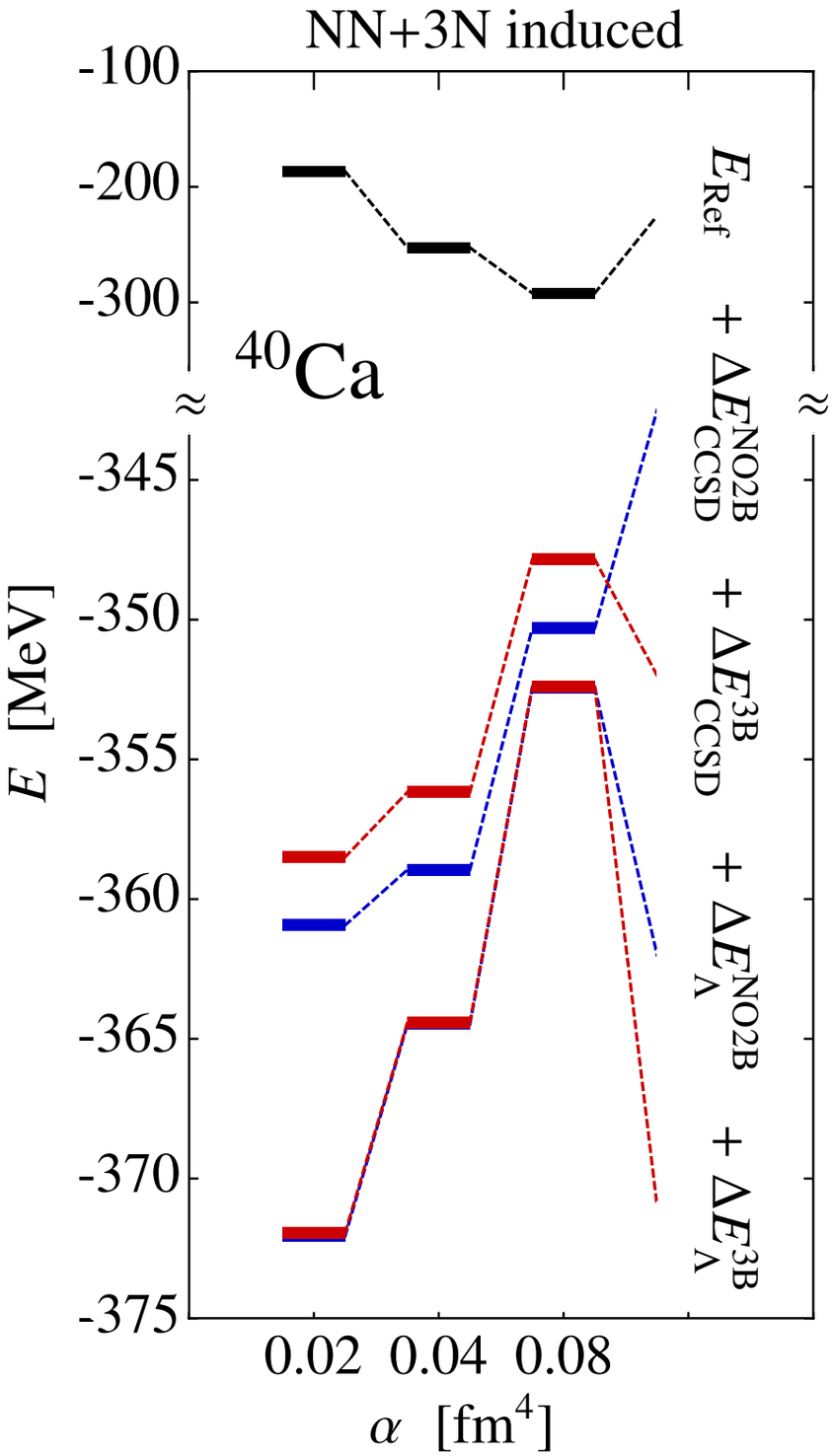
- $E_{\Lambda\mathrm{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\mathrm{CCSD}} + \Delta E_{\Lambda\mathrm{CCSD(T)}}$

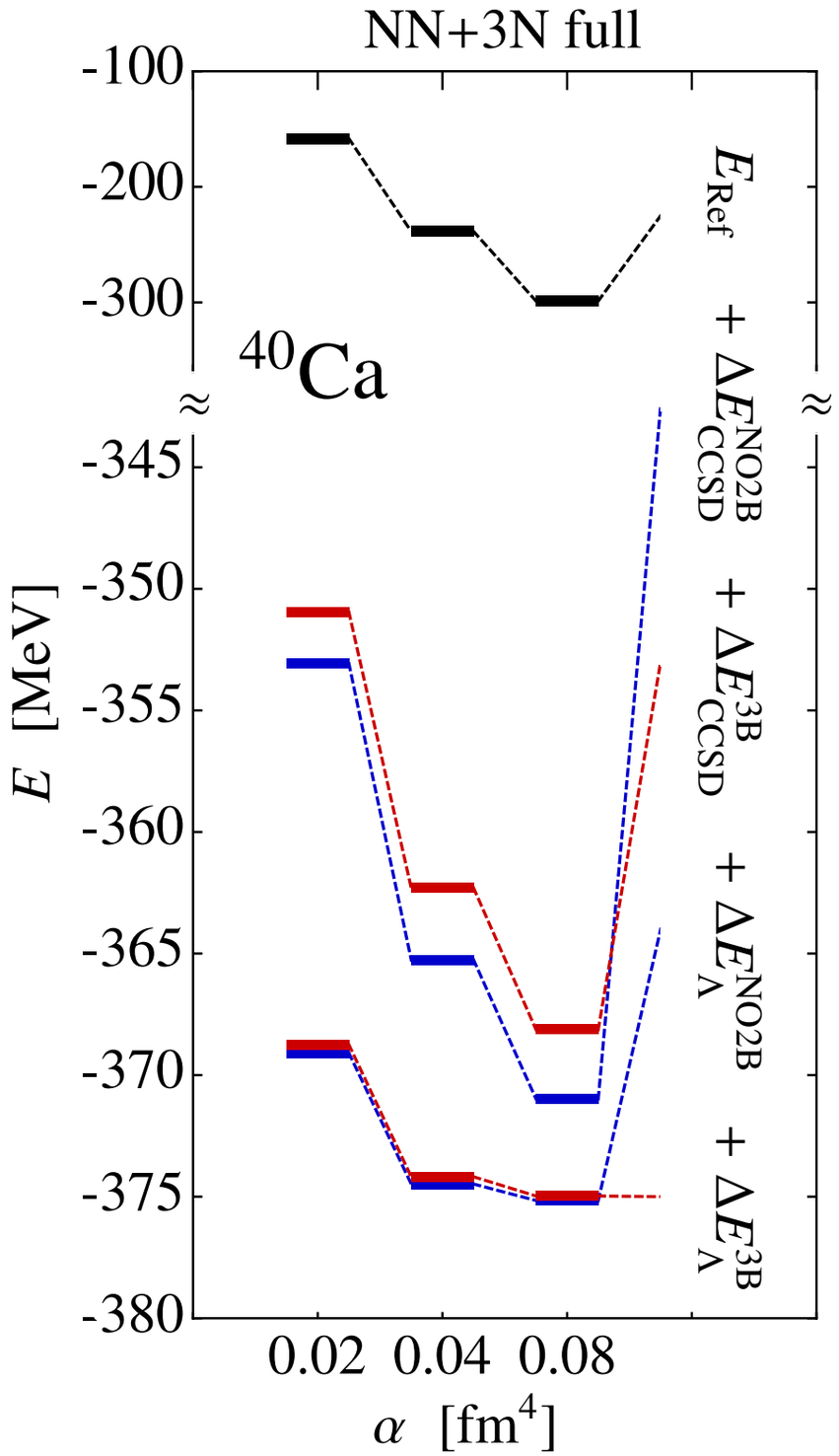
$$\Delta E_{\mathrm{CCSD}} = \Delta E^{\mathrm{NO2B}}_{\mathrm{CCSD}} + \Delta E^{\mathrm{3B}}_{\mathrm{CCSD}}\ , \quad \text{etc.}$$

- 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





ΛCCSD(T)3B

HF basis

e_{max} = 10

E_{3max} = 12

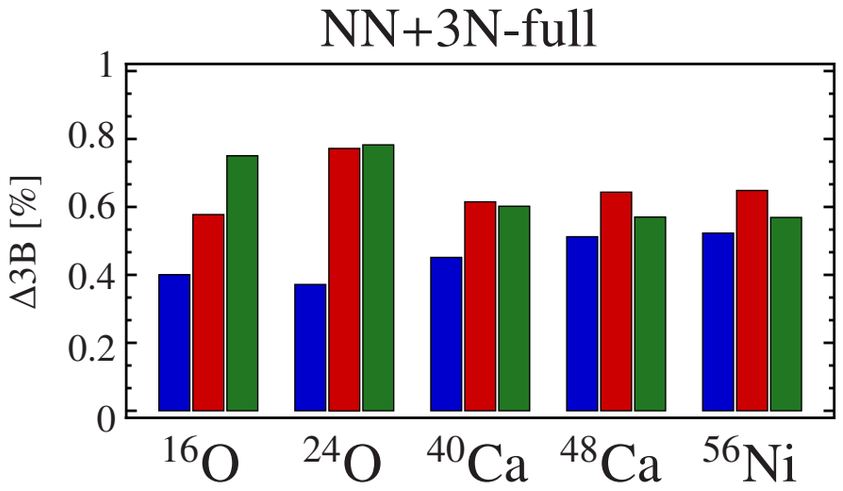
$\hbar\Omega$ = 24 MeV

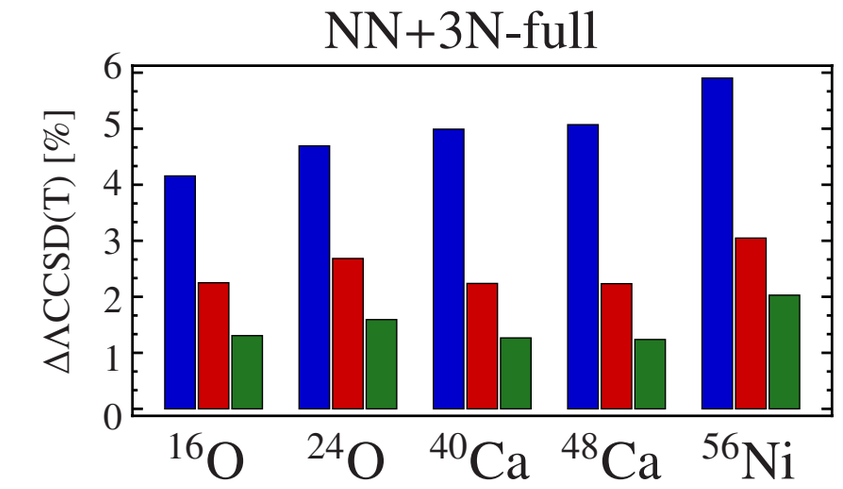
Uncertainty Summary

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

- **Normal-Ordering 2B Approximation**
  - ☑ error in light nuclei: 1-2%,
  - ☑ error in medium-mass nuclei: <1%
  - ☑ error independent of mass number etc.
  - ☑ residual 3N significant for CCSD only

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



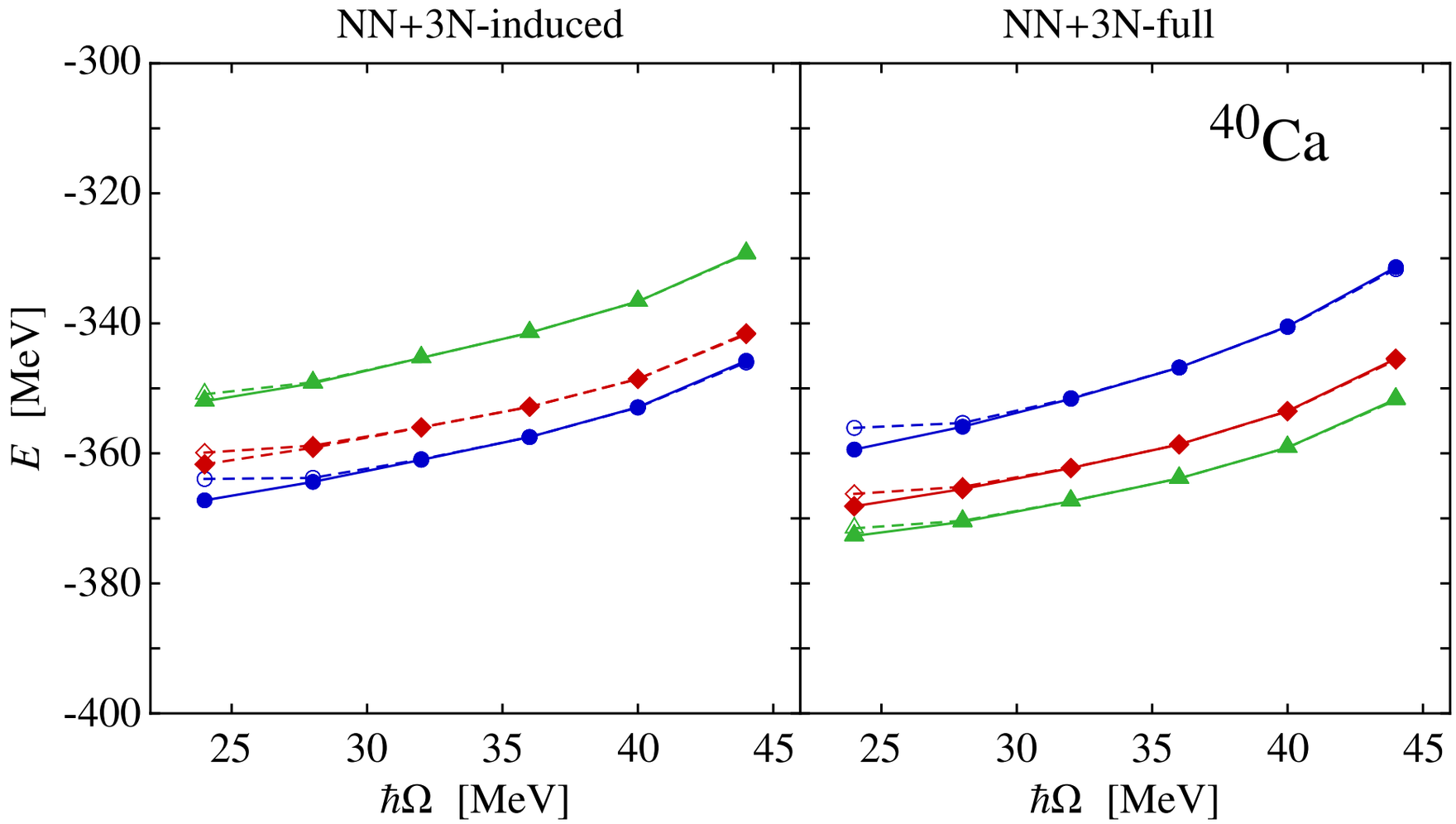


Frequency Conversion

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**)



CCSD
conv./ no conv.

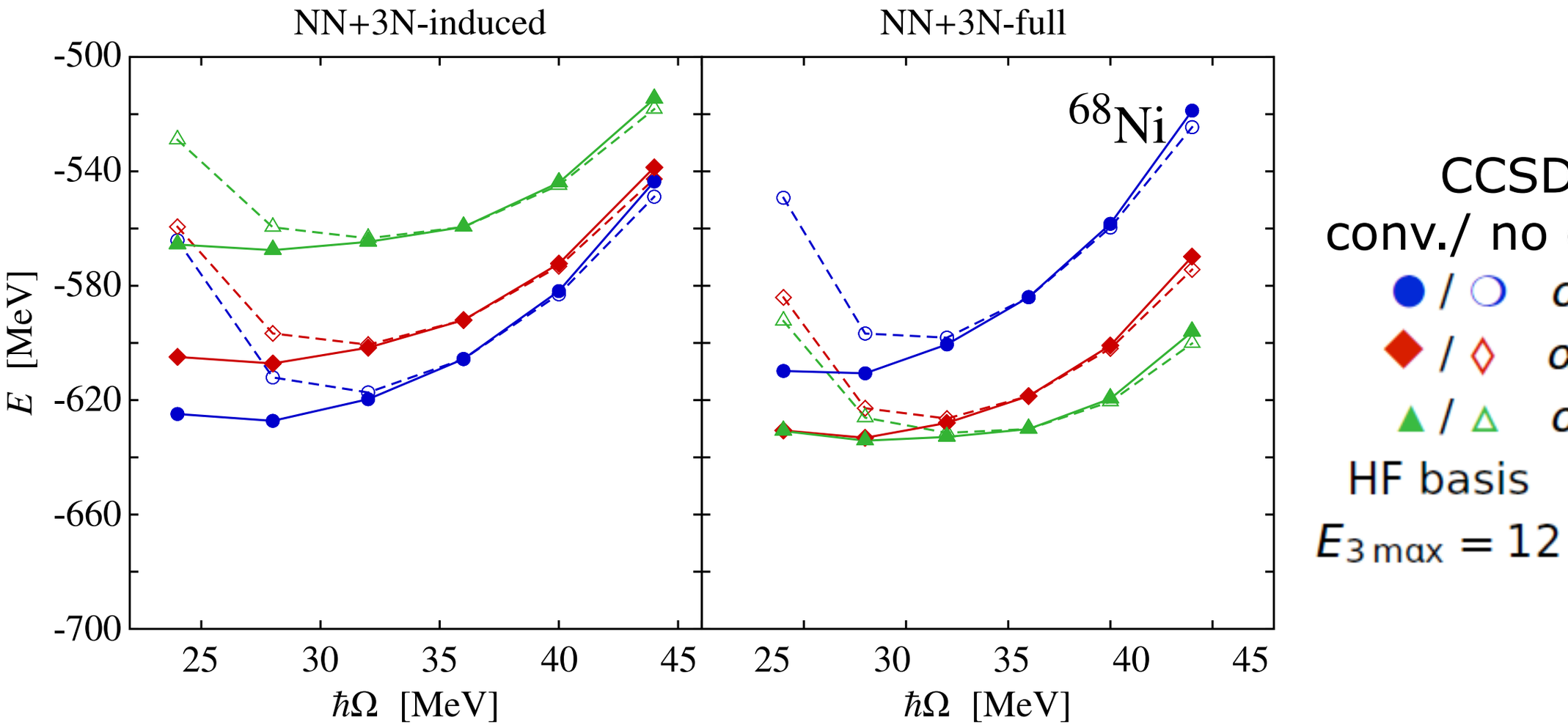
- ● / ○ $\alpha = 0.02\,\mathrm{fm}^4$
- ◆ / ◇ $\alpha = 0.04\,\mathrm{fm}^4$
- ▲ / △ $\alpha = 0.08\,\mathrm{fm}^4$

HF basis

$E_{3\,\mathrm{max}} = 12$

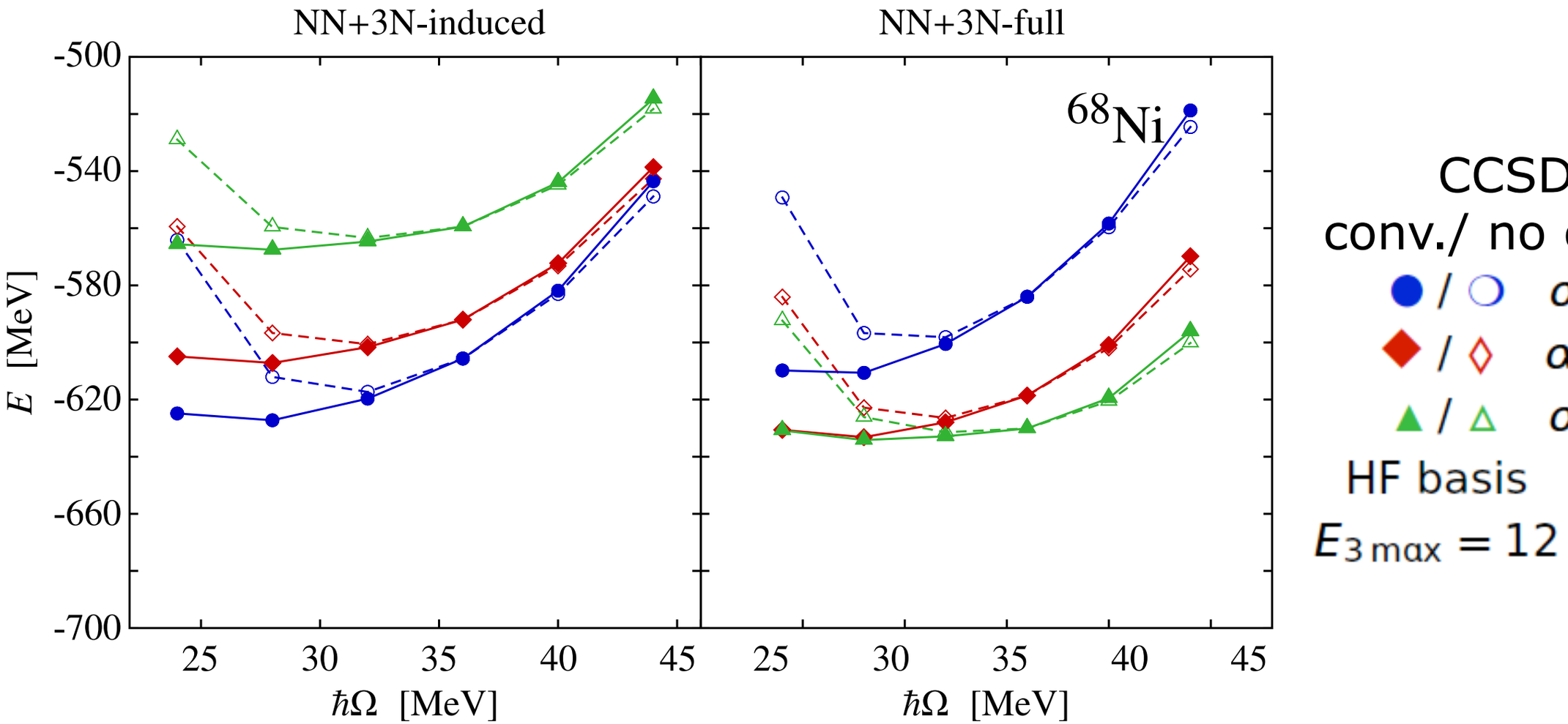
- $\hbar\Omega = 36$ MeV used for conversion

Frequency Conversion



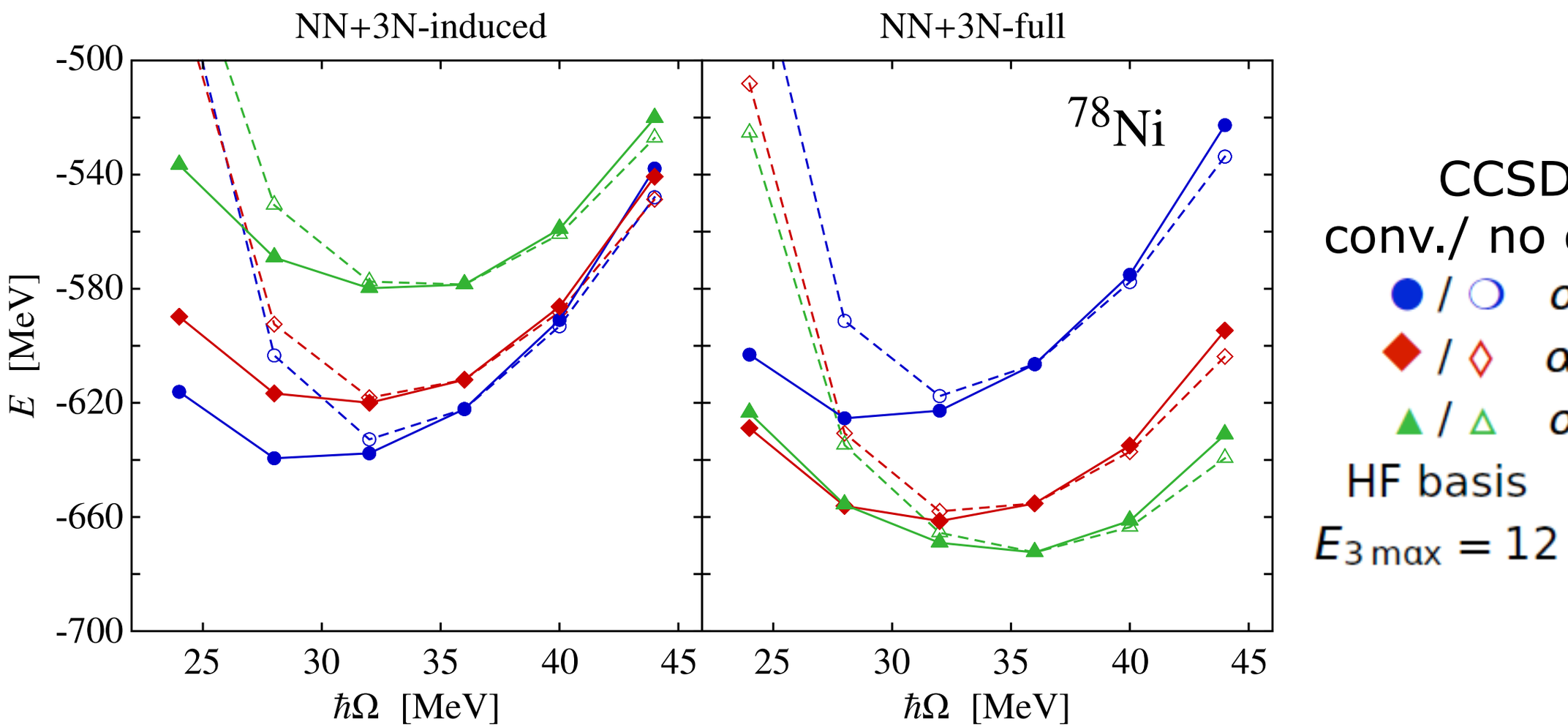
- without conversion: **energy minimum** artificially shifted towards larger frequencies
- **frequency conversion** mandatory for heavier nuclei

Frequency Conversion



- without conversion: **energy minimum** artificially shifted towards larger frequencies
- **frequency conversion** mandatory for heavier nuclei

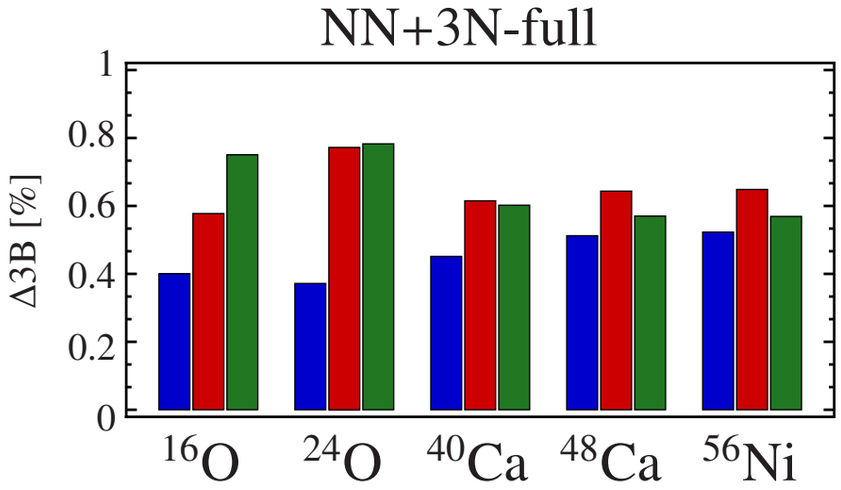
Frequency Conversion

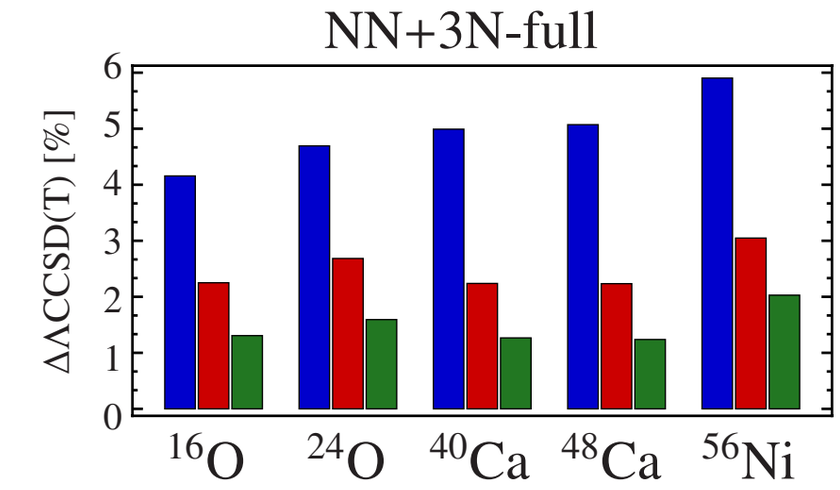


- without conversion: **energy minimum** artificially shifted towards larger frequencies
- **frequency conversion** mandatory for heavier nuclei

Uncertainty Summary

- **Similarity Renormalization Group**
  - ☑ α-dependence: low-cutoff 3N interaction
  - ☑ small frequencies: conversion
- **Normal-Ordering 2B Approximation**
  - ☑ error in light nuclei: 1-2%,
  - ☑ error in medium-mass nuclei: <1%
  - ☑ error independent of mass number etc.
  - ☑ residual 3N significant for CCSD only
- **Cluster Truncation**
  - ☐ up to 6% contributions from ΛCCSD(T)
  - ☑ soft interactions: only 1-2%
  - ☑ no strong increase with mass number





E3Max Truncation

$E_{3\max}$ Truncation

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

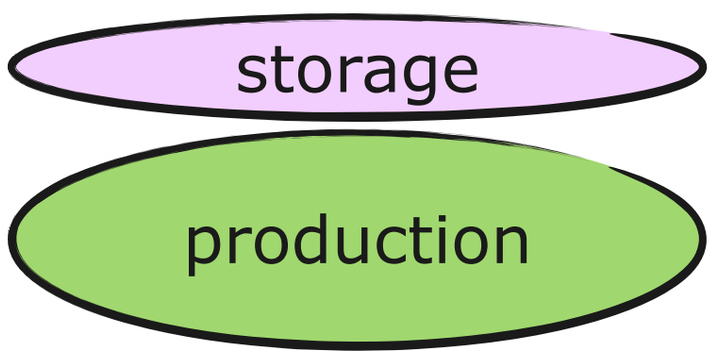
- **$E_{3\max}$ truncation**: use $\hat{W}_{3\mathrm{B}}$ matrix elements $\langle pqr|\hat{W}_{3\mathrm{B}}|stu\rangle$ with

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

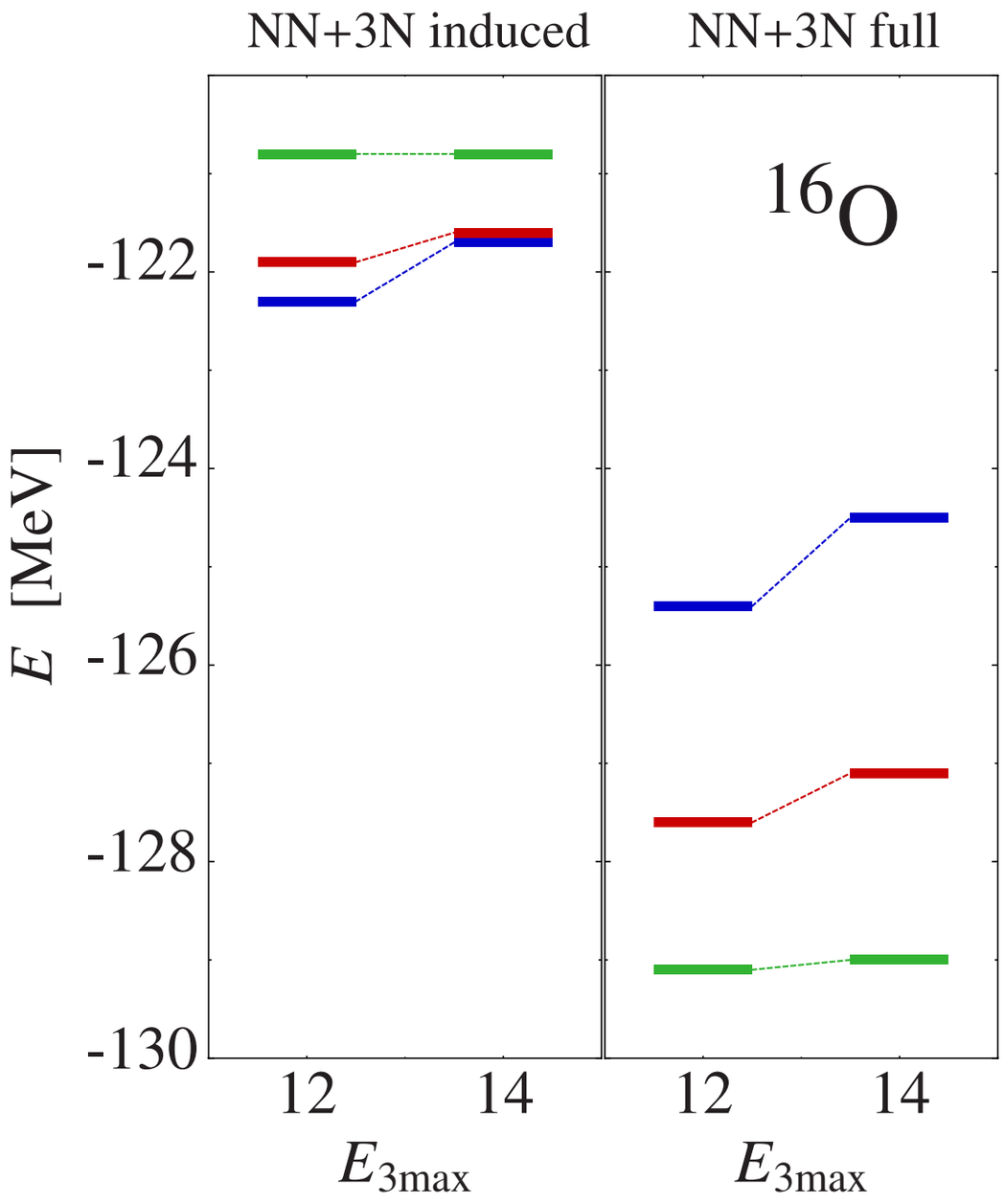
$$e_p = 2n_p + l_p$$

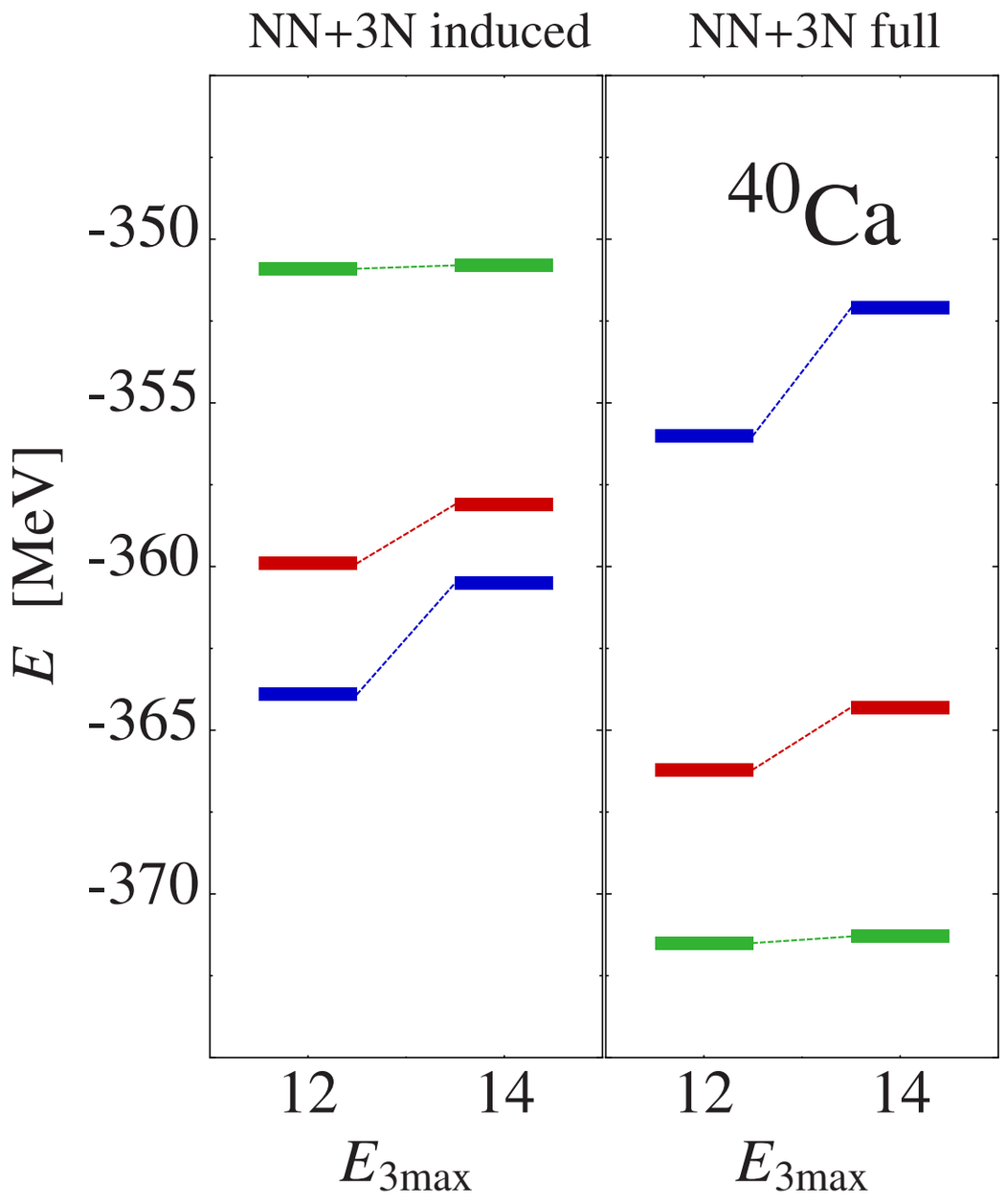
- **current limits**:

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



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





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

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

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

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

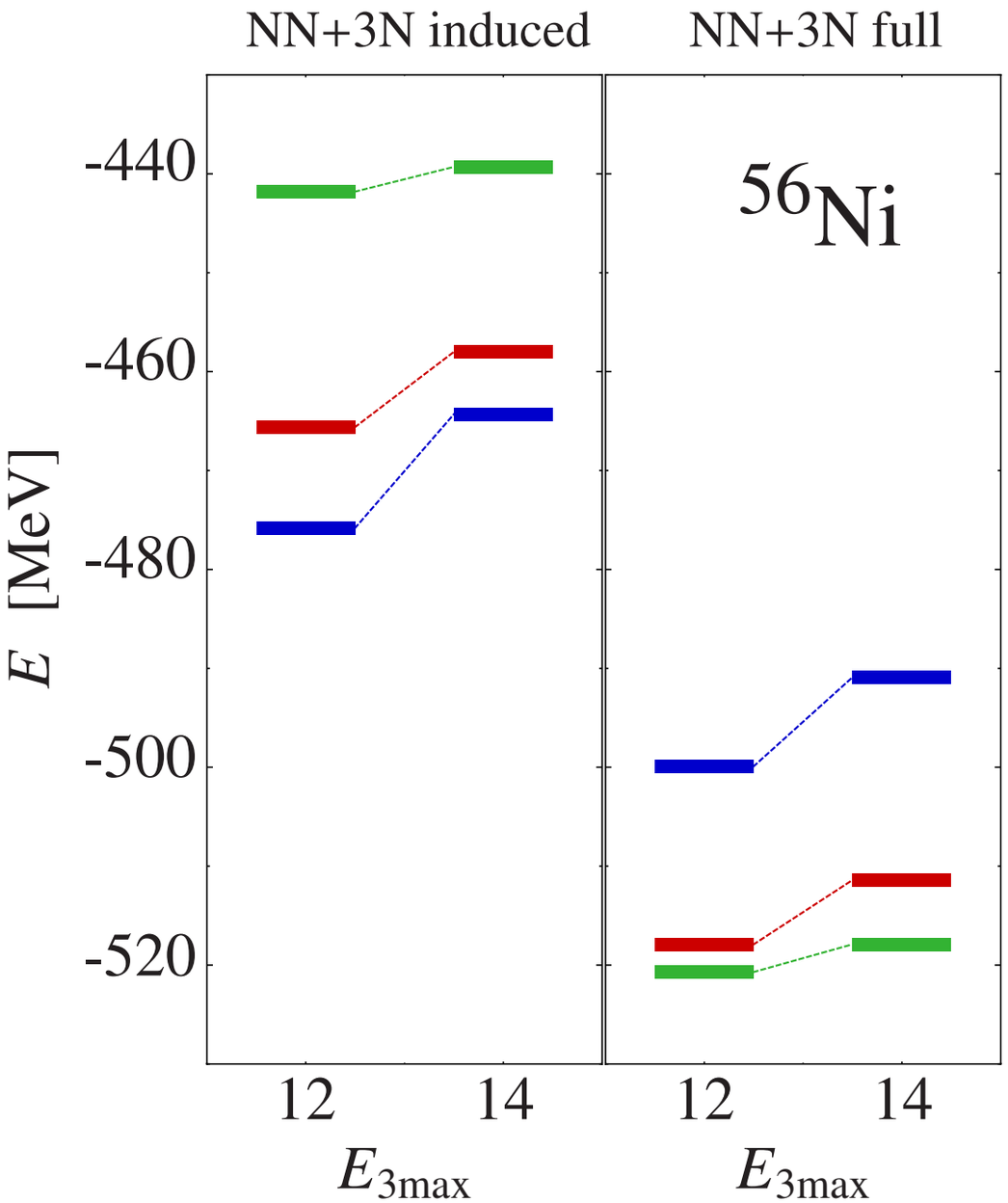
- E_{3max} not significant for **soft interactions** up to A<50
- **harder interactions**: up to 2% change in g.s. energies for E_{3max} 12 → 14
- α-dependence for **NN+3N induced** gets **reduced** for larger E_{3max}
- α-dependence for **NN+3N full** gets **enhanced** for larger E_{3max}

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

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

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

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



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

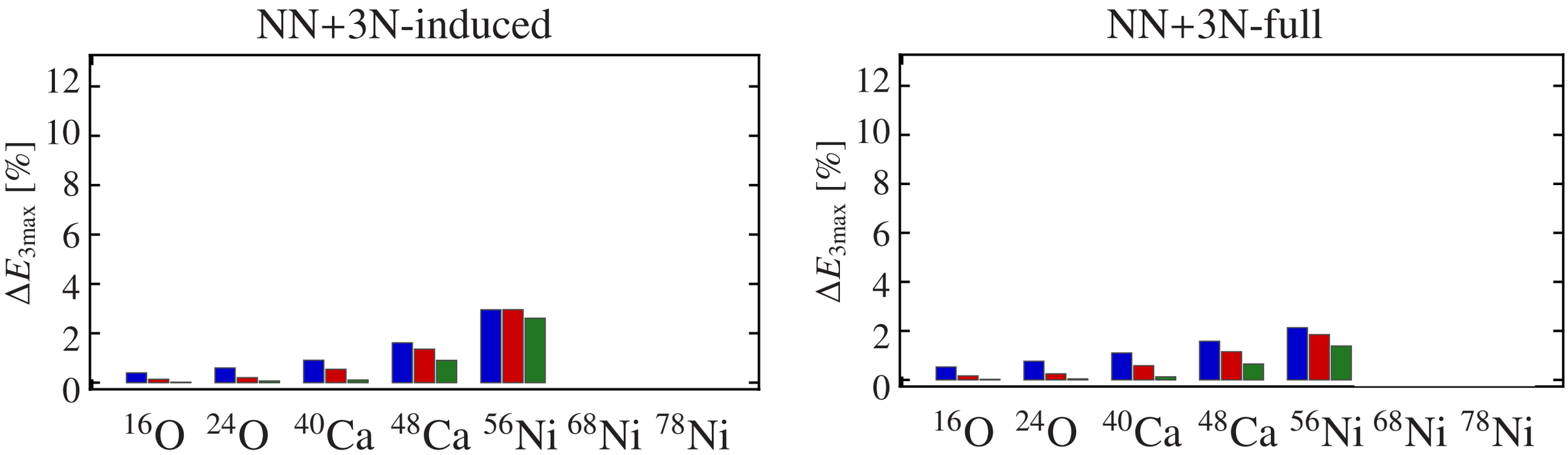
$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

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

- E_{3max} 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}

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

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



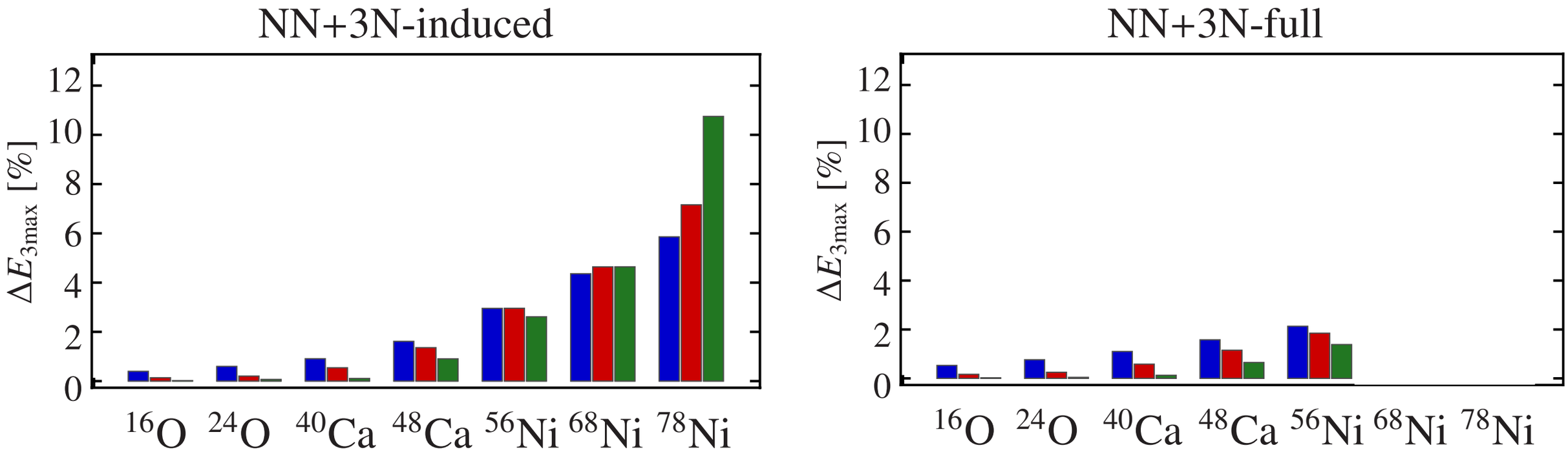
$\alpha = 0.02\,\mathrm{fm}^4$ $\Lambda = 2.66\,\mathrm{fm}^{-1}$

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

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

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

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



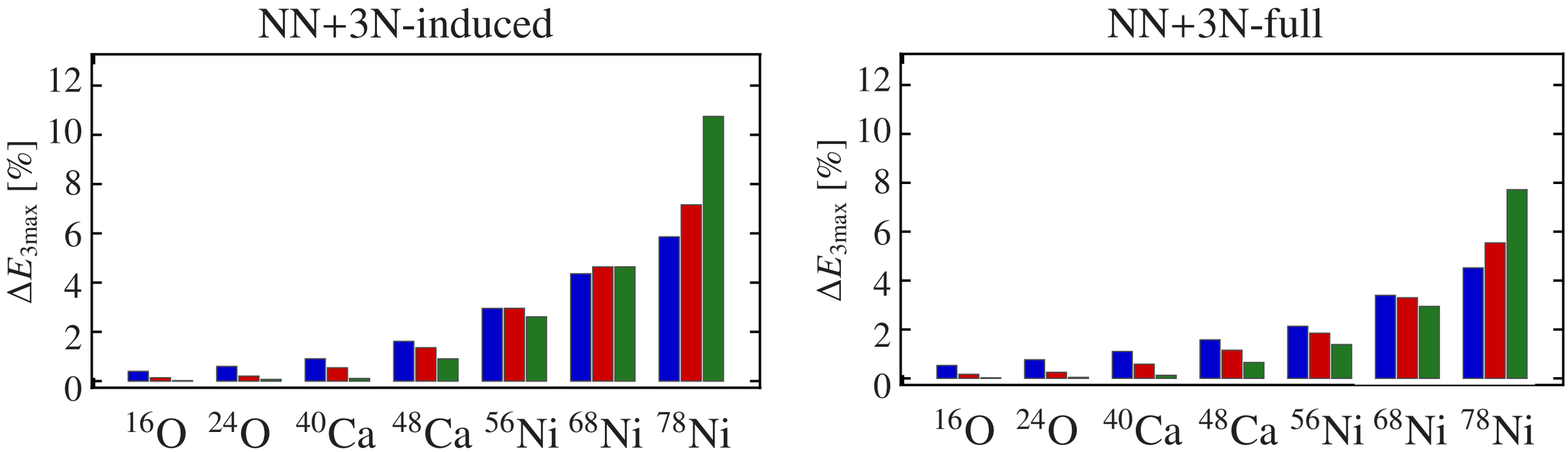
$\alpha = 0.02\,\mathrm{fm}^4$ $\Lambda = 2.66\,\mathrm{fm}^{-1}$

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

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

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

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



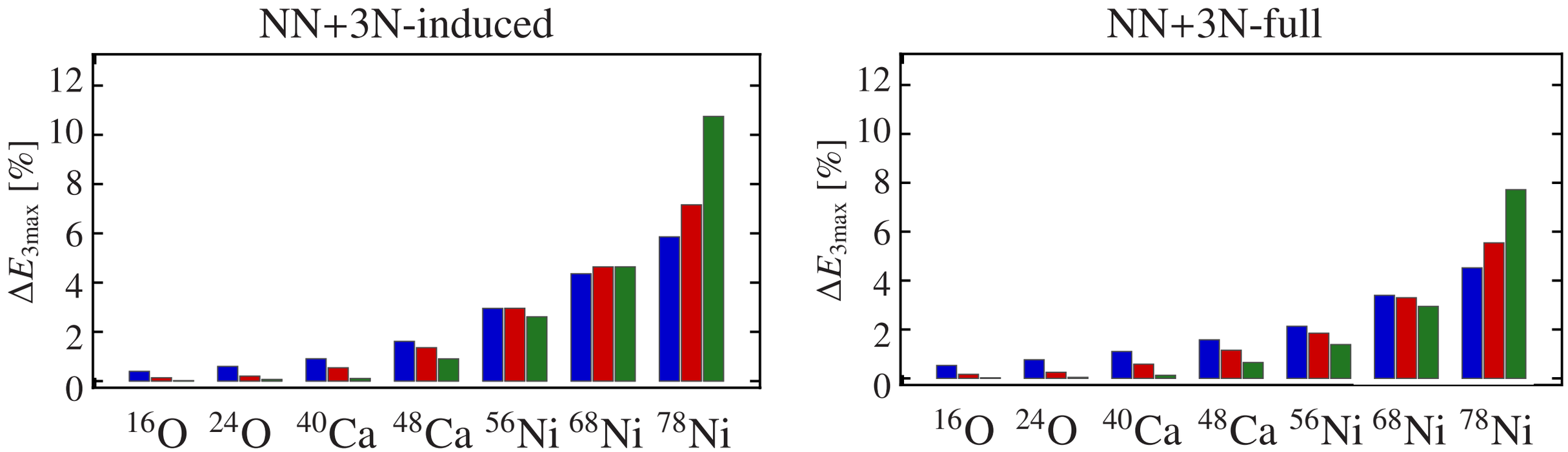
$\alpha = 0.02\,\mathrm{fm}^4$ $\Lambda = 2.66\,\mathrm{fm}^{-1}$

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

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

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

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



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

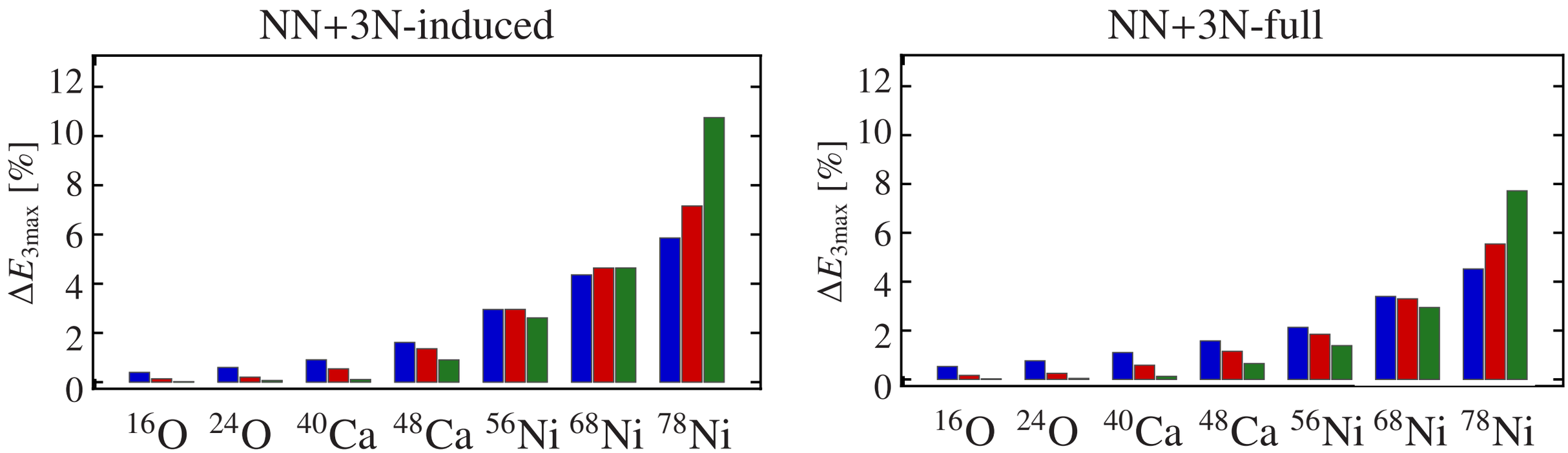
$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

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

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

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

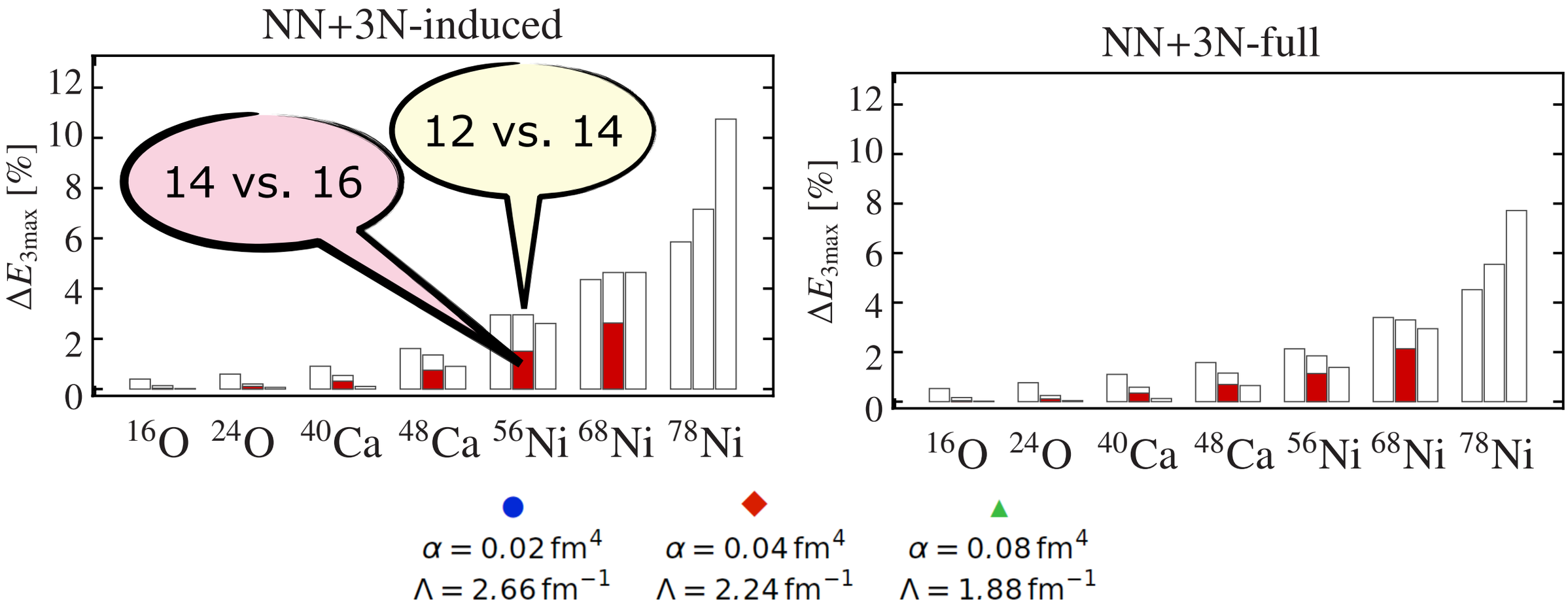
- $E_{3Max}=12$ vs. $E_{3Max}=14$



- Relevance of E_{3Max} grows rapidly with **mass number**
- **soft interactions** do not reduce uncertainties far from convergence

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

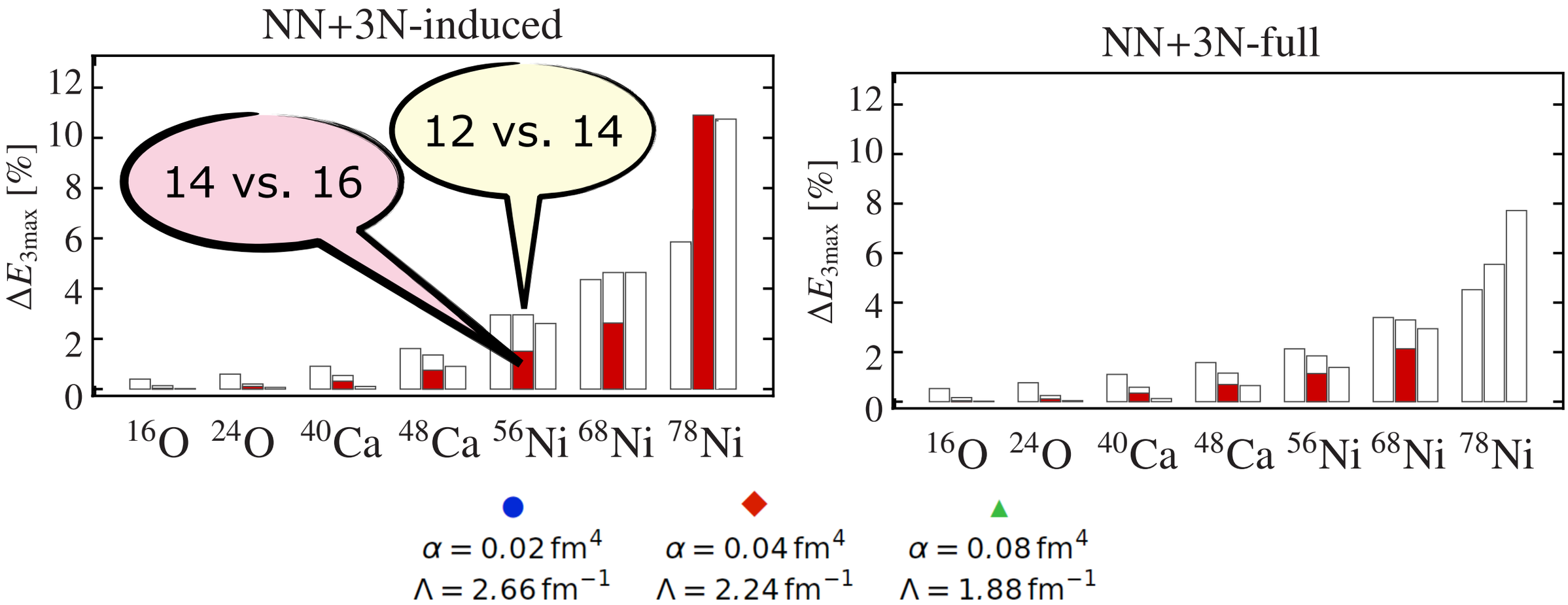
- E_{3Max}=14 vs. E_{3Max}=16 (HF reference state with explicit E_{3Max}=14 used)



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

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

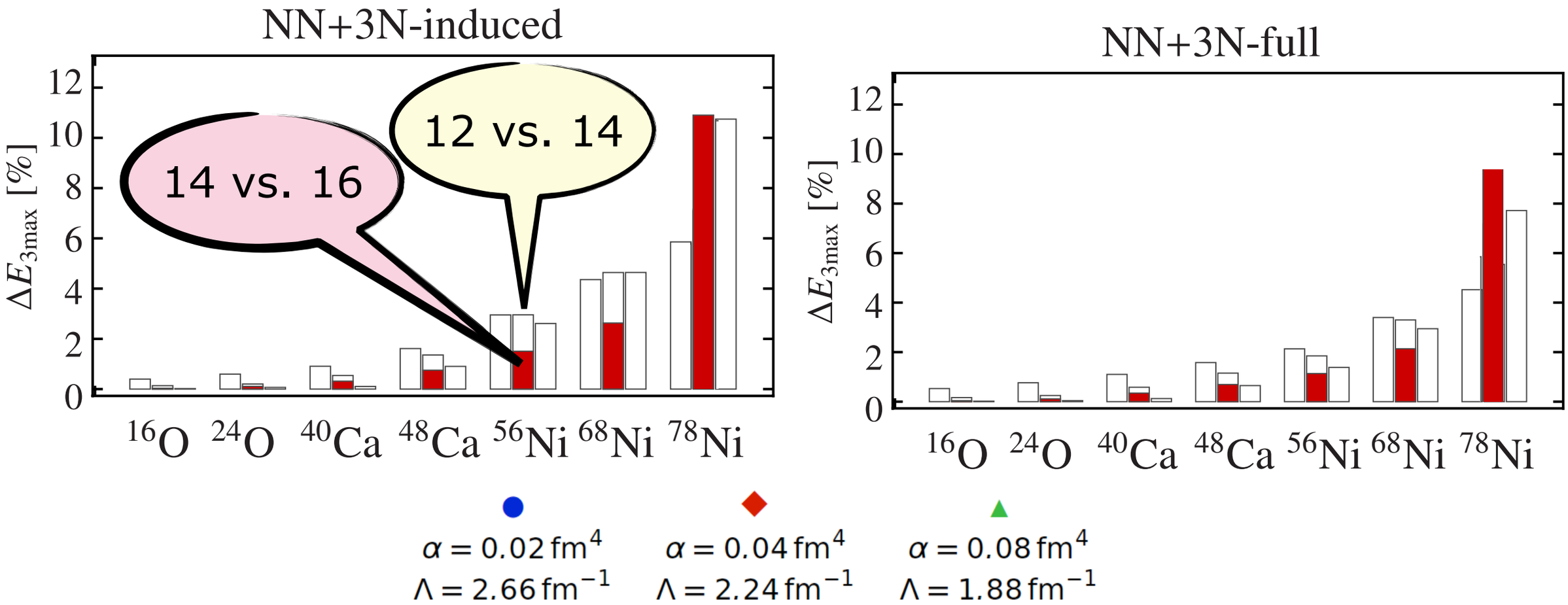
- E_{3Max}=14 vs. E_{3Max}=16 (HF reference state with explicit E_{3Max}=14 used)



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

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

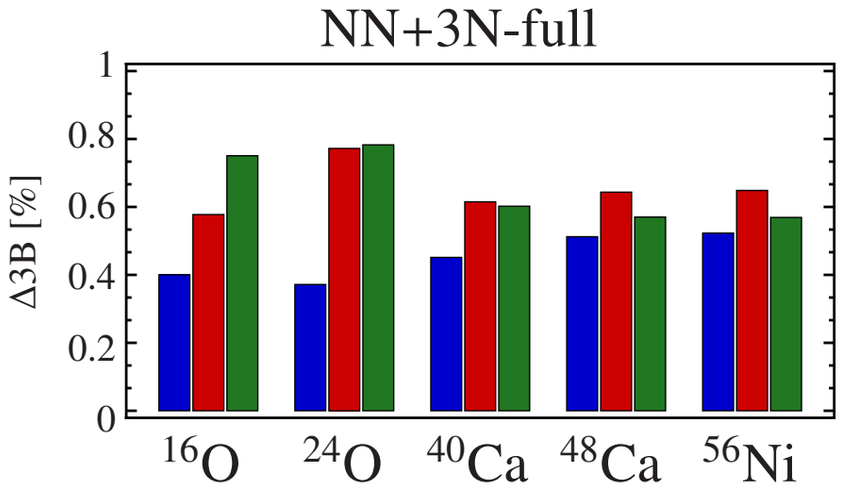
- E_{3Max}=14 vs. E_{3Max}=16 (HF reference state with explicit E_{3Max}=14 used)

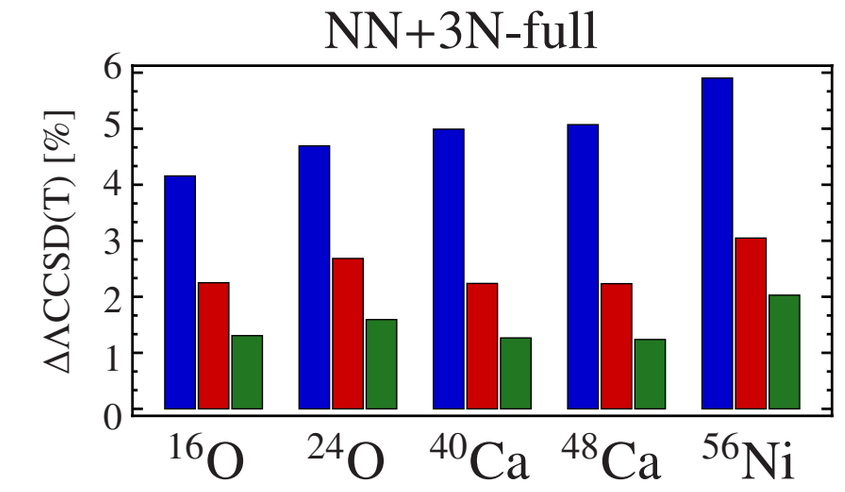


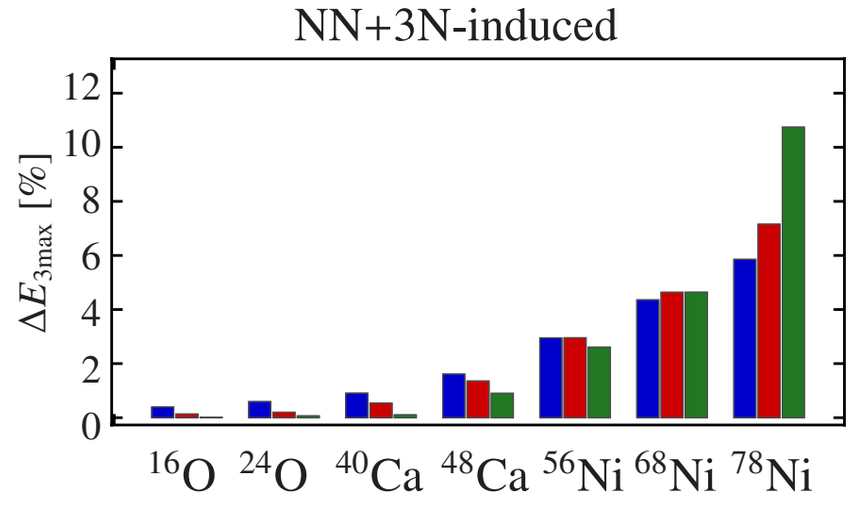
- E_{3Max}=16 **not sufficient** beyond ^{56}Ni

Uncertainty Summary

- **Similarity Renormalization Group**
  - ☑ α-dependence: low-cutoff 3N interaction
  - ☑ small frequencies: conversion
- **Normal-Ordering 2B Approximation**
  - ☑ error in light nuclei: 1-2%,
  - ☑ error in medium-mass nuclei: <1%
  - ☑ error independent of mass number etc.
  - ☑ residual 3N significant for CCSD only
- **Cluster Truncation**
  - ☐ up to 6% contributions from ΛCCSD(T)
  - ☑ soft interactions: only 1-2%
  - ☑ no strong increase with mass number
- **E_{3Max} Cutoff**
  - ☐ up to ^{56}Ni: 2-3% effect for E_{3Max}=12-14
  - ☑ 0.5% for soft interaction
  - ☐ rapid increase with mass number
  - ☐ E_{3Max}=16 not sufficient for A>60





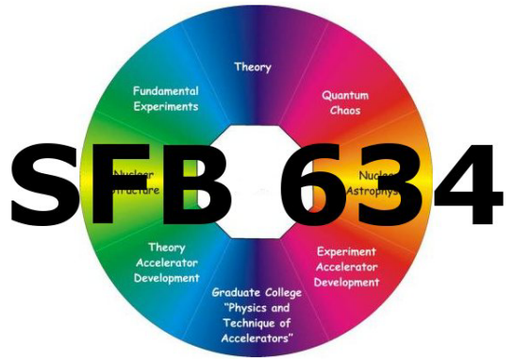


Conclusions

- **medium-mass nuclei** are accessible with **ab initio methods**
- various **truncations** involved ⇒ **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**
  - A. Calci, E. Gebrerufael, P. Isserstedt, H. Krutsch, J. Langhammer, S. Reinhard, R. Roth, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth



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

Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

Computing Time

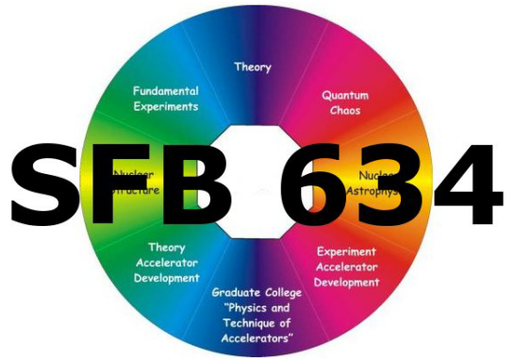
JÜLICH FORSCHUNGSZENTRUM

NERSC

CSC Center for Scientific Computing Frankfurt

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



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

LENPIC

Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

Computing Time

JÜLICH FORSCHUNGSZENTRUM

NERSC

CSC Center for Scientific Computing Frankfurt

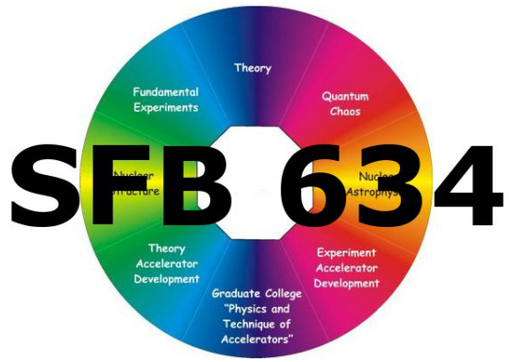
Epilogue

- **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

- P. Navrátil
  TRIUMF, Canada
- P. Piecuch
  Michigan State University, USA
- J. Vary, P. Maris
  Iowa State University, USA
- H. Hergert, K. Hebeler
  The Ohio State University, USA
- C. Forssén
  Chalmers University, Sweden
- U. Feldmeier, T. Neff
  [illegible]um
- [illegible]nou

Thanks for your attention!

LENPIC



SFB 634

Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

Computing Time

JÜLICH FORSCHUNGSZENTRUM

NERSC

CSC Center for Scientific Computing Frankfurt