Ab Initio Coupled Cluster Calculations of Medium-Mass Nuclei

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Similarity Renormalization Group

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

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

$$\widetilde{H}_\alpha = U_\alpha^\dagger \, H \, U_\alpha$$

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

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

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

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

Calculations in *A*-Body Space

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

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

- truncation of cluster series inevitable
  and invariance of energy eigenvalues

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 all three-body terms

Coupled Cluster Method

G. Hagen, T. Papenbrock, D.J. Dean, and 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

$$|\Psi\rangle = \hat{\Omega}|\Phi_0\rangle = e^{\hat{T}_1+\hat{T}_2+\hat{T}_3+\cdots+\hat{T}_A}|\Phi_0\rangle$$

- $\hat{T}_n$: ***n*p*n*h excitation** ("cluster") operators

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

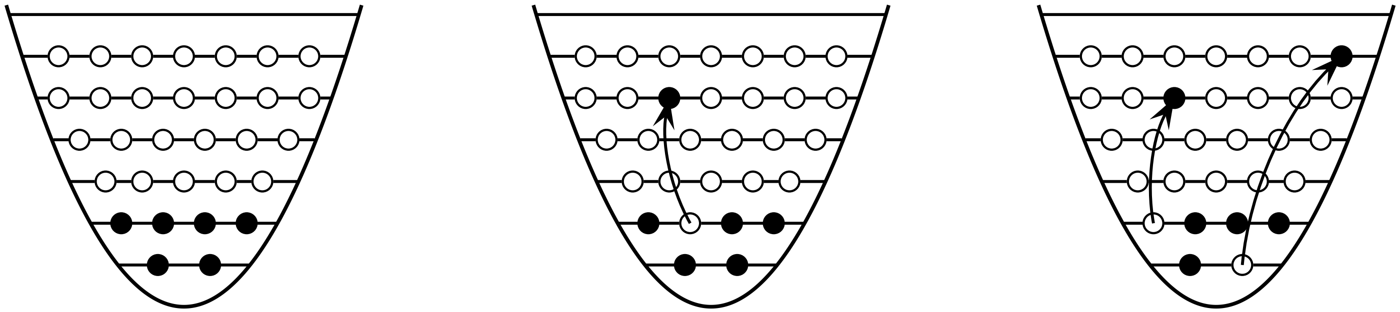
- **similarity transformed** Schrödinger Eq.

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

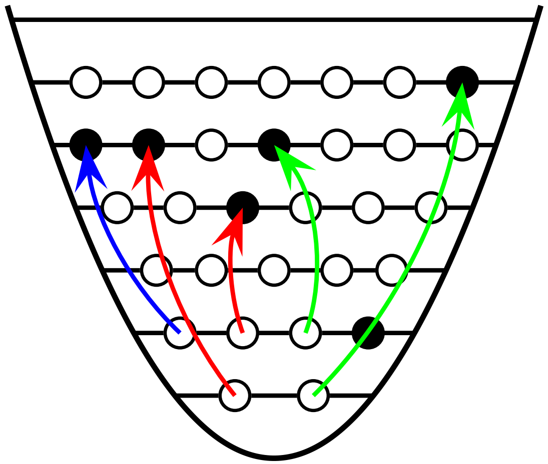
- $\hat{\mathcal{H}}$: non-Hermitian **effective Hamiltonian**

Coupled Cluster Approach

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



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



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

- CCSD equations

$$\Delta E_{\mathrm{CCSD}} = \langle\Phi_0|\,\hat{\mathcal{H}}\,|\Phi_0\rangle$$
$$0 = \langle\Phi_i^a|\,\hat{\mathcal{H}}\,|\Phi_0\rangle$$
$$0 = \langle\Phi_{ij}^{ab}|\,\hat{\mathcal{H}}\,|\Phi_0\rangle$$

Normal-Ordered 3N Interaction

Hagen, Papenbrock, Dean et al. — Phys. Rev. C 76, 034302 (2007)
Roth, Binder, Vobig et al. — Phys. Rev. Lett 109, 052501 (2012)
Binder, Langhammer, 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)

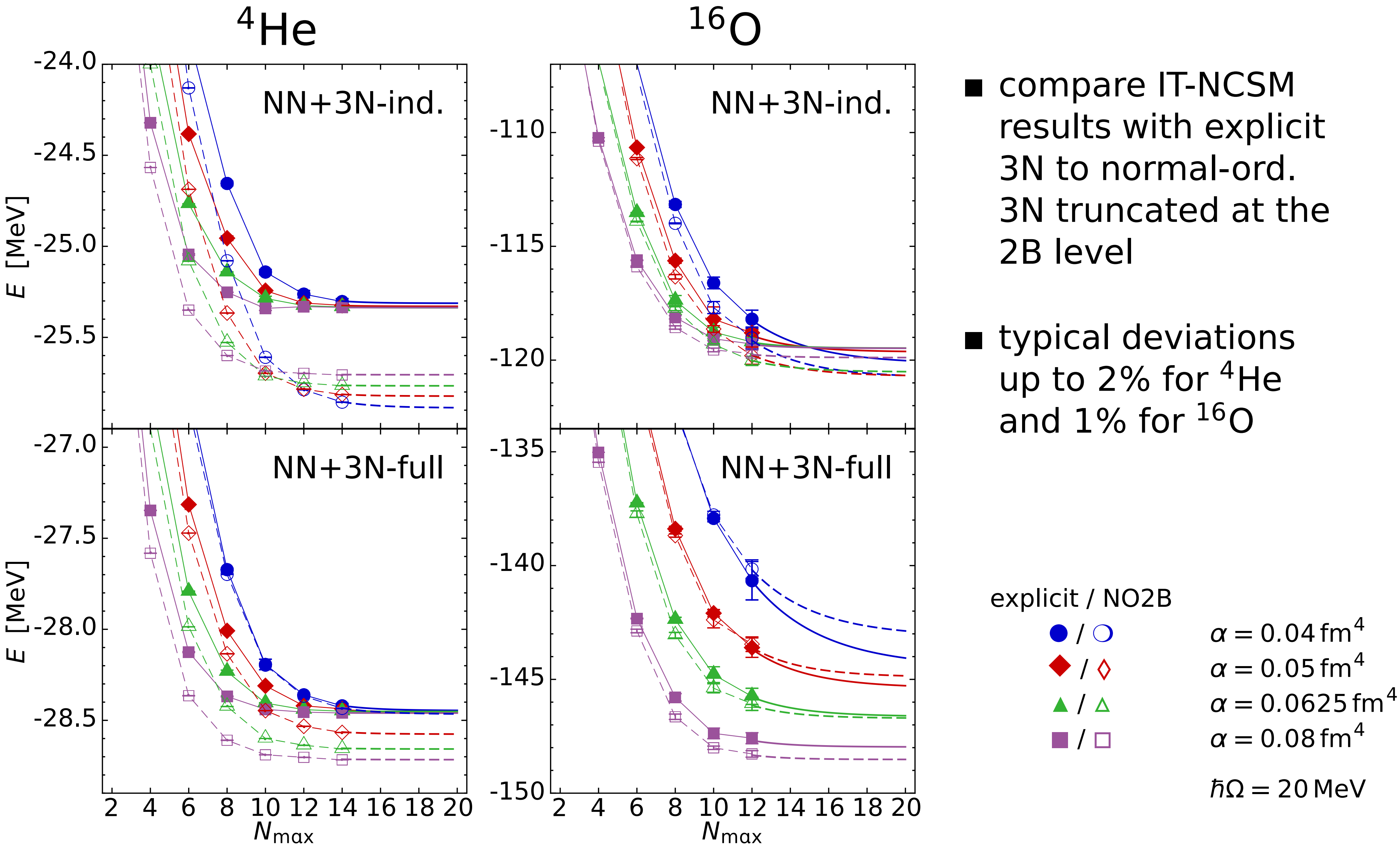
$$\hat{V}_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ}\, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

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

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

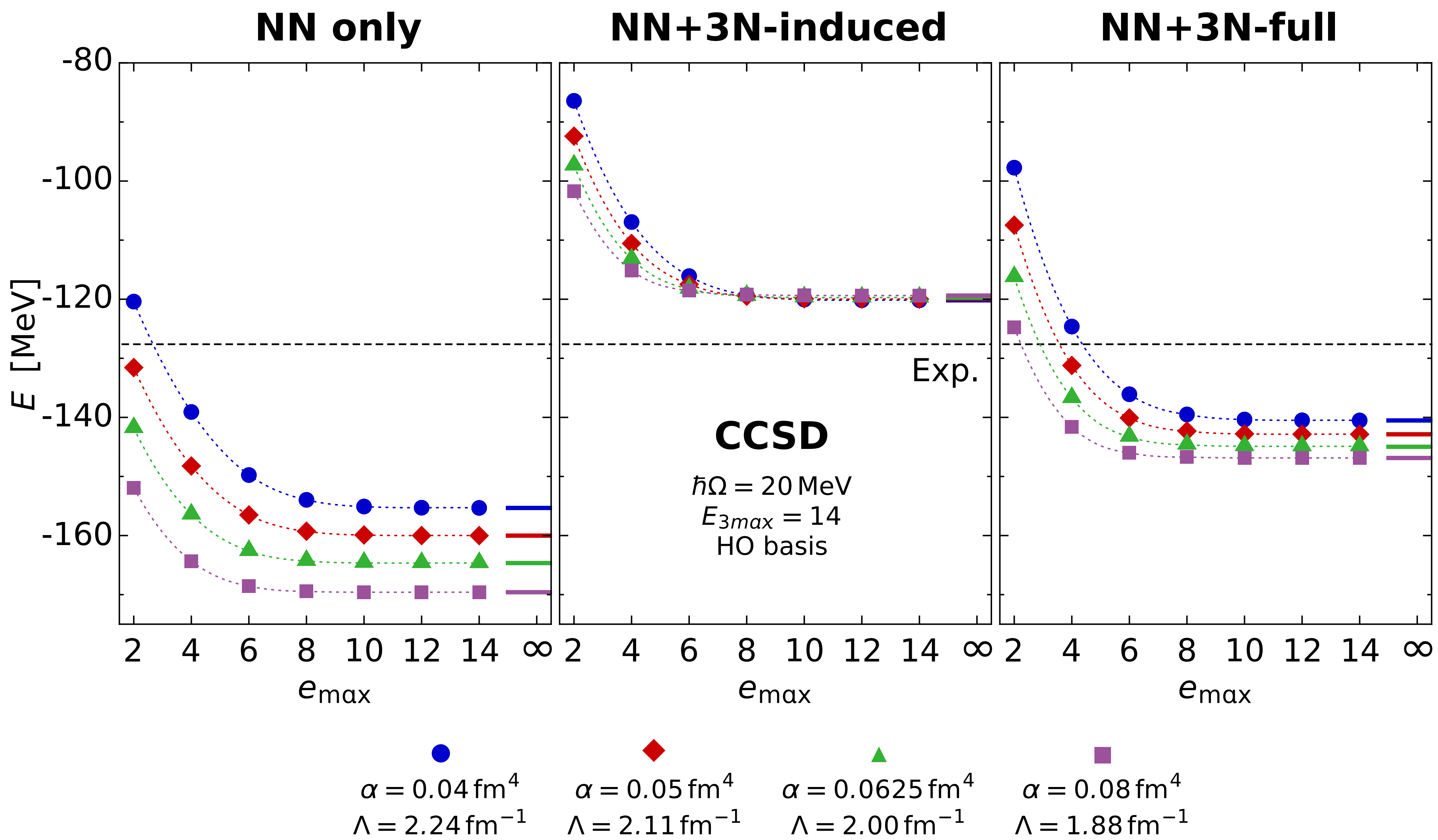
- **Normal-Ordering Approximation** (NO2B): discard residual 3B part W^{3B}

Benchmark of Normal-Ordered 3N

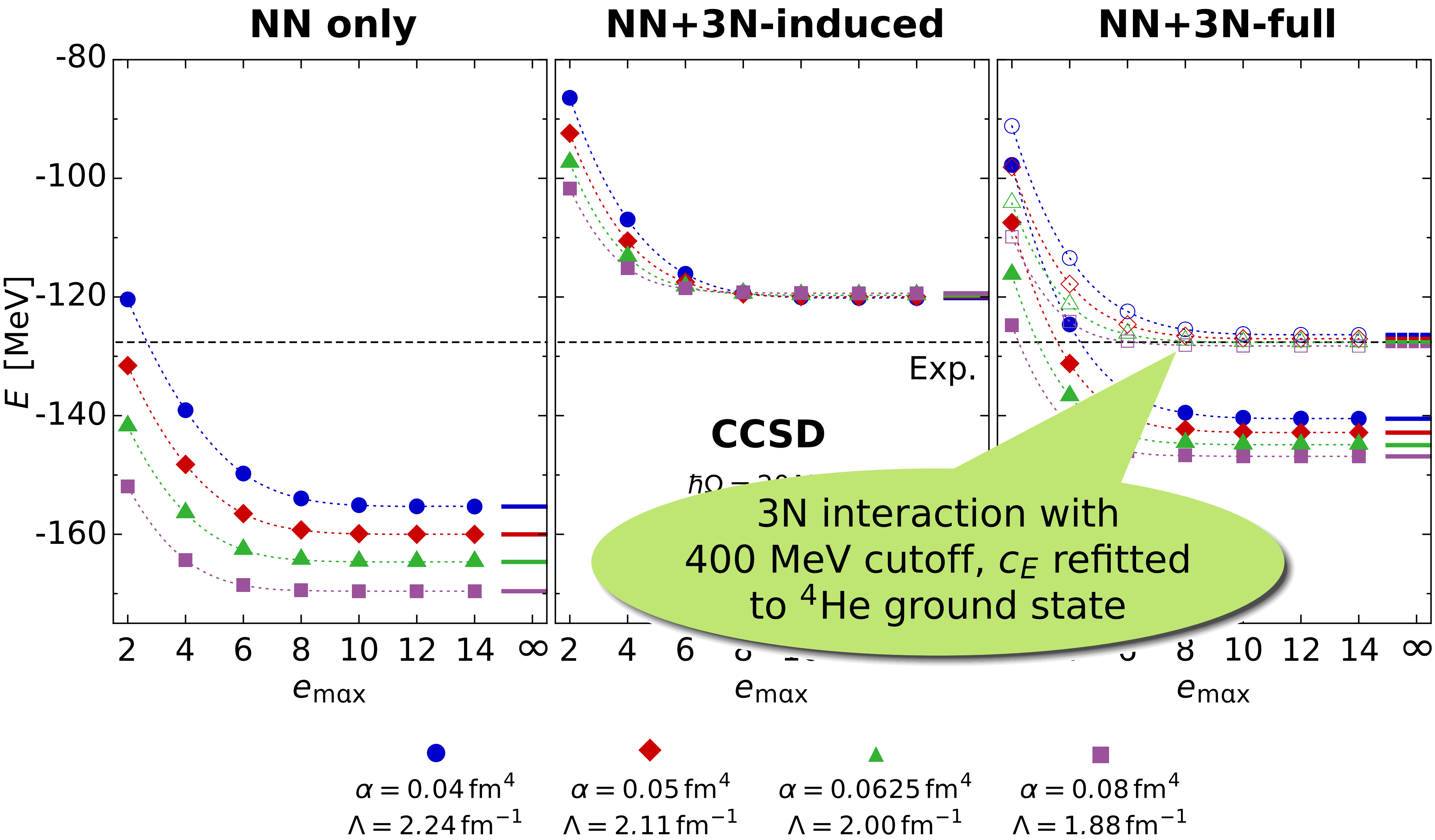


- compare IT-NCSM results with explicit 3N to normal-ord. 3N truncated at the 2B level
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O

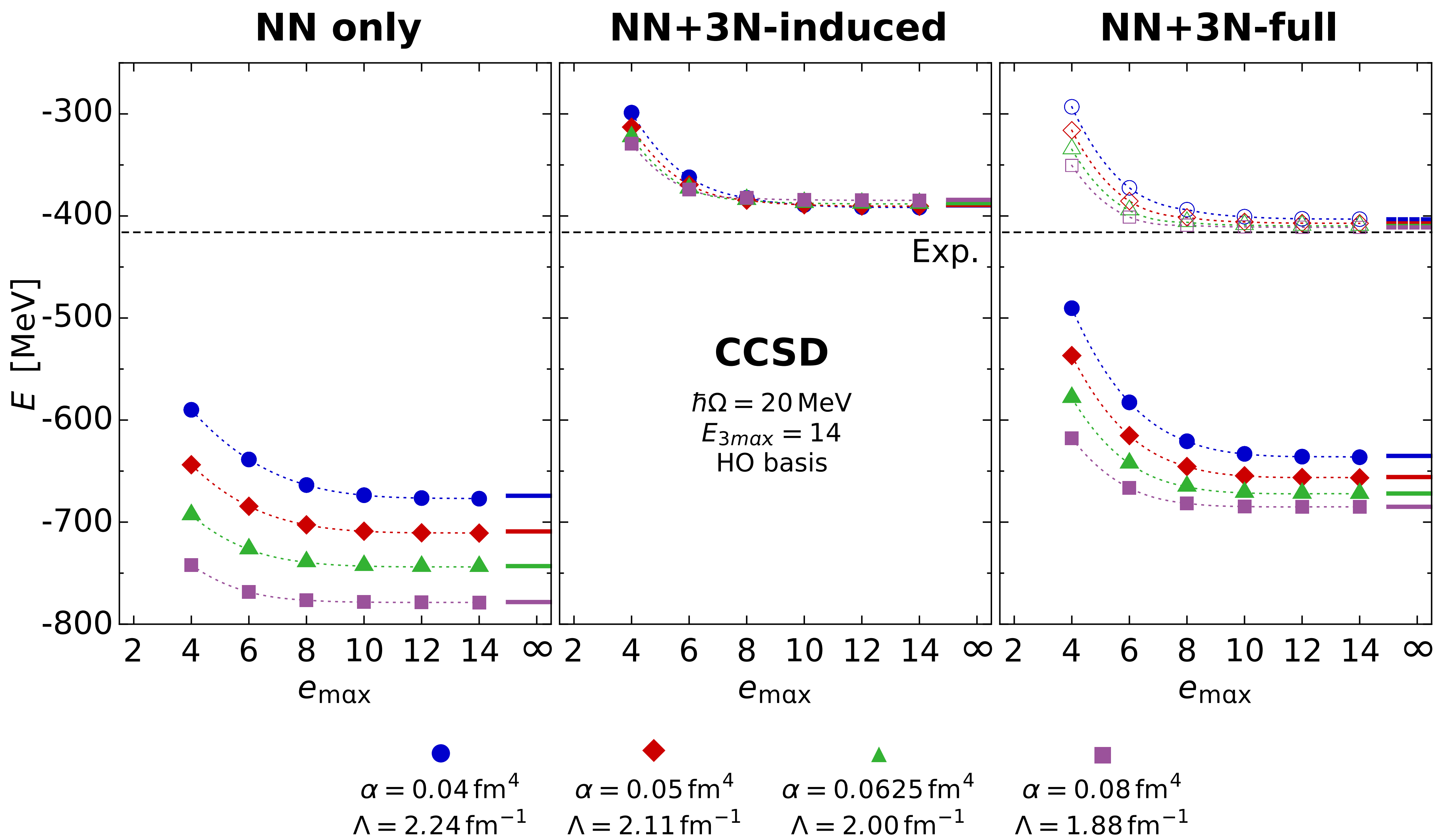
^{16}O: Coupled-Cluster with $3N_{NO2B}$



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



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



CCSD with Explicit 3N Interactions (CCSD3B)

Hagen, Papenbrock, Dean et al. — Phys. Rev. C 76, 034302 (2007)
Binder, Langhammer, Calci et al. — Phys. Rev. C 82, 021303 (2013)

The CCSD3B Equations

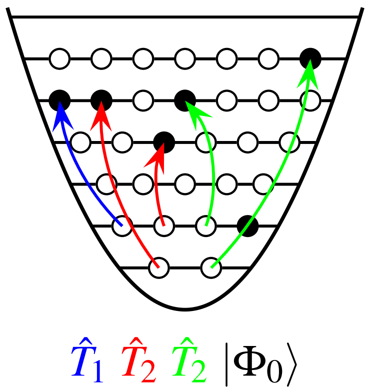
- the CCSD equations with explicit 3N read

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

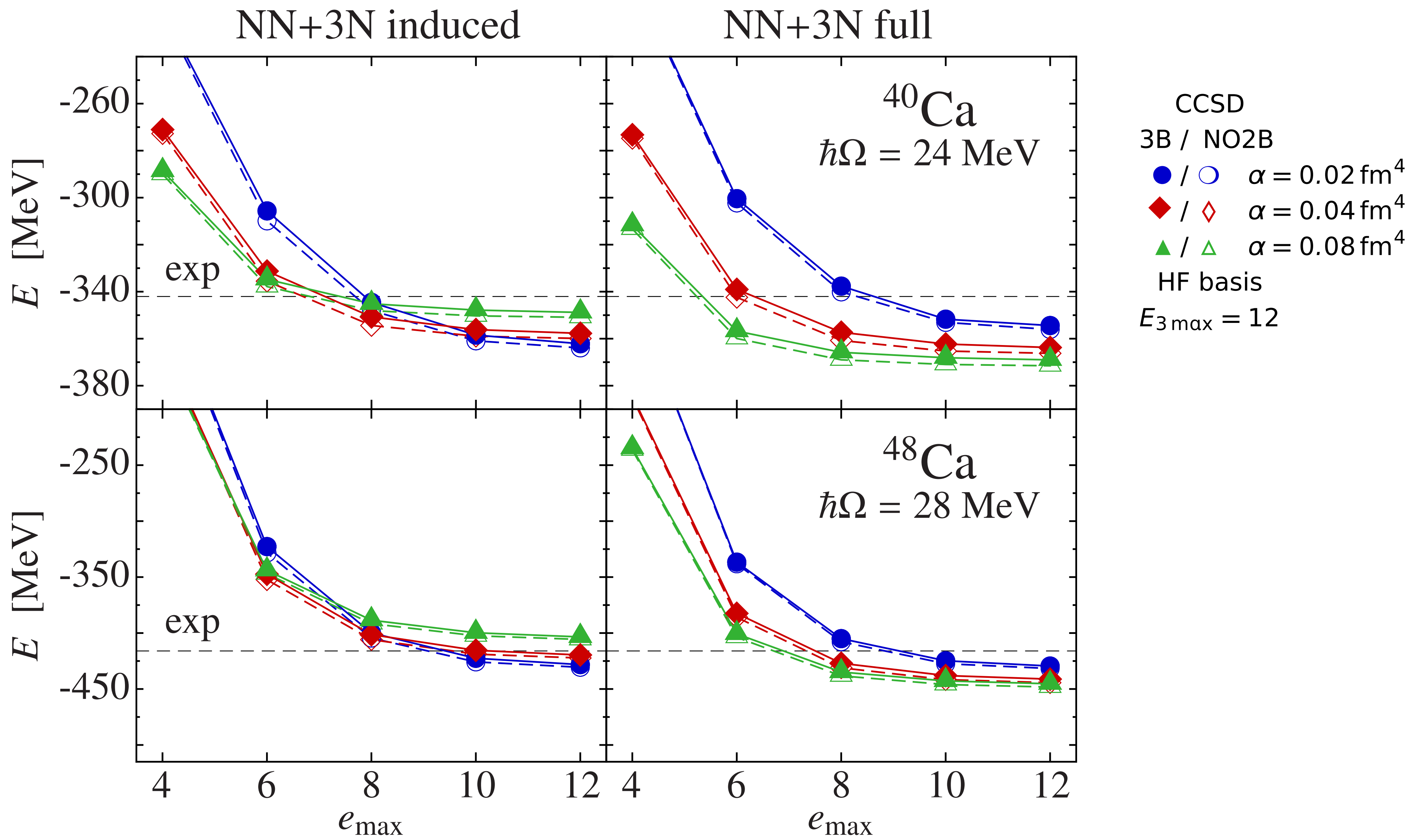
$$0 = T^{NO2B}_{1,\mathrm{CCSD}} + \left\langle \Phi_i^a \right| \hat{W}_{3B}(\hat{T}_2 + \tfrac{1}{2}\hat{T}_1^2 + \hat{T}_1\hat{T}_2 + \tfrac{1}{2}\hat{T}_2^2 + \tfrac{1}{3!}\hat{T}_1^3 + \tfrac{1}{2}\hat{T}_1^2\hat{T}_2 + \tfrac{1}{4!}\hat{T}_1^4) \left| \Phi_0 \right\rangle_C$$

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

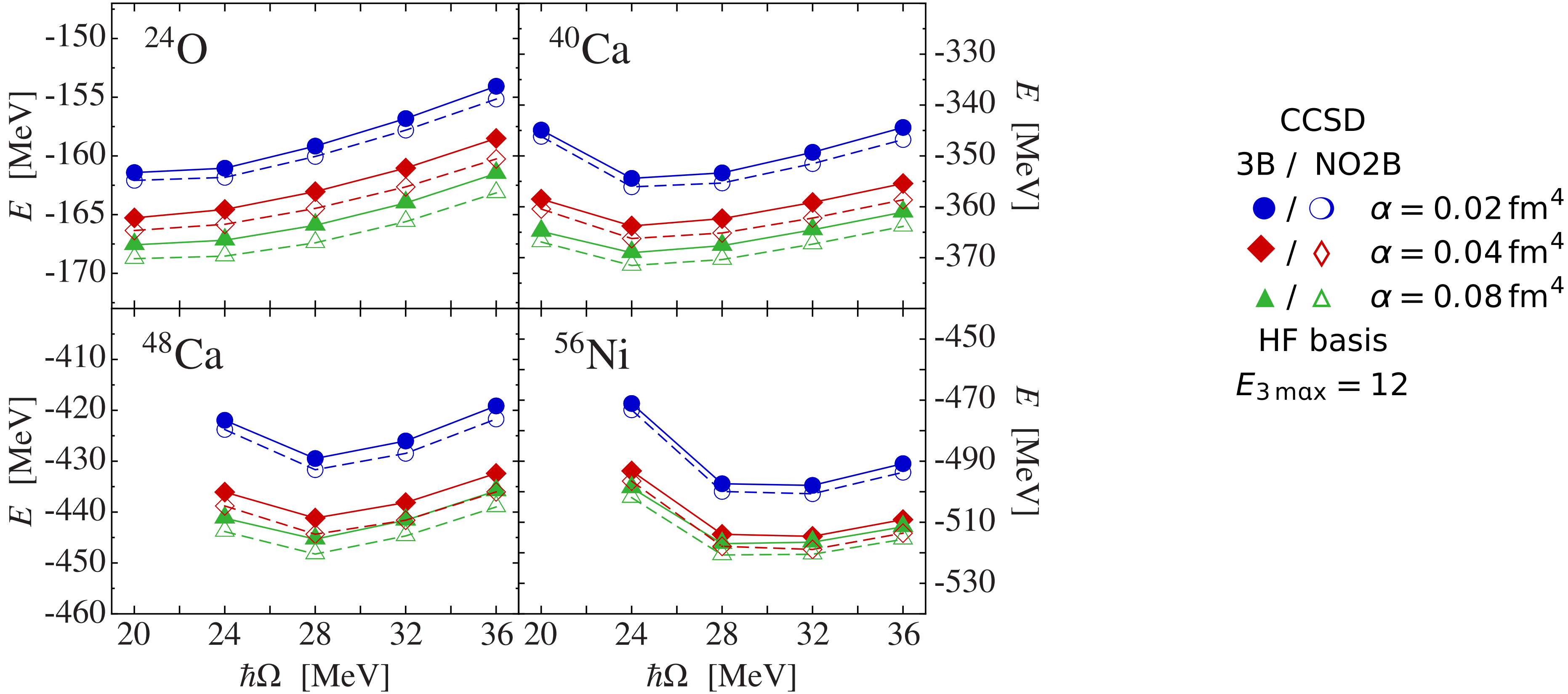
- all new contributions stem from $\hat{W}_{3B}$
- CCSD3B probes new **parts of the Hamiltonian** and new **excitation types**



CCSD with Explicit 3N Interaction



CCSD with Explicit 3N Interaction



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

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

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

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

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

$$e_p = 2n_p + l_p$$

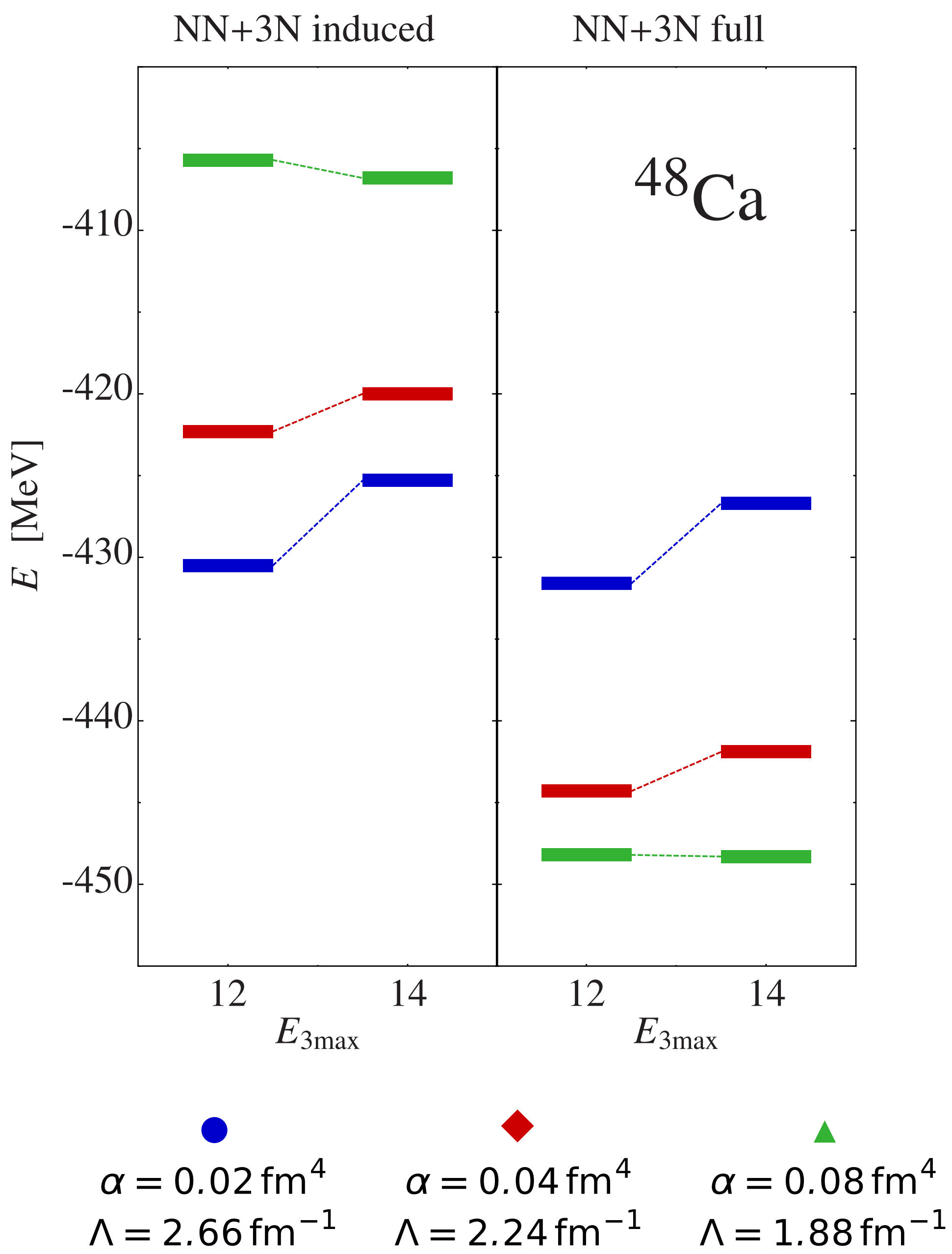
- **current limits**:

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

storage

production

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



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

ΛCCSD(T) - Improving upon CCSD

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

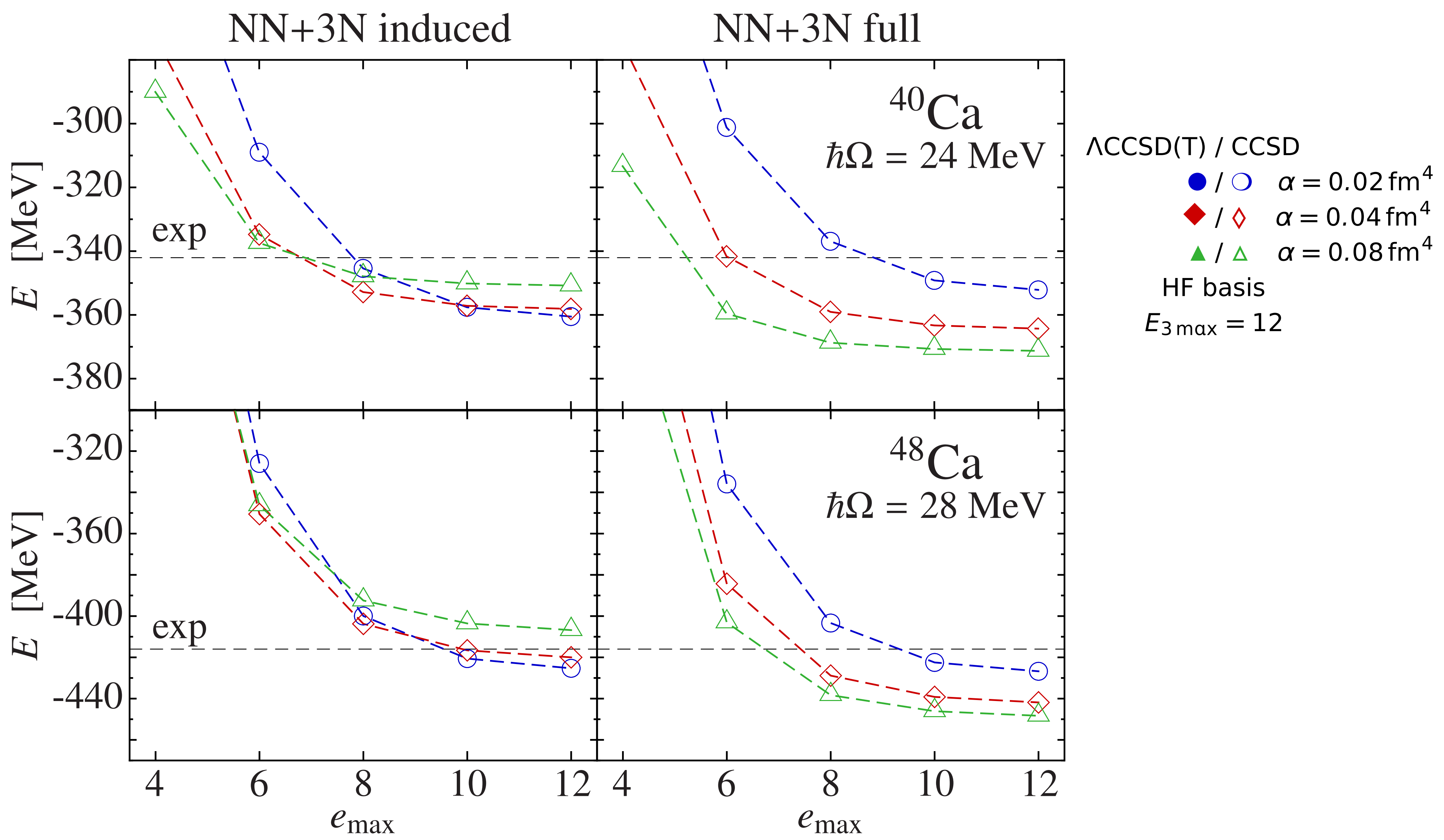
- solution of the Coupled Cluster Λ equations give **a posteriori** fourth order correction to CC energy functional

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

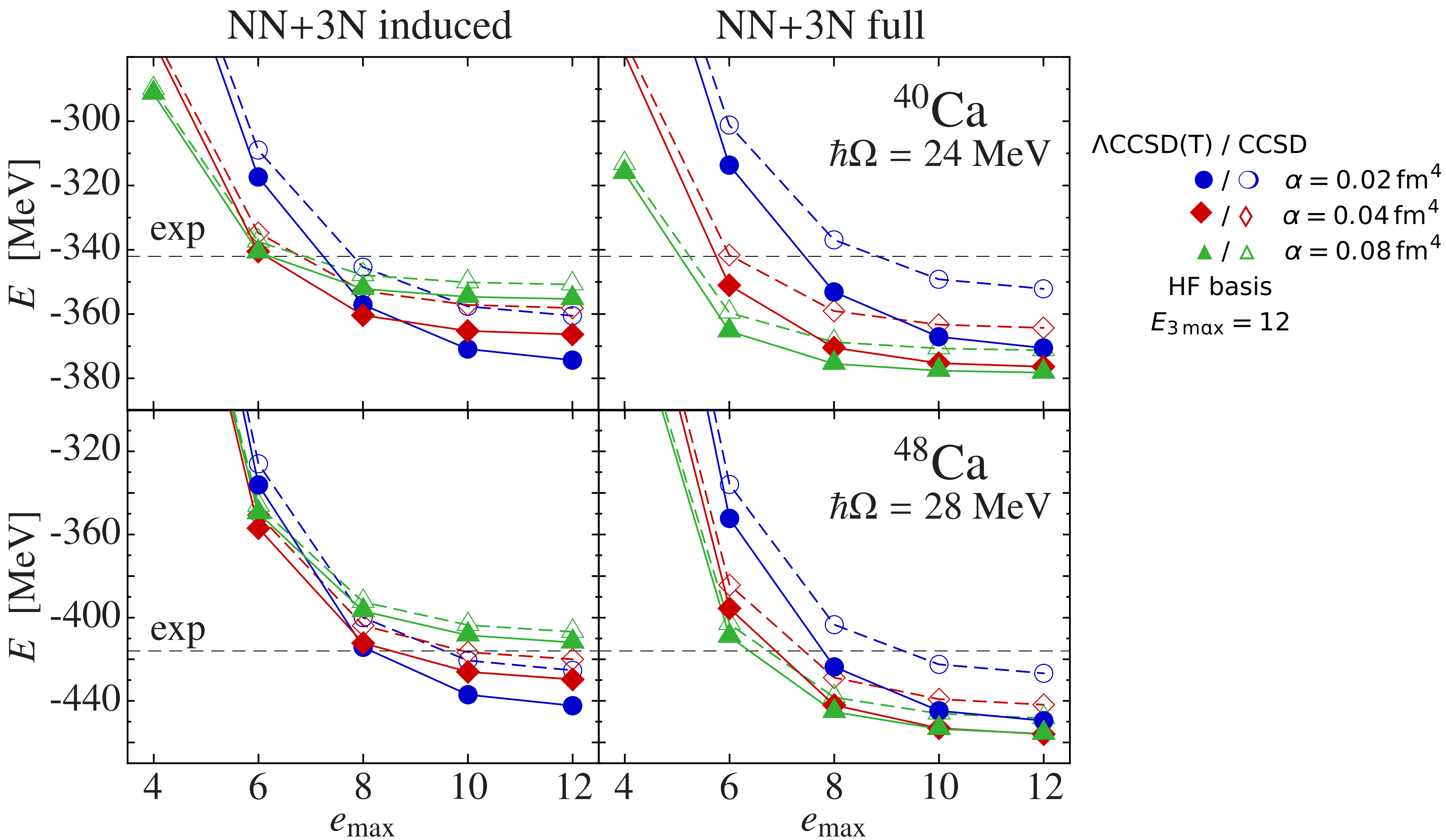
due to triples excitations

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

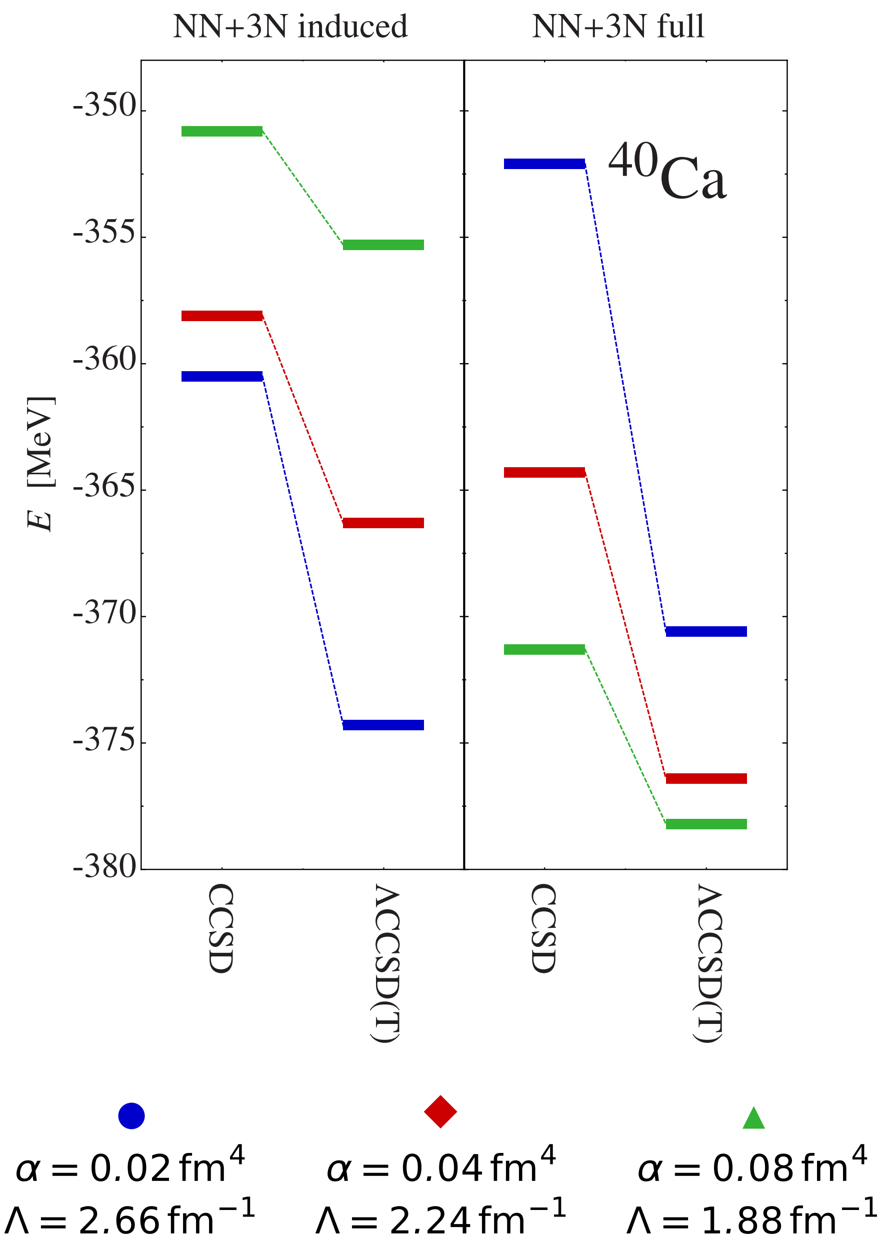
ΛCCSD(T)$_{\text{NO2B}}$



ΛCCSD(T)$_{\text{NO2B}}$



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



- inclusion of **triples excitations mandatory** (up to 6 % more binding for heavier nuclei)
- cluster truncation works better for **softer interactions**
- $\alpha = 0.02\ \mathrm{fm}^4$ results not necessarily closer to **exact result** than $\alpha = 0.08\ \mathrm{fm}^4$
- $\Rightarrow$ calculations with **bare** 3N interaction suffer from cluster truncation and $E_{3\mathrm{max}}$ cut

ΛCCSD(T) with Explicit 3N Interactions

Binder, Langhammer, Calci, Navrátil, Roth — in prep.

ΛCCSD(T)3B

- $\hat{\mathcal{H}} = e^{-\hat{T}} \hat{H}_N e^{\hat{T}} = \hat{\mathcal{H}}_{\text{NO2B}} + 116 \text{ terms } + \ldots$
- ΛCCSD(T)3B energy correction

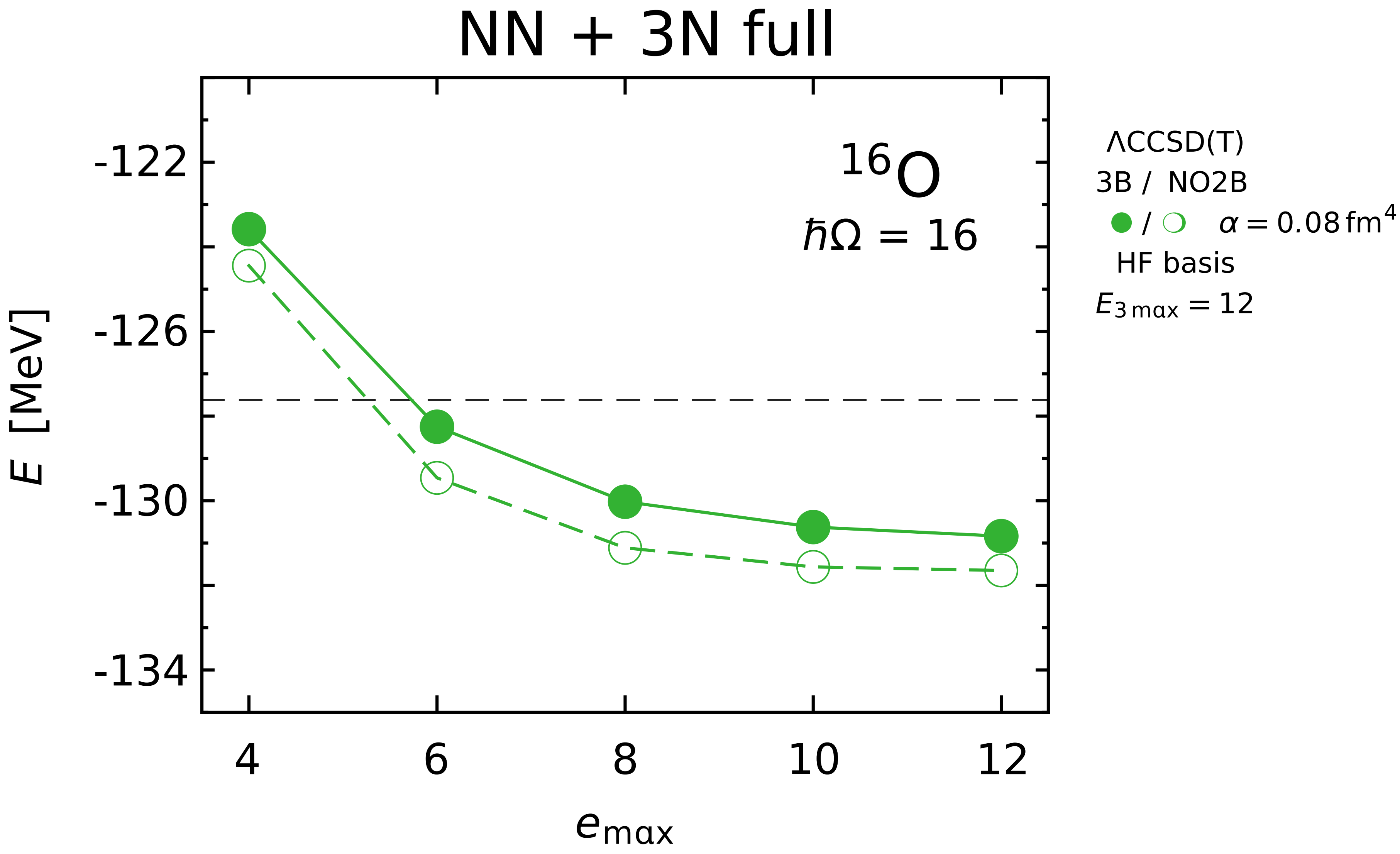
$$\delta E_{\Lambda\text{CCSD(T)}} = \frac{1}{(3!)^2} \sum_{\substack{abc \\ ijk}} \tilde{\lambda}^{ijk}_{abc} \frac{1}{\epsilon^{abc}_{ijk}} \tilde{t}^{abc}_{ijk}$$

- contributions from $\hat{W}_{3\text{B}}$ to $\tilde{\lambda}^{ijk}_{abc}$, $\tilde{t}^{abc}_{ijk}$

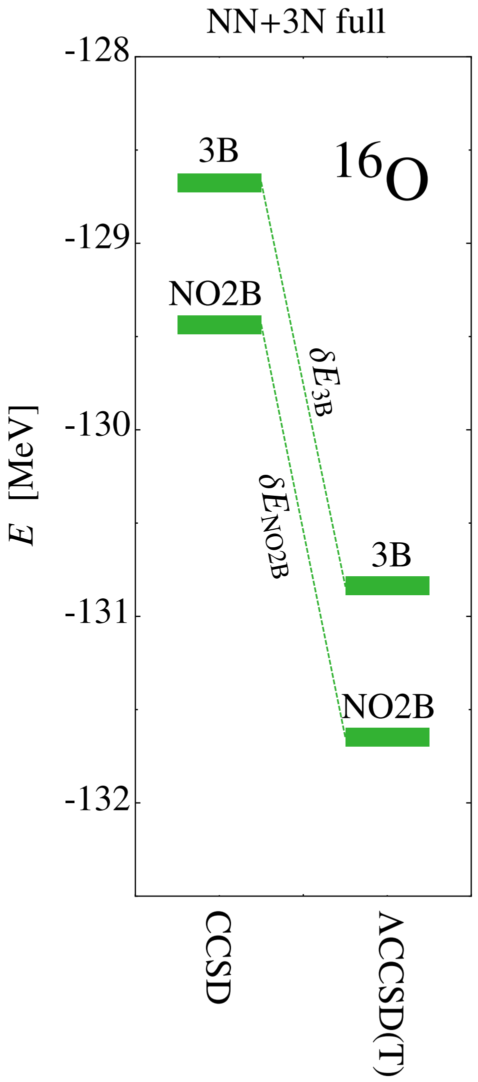
$$\tilde{\lambda}^{ijk}_{abc} = \tilde{\lambda}^{ijk}_{abc}[\text{NO2B}] - \hat{P}_{ab/c} \sum_{l} w^{ijk}_{abl} \lambda^{l}_{c} + \hat{P}_{ij/k} \sum_{d} w^{ijd}_{abc} \lambda^{k}_{d}$$
$$+ \tfrac{1}{2} \hat{P}_{ij/k} \sum_{de} w^{dek}_{abc} \lambda^{ij}_{de} + \tfrac{1}{2} \hat{P}_{ab/c} \sum_{lm}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

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

ΛCCSD(T)3B


NN + 3N full
^{16}O
$\hbar\Omega = 16$
-122
-126
-130
-134
E [MeV]
4
6
8
10
12
e_{max}
ΛCCSD(T)
3B / NO2B
$\alpha = 0.08\,\mathrm{fm}^4$
HF basis
$E_{3\,\mathrm{max}} = 12$

ΛCCSD(T)3B



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

- NO2B shows **excellent agreement** also for ΛCCSD(T)
  - residual 3N contribute **0.75 MeV** or **0.7 %** to $E_{\Lambda\text{CCSD(T)}}$
- $E_{\Lambda\text{CCSD(T)}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\text{CCSD}} + \delta E_{\Lambda\text{CCSD(T)}}$
- residual 3N 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}
  - **0.05 MeV** or **2.2 %** to $\delta E_{\Lambda\text{CCSD(T)}}$
- significant contribution of residual 3N **only for ΔE_{CCSD}**
- $E_{\Lambda\text{CCSD(T)}\mathbf{3B}} \approx \langle\Phi_0|\hat{H}|\Phi_0\rangle + \Delta E_{\text{CCSD}\mathbf{3B}} + \delta E^{\mathbf{NO2B}}_{\Lambda\text{CCSD(T)}}$

CCSDT?

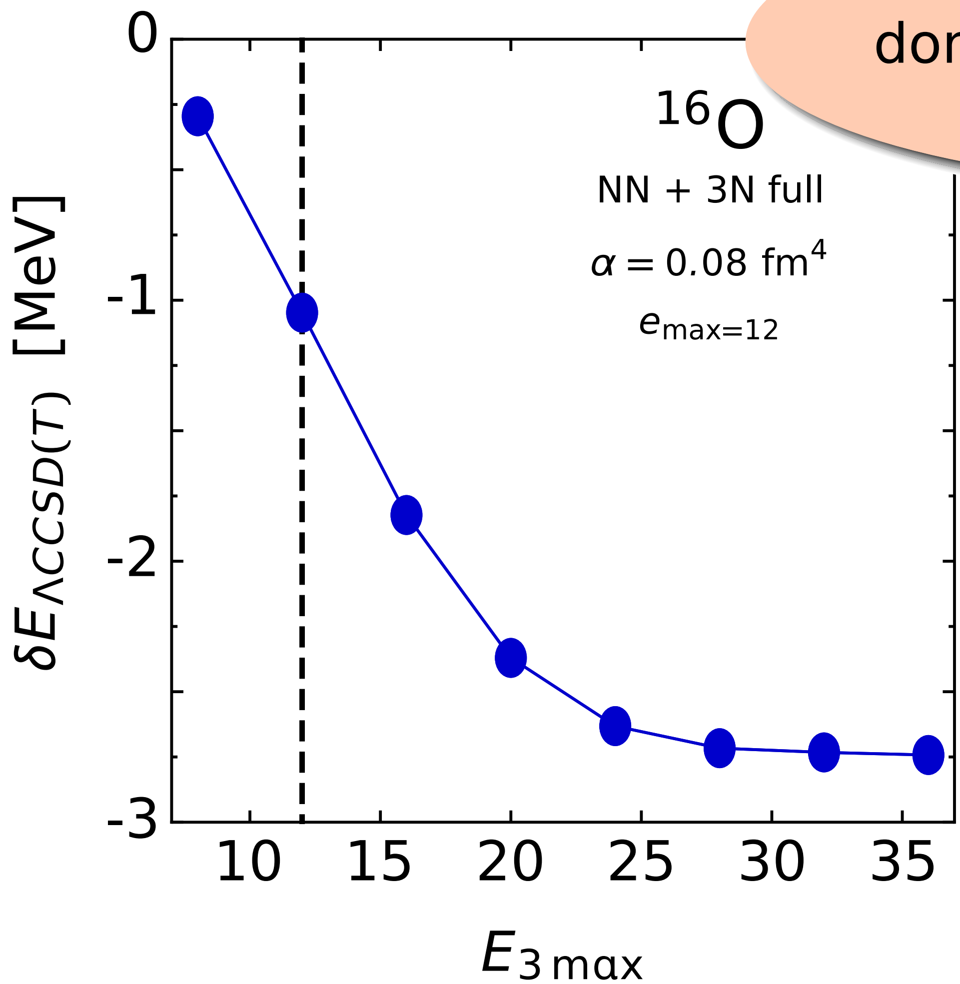
- **No, thanks!**
- ΛCCSD(T) energy correction (**non-iterative**)

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

$$\tilde{t}^{abc}_{ijk} \approx \langle abc|\hat{t}_3|ijk\rangle$$

- CCSDT is **iterative** $\Rightarrow$ solve for and **store** $\langle abc|\hat{t}_3|ijk\rangle$
- need $E_{3\mathrm{max}}$ truncation for $\langle abc|\hat{t}_3|ijk\rangle$
- assume $E_{\mathrm{CCSDT}}(E_{3\mathrm{max}}) \approx E_{\Lambda\mathrm{CCSD(T)}}(E_{3\mathrm{max}})$

CCSDT?



realistic E_{3max} cuts don't allow for reasonable CCSDT calculations

Epilogue

- **thanks to my group & my collaborators**

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