Ab Initio Calculations of Medium-Mass Nuclei and Normal-Ordered Chiral NN+3N Interactions

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Road Map

Nuclear
Structure & Reaction Observables

Importance Truncated NCSM
ab initio studies in the p- & sd-shell

Applications to Nuclear Spectra
spectroscopy and sensitivity on 3N

Coupled Cluster Approach
systematic extension to heavy nuclei

...

Similarity Renormalization Group
pre-diagonalization of Hamiltonian by unitary transformation
computational technology for 3N matrix elements

Chiral Effective Field Theory
systematic low-energy effective theory of QCD
consistent & improvable NN, 3N,... interactions

Low-Energy Quantum Chromodynamics

Reminder: Similarity Renormalization Group

...yields an evolved Hamiltonian with **improved convergence properties** in many-body calculations

- **unitary transformation** of Hamiltonian driven by

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha] \qquad \eta_\alpha = (2\mu)^2 [T_{int}, \widetilde{H}_\alpha]$$

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

Coupled Cluster Method

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

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

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

- **similarity transformed** 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 - Equations

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

- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

$$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i|\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i|\Phi_0\rangle \right\}$$

leads to **CCSD equations**

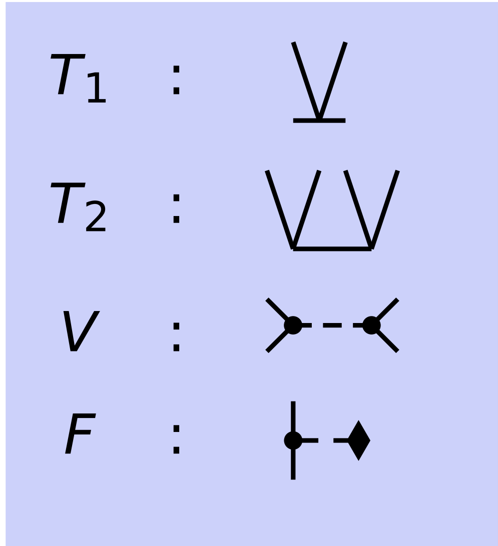
- $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(\hat{T}_2 + \hat{T}_1 + \frac{1}{2}\hat{T}_1^2)|\Phi_0\rangle_C$

- $0 = \langle\Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(1 + \hat{T}_2 + \hat{T}_1 + \hat{T}_1\hat{T}_2 + \frac{1}{2}\hat{T}_1^2 + \frac{1}{3!}\hat{T}_1^3)|\Phi_0\rangle_C$

- $0 = \langle\Phi_{ij}^{ab}|\hat{\mathcal{H}}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(1 + \hat{T}_2 + \frac{1}{2}\hat{T}_2^2 + \hat{T}_1 + \hat{T}_1\hat{T}_2$
$\quad + \frac{1}{2}\hat{T}_1^2 + \frac{1}{2}\hat{T}_1^2\hat{T}_2 + \frac{1}{3!}\hat{T}_1^3 + \frac{1}{4!}\hat{T}_1^4)|\Phi_0\rangle_C$

Coupled Cluster - Equations

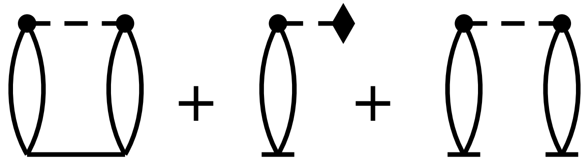
- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



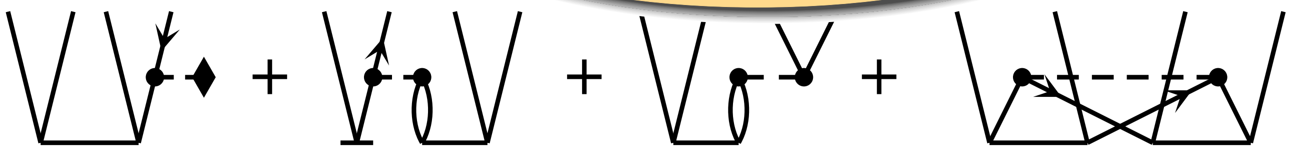
- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

  $\left\{ \, |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle \, \right\}$

  leads to **CCSD equations**

  - $\Delta E = \langle \Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle =$ 

  - $0 = \langle \Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle =$  $\dots$

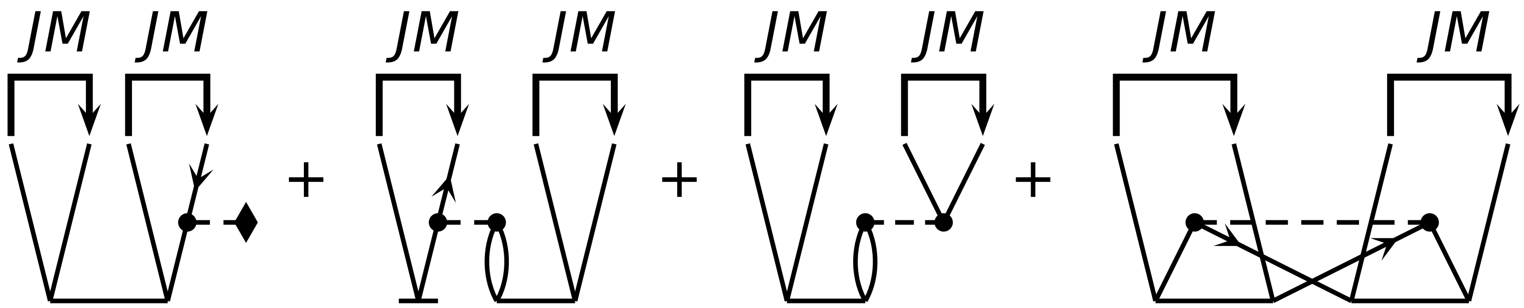
  - $0 = \langle \Phi_{ij}^{ab}|\hat{\mathcal{H}}|\Phi_0\rangle =$  $\dots$

linked diagrams only
$\Rightarrow$ size extensive

Coupled Cluster - Spherical Scheme

- **coupling of external lines** to good J

$0 =$



$\ldots$

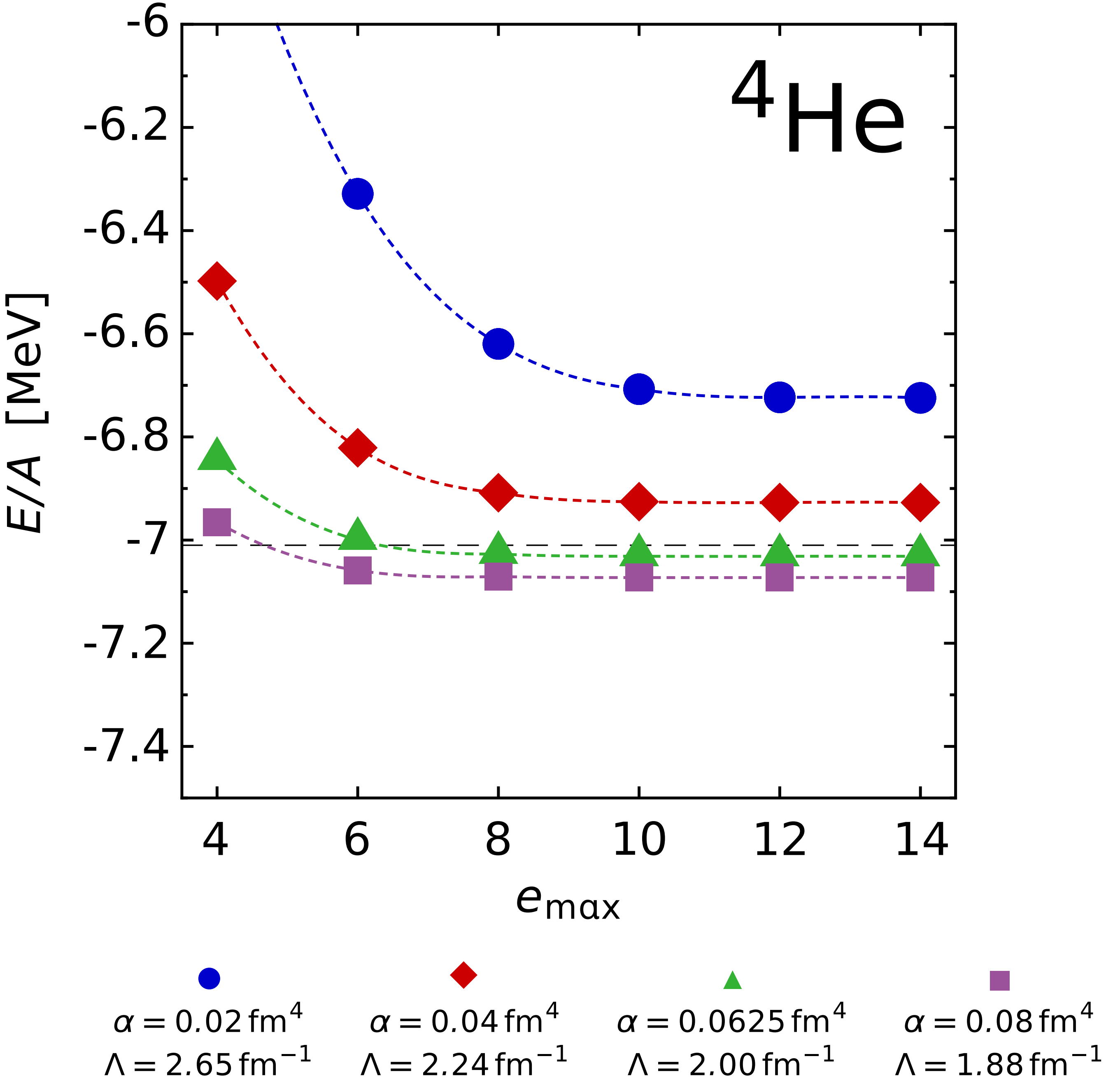
etc.

- express CCSD equations in terms of

$$\langle \overbrace{p\quad q}^{J0} \| \overbrace{r\quad s}^{J0} \rangle\,,\quad \langle \overbrace{a\quad b}^{J0} | t | \overbrace{i\quad j}^{J0} \rangle\,,\quad \langle \overbrace{\tilde{a} | t | i}^{00} \rangle\,,\quad etc.$$

- $\Rightarrow$ **drastic reduction** of number of amplitudes

Coupled Cluster - Convergence Rate

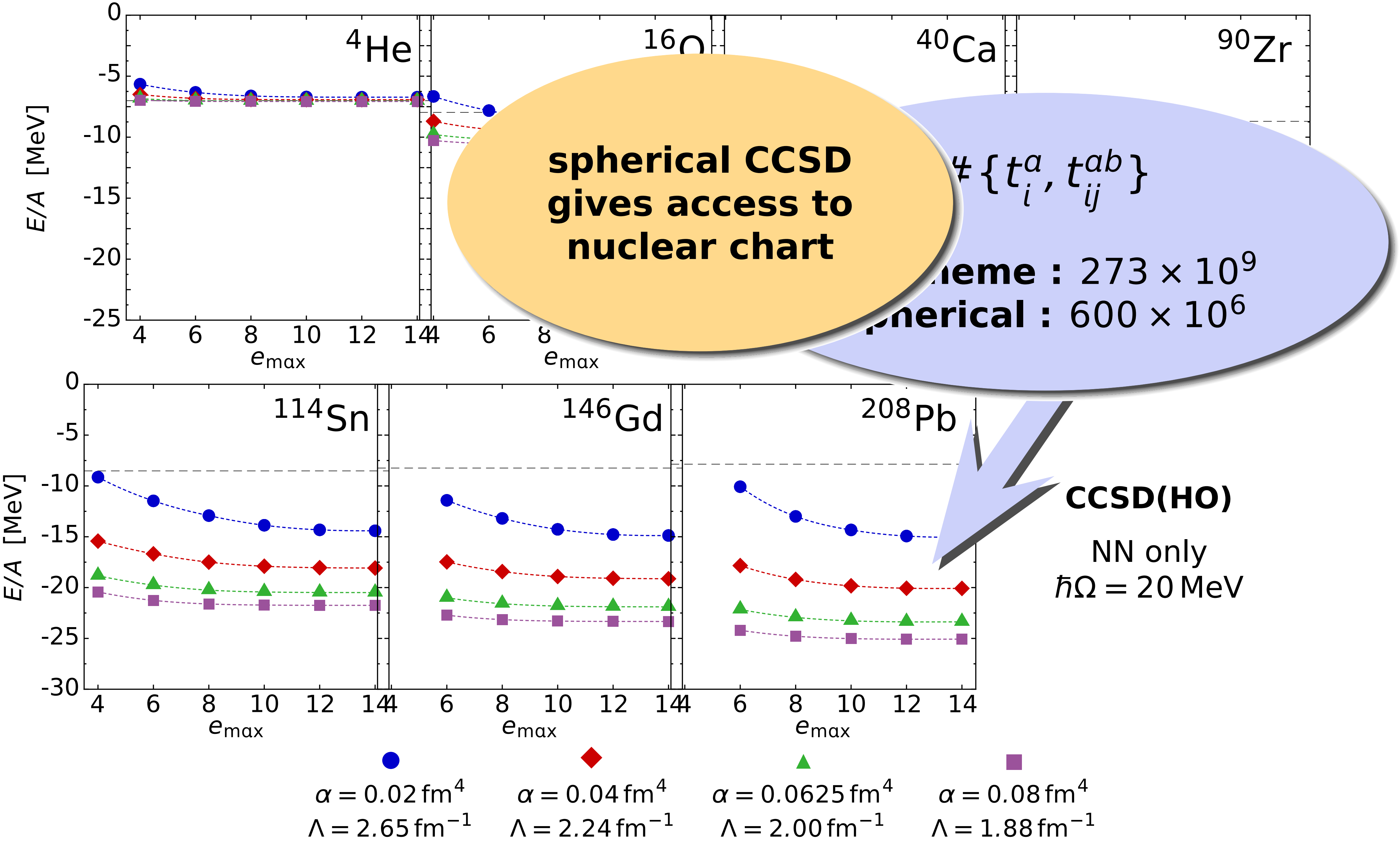


CCSD(HO)

NN only

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

Coupled Cluster - Convergence Rate



Normal-Ordered 3N Interaction

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

Normal-Ordered 3N Interaction

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

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

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

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

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

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

Normal-Ordered 3N Interaction

- compute NO2B contributions to original $H_{0B},\ H_{1B}, H_{2B}$

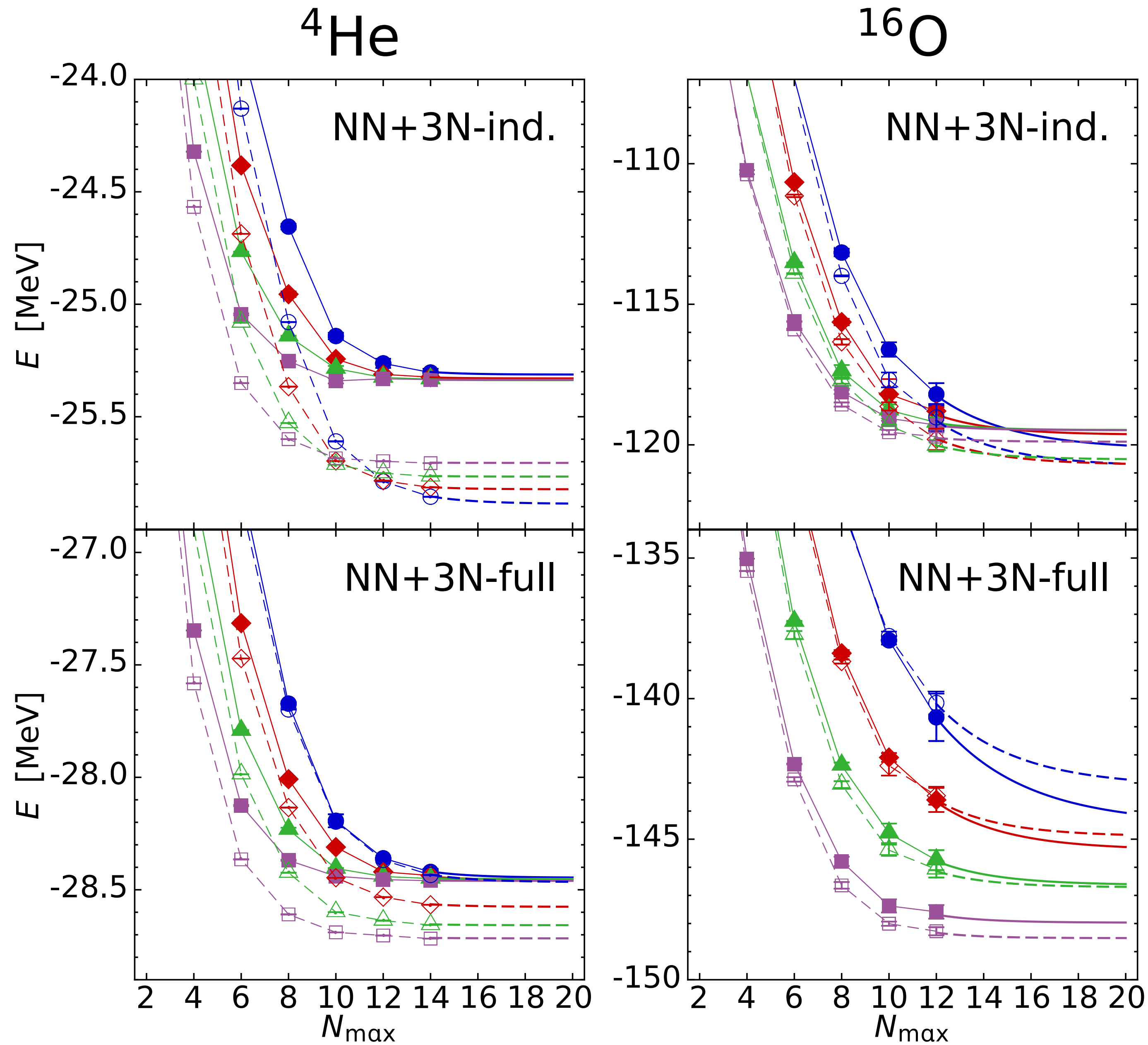
$$
\begin{aligned}
H_{0B} &\leftarrow \frac{1}{6}\sum_{ijk}\langle ijk|v|ijk\rangle \\
\langle p|H_{1B}|q\rangle &\leftarrow \frac{1}{2}\sum_{ij}\langle ijp|v|ijq\rangle \\
\langle pq|H_{2B}|rs\rangle &\leftarrow \frac{1}{4}\sum_{i}\langle ipq|v|irs\rangle
\end{aligned}
$$

✓ embarrassingly parallel

✓ HO and HF basis

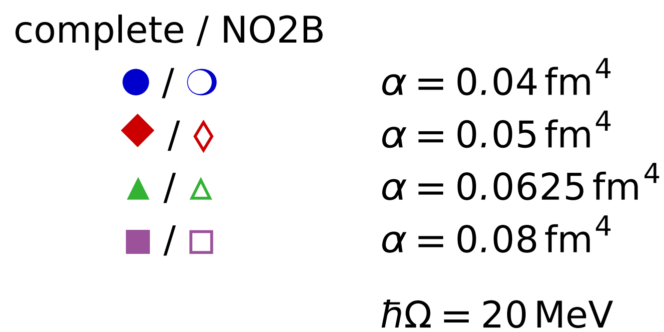
- $\langle pqr|v|stu\rangle$: $E_{3,\max} = \max\left\{\ 2\,e_{\max} + e_{\max}\left(\Phi_0\right)\ ,\ 14\ \right\}$

Benchmark of Normal-Ordered 3N

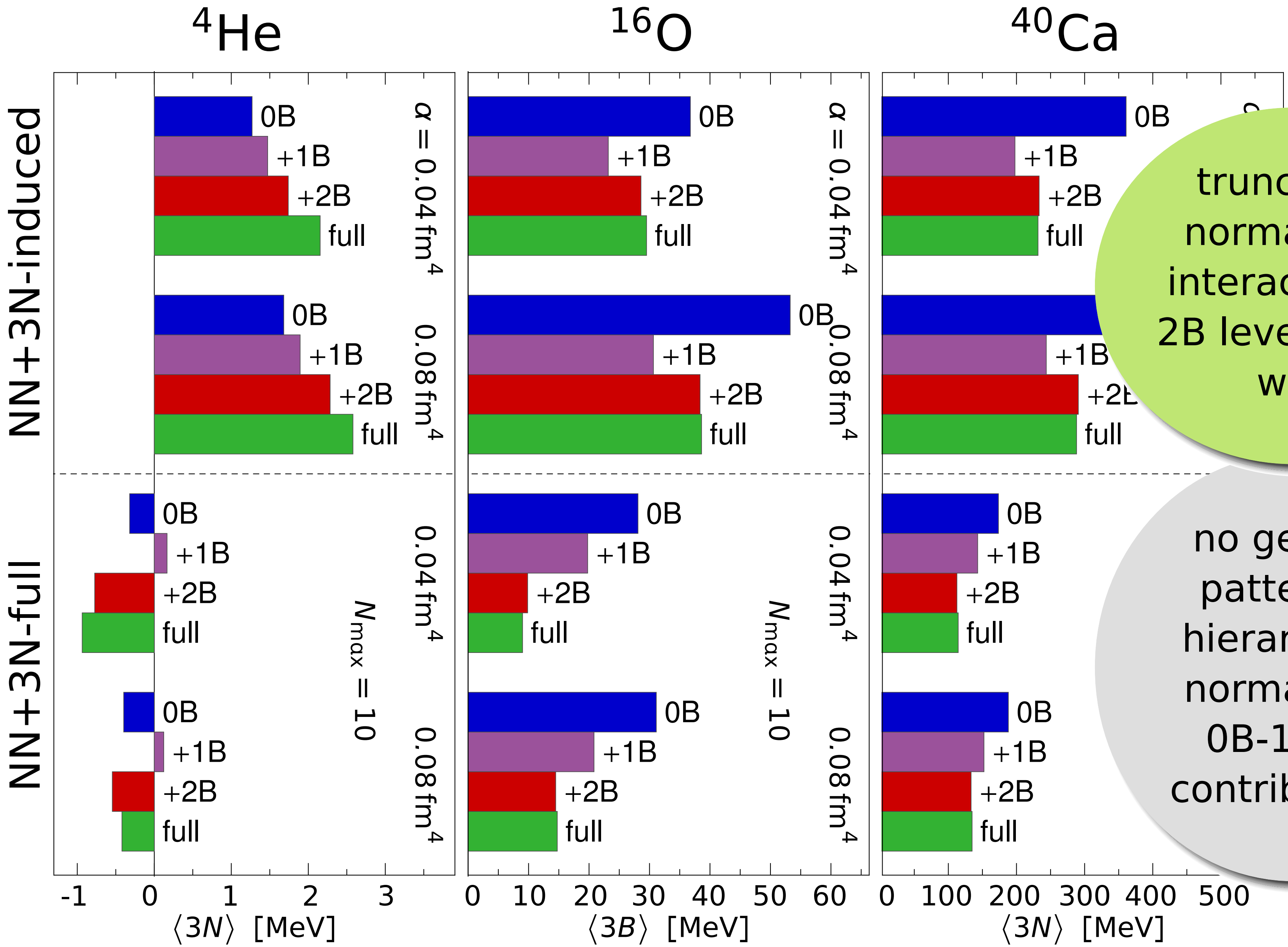


- compare IT-NCSM results with complete 3N to normal-ord. 3N truncated at the 2B level

- typical deviations up to 2% for ^{4}He and 1% for ^{16}O



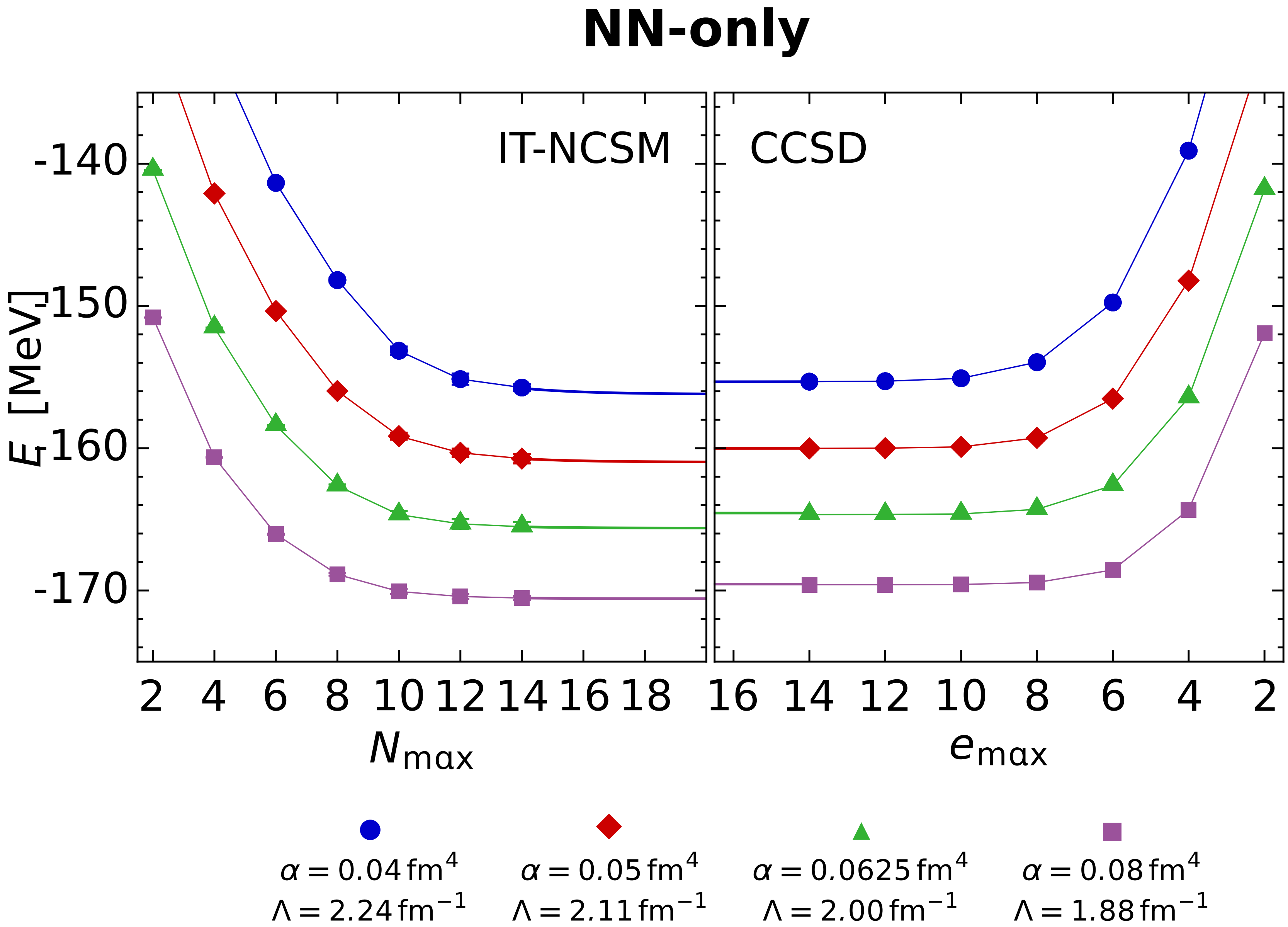
Anatomy of Normal-Ordered 3N



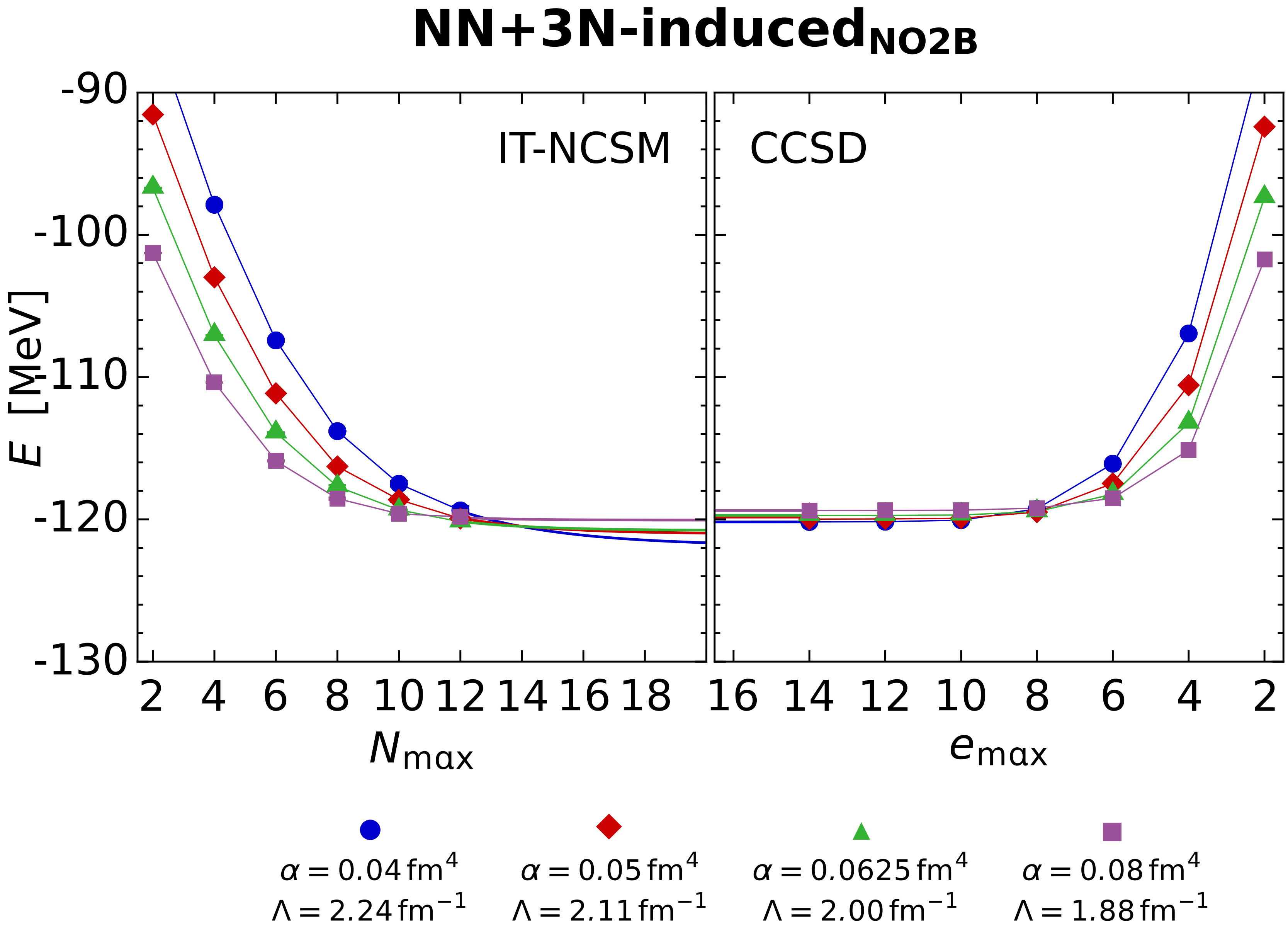
truncating normal-ord. interaction at 2B level works well

no general pattern or hierarchy in normal-ord. 0B-1B-2B contributions

^{16}O: IT-NCSM vs. Coupled-Cluster



^{16}O: IT-NCSM vs. Coupled-Cluster



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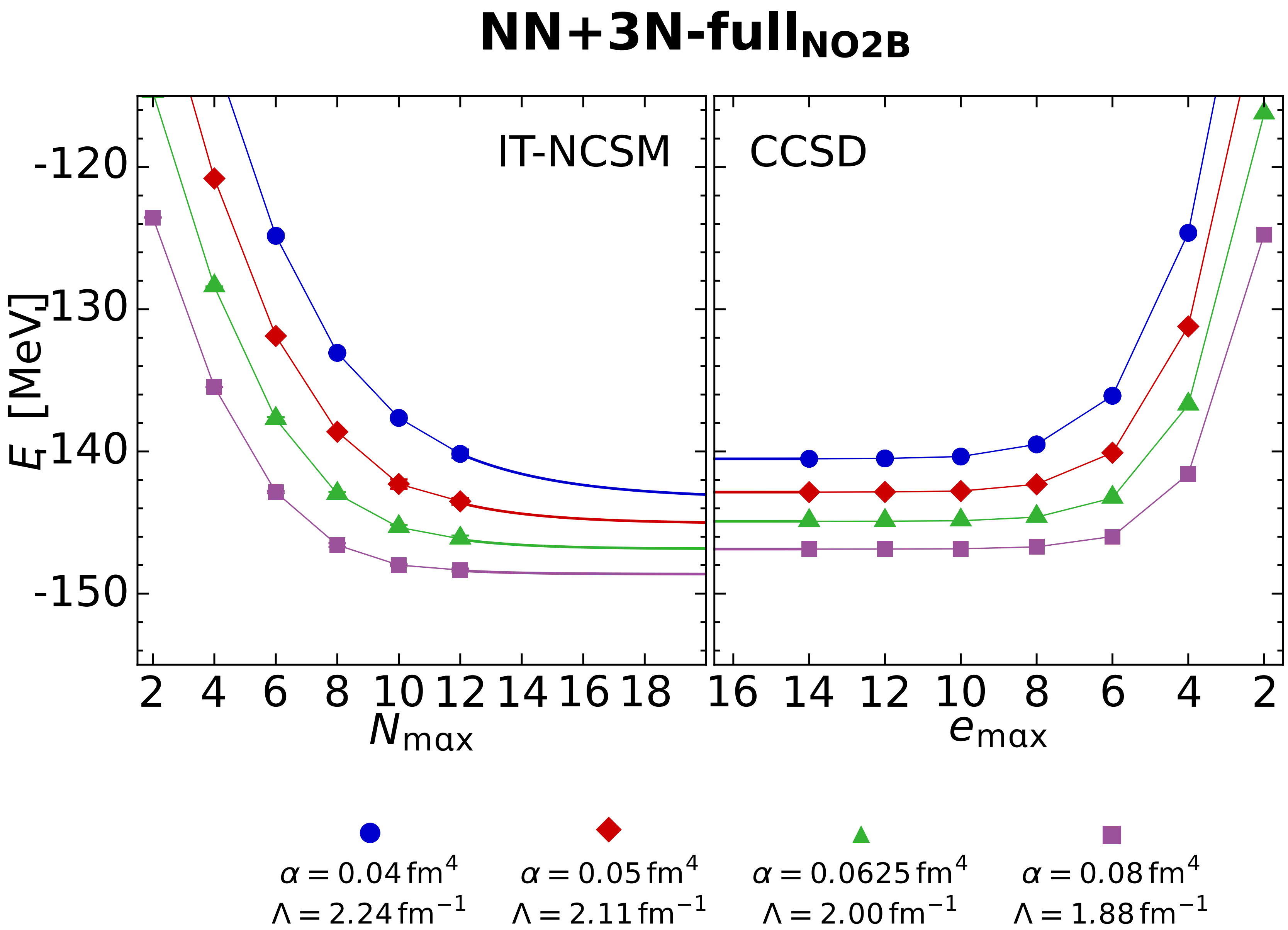
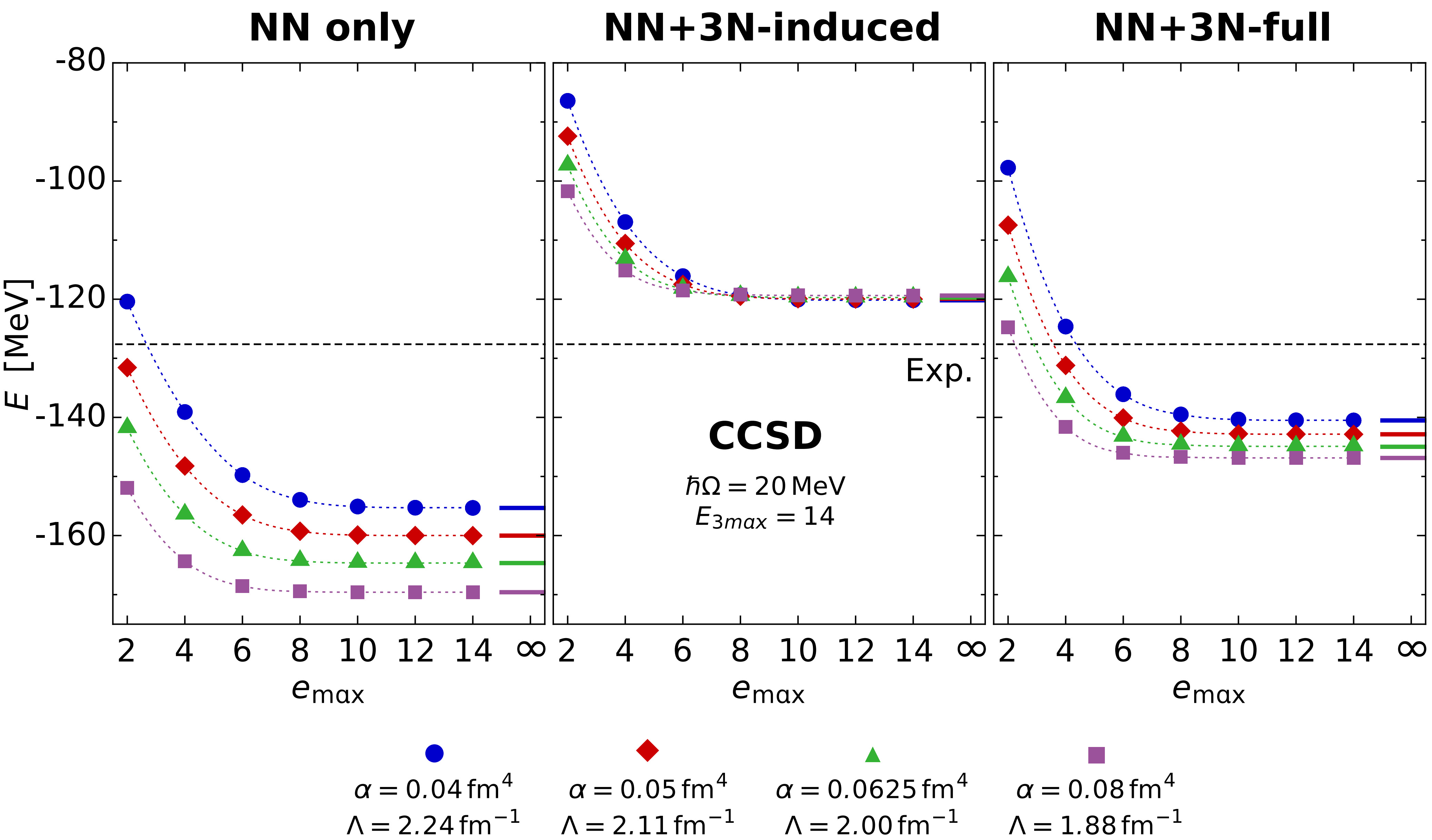


^{16}O: Coupled-Cluster with $3N_{NO2B}$



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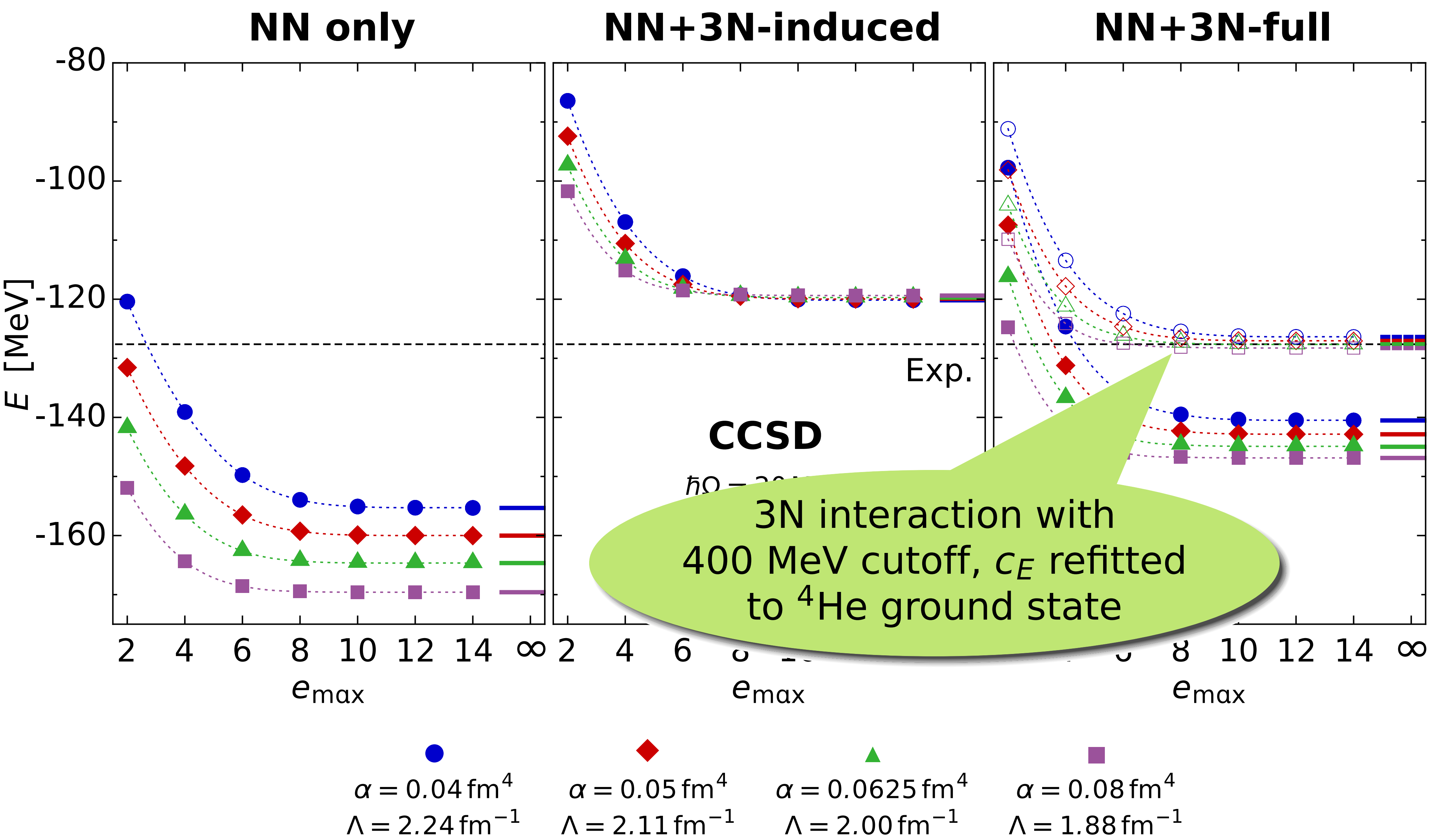
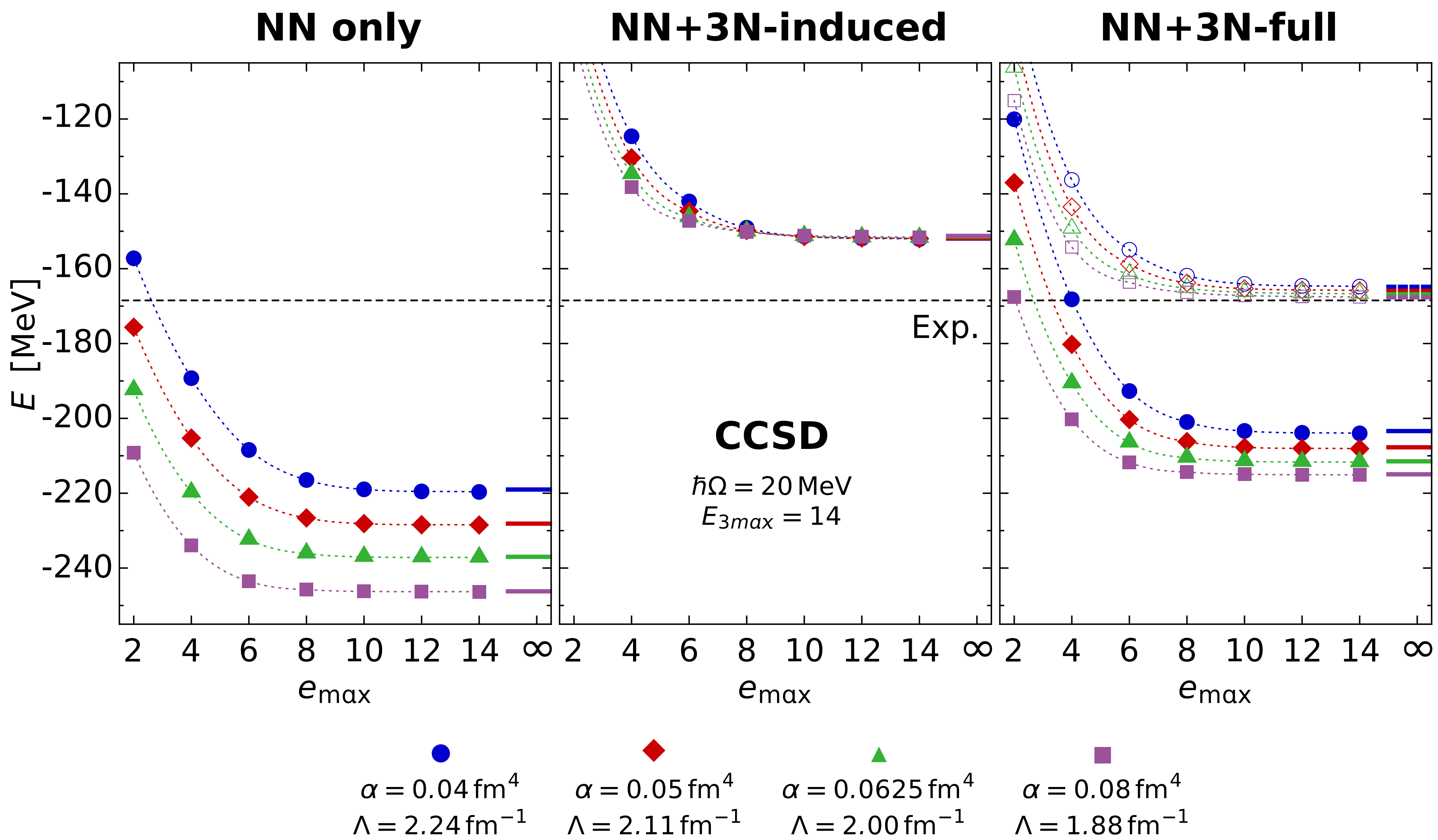
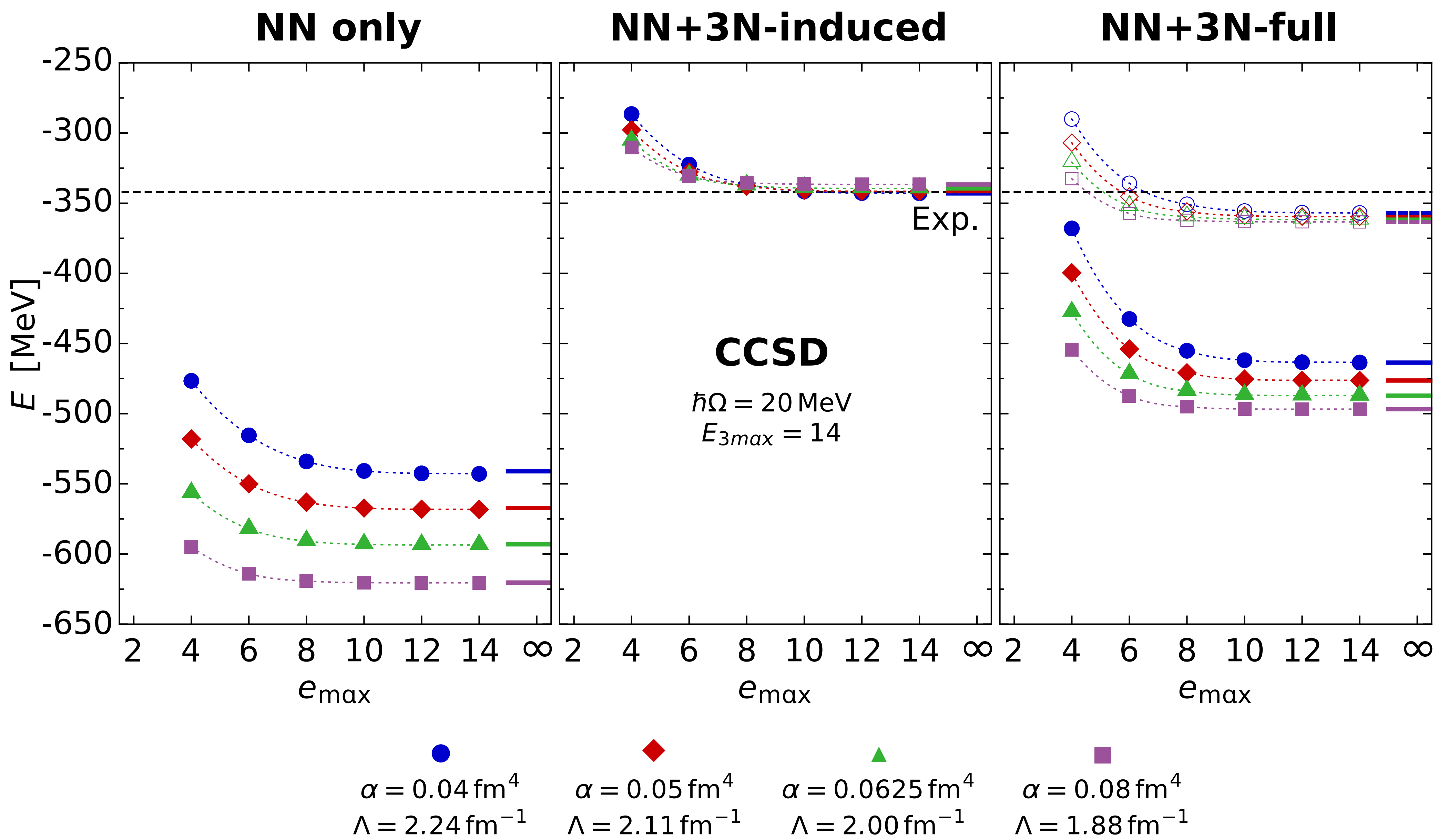


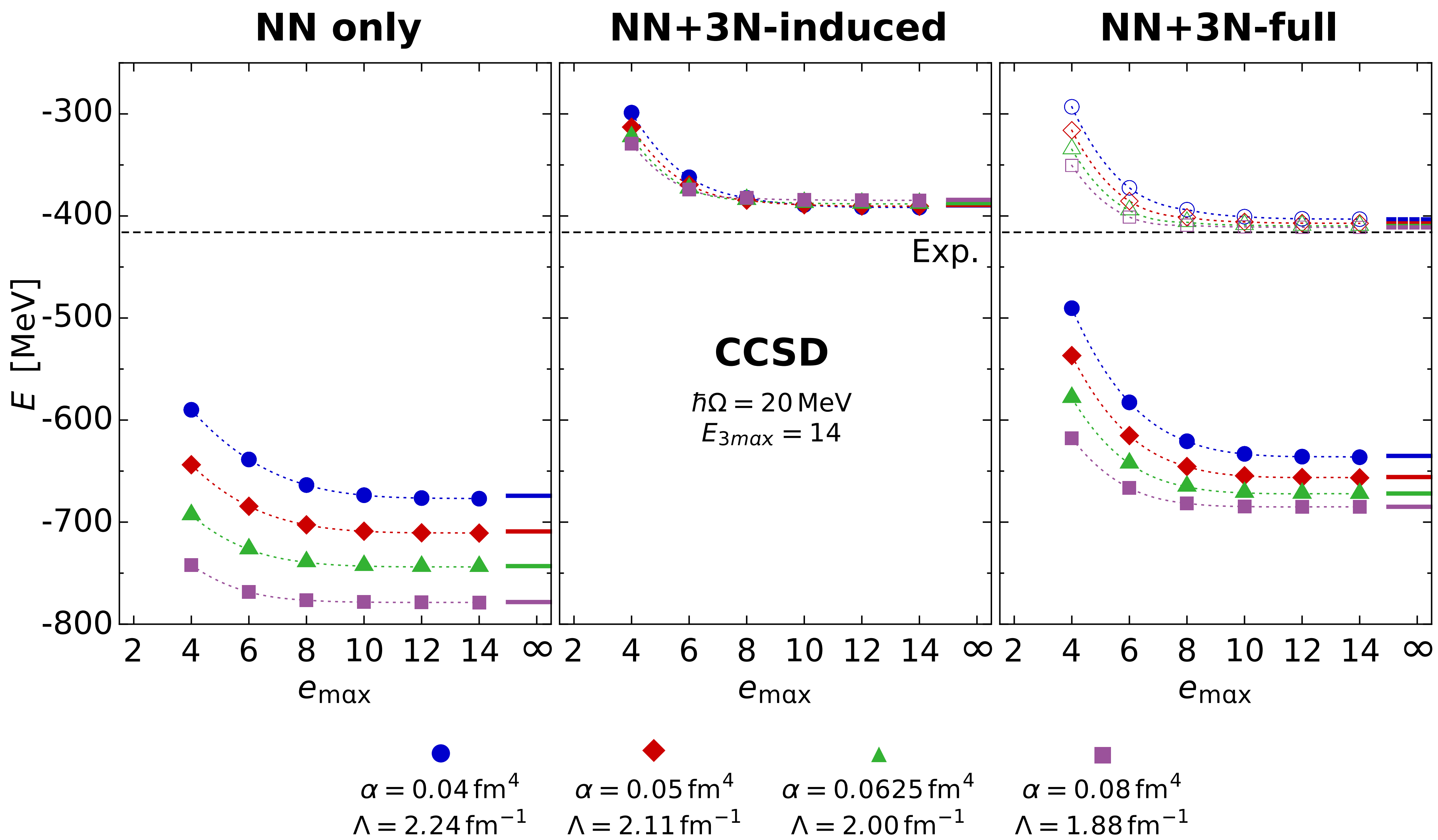
^{24}O: Coupled-Cluster with $3N_{NO2B}$



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

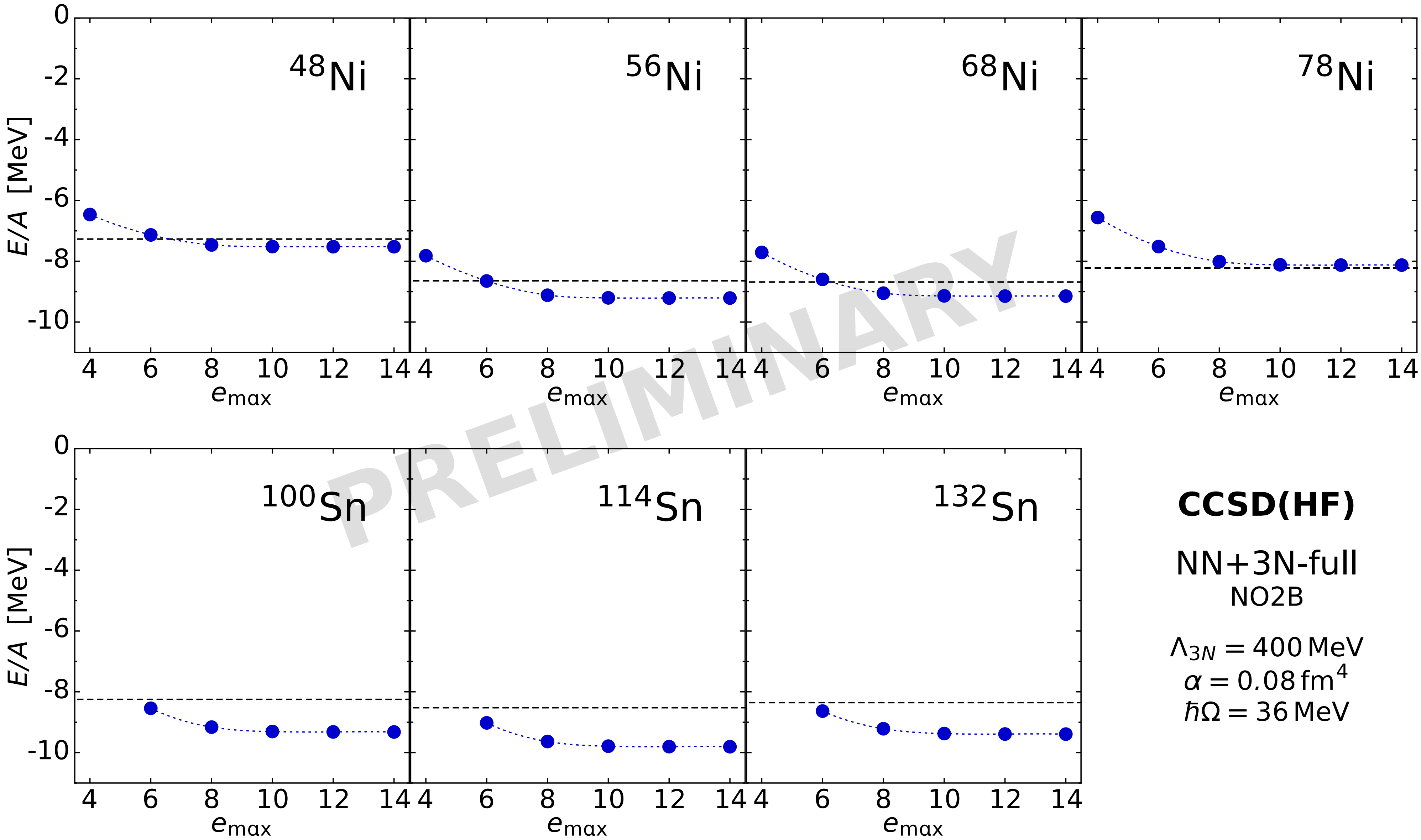


^{48}Ca: Coupled-Cluster with $3N_{NO2B}$



Outlook

Chiral 3N for Heavy Nuclei



CCSD(HF)

NN+3N-full
NO2B

$\Lambda_{3N} = 400\,\mathrm{MeV}$
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 36\,\mathrm{MeV}$

ΛCCSD(T) - Improving upon CCSD

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

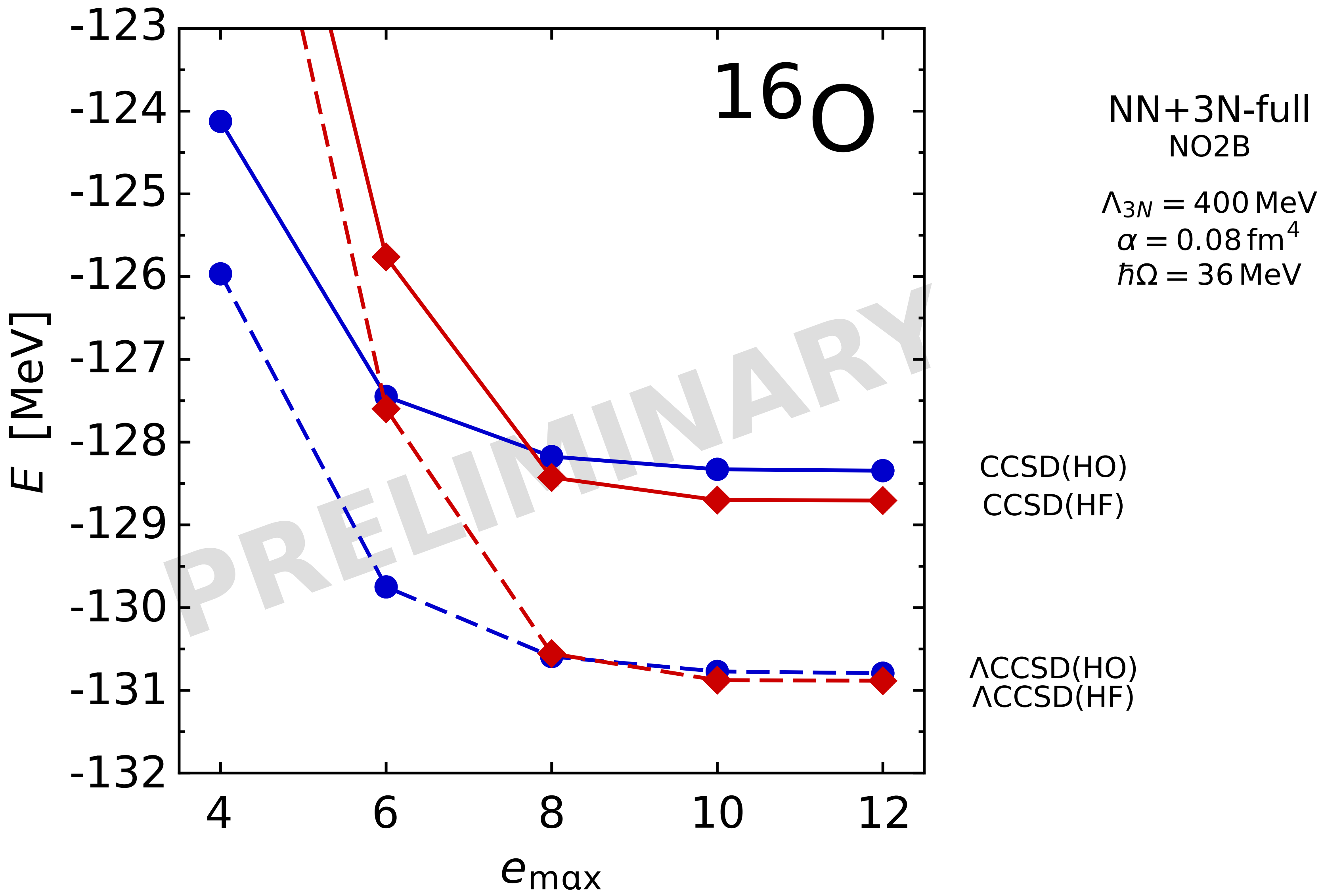
- solution of Λ equations give **a posteriori** fourth order correction to CC energy functional

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

due to triples excitations

ΛCCSD(T)

ΛCCSD(T) - Improving upon CCSD



EOMCCSD

- **excited states** : linear excitations on top of $|\Psi\rangle$

$$|\Psi_k\rangle = \hat{R}_k e^{\hat{T}} |\Phi_0\rangle$$

- EOMCCSD :

$$\hat{R}_k = (r^k)_0 + \sum_{ia} (r^k)_i^a \, \{\hat{a}_a^\dagger \hat{a}_i\} + \frac{1}{2} \sum_{ijab} (r^k)_{ij}^{ab} \, \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\}$$

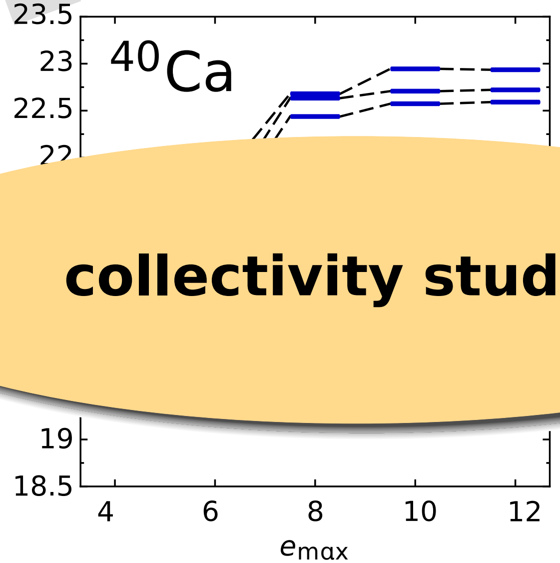
- non-Hermitian EVP : $\left(\hat{\mathcal{H}} \hat{R}_k\right)_C |\Phi_0\rangle = \omega_k \hat{R}_k |\Phi_0\rangle$

$J^\pi = 2^+$

EOMCCSD(HF)

NN+3N-full
NO2B

$\Lambda_{3N} = 400\,\mathrm{MeV}$
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 32\,\mathrm{MeV}$



collectivity studies

Epilogue

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LOEWE-CSC — CSC Center for Scientific Computing Frankfurt
HOPPER — NERSC

COMPUTING TIME

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Deutsche Forschungsgemeinschaft
DFG
HIC for FAIR
Helmholtz International Center
LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz
HELMHOLTZ GEMEINSCHAFT
Bundesministerium für Bildung und Forschung