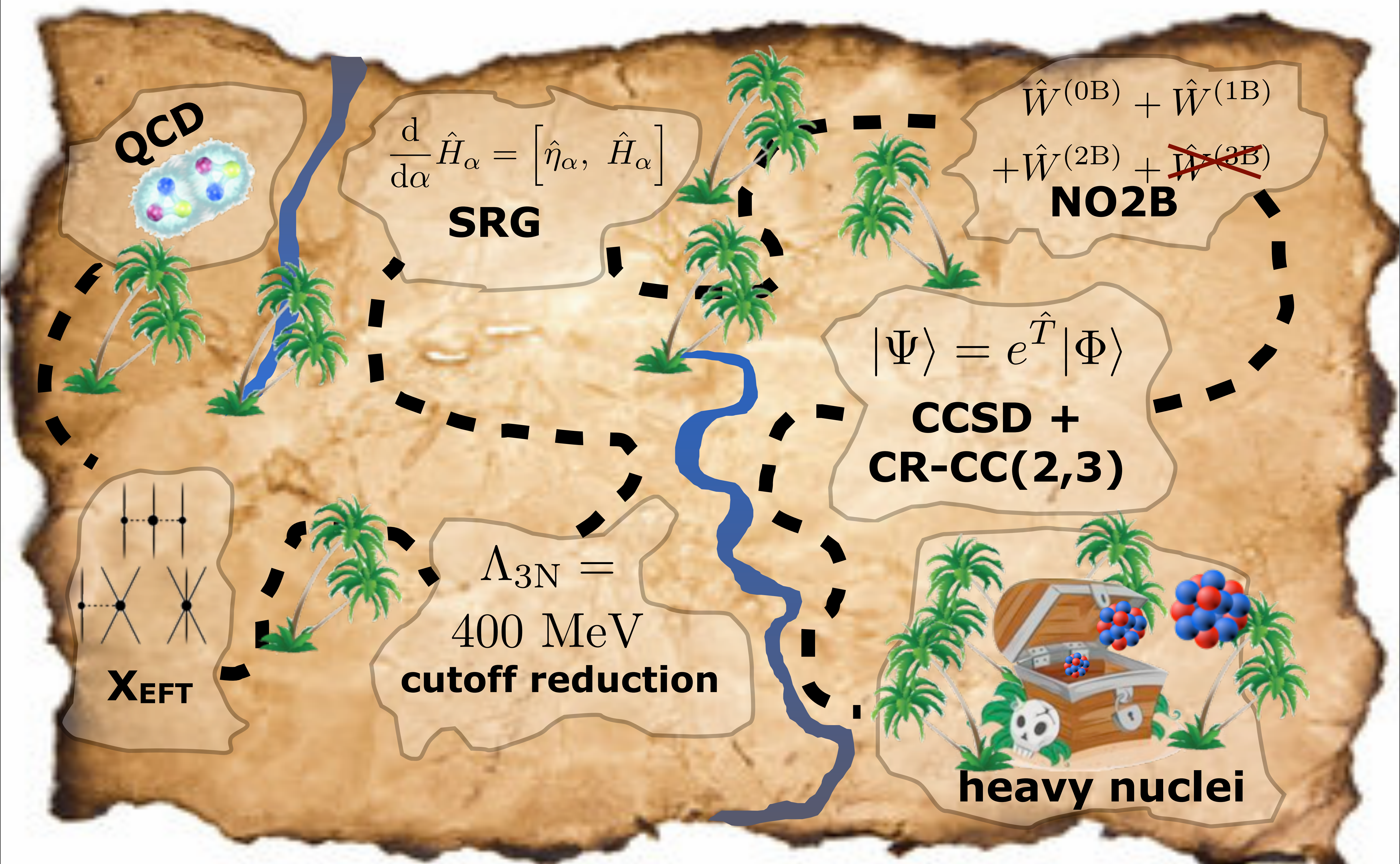
Heavy Nuclei *Ab Initio*

Sven Binder

INSTITUT FÜR KERNPHYSIK

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Path to Heavy Nuclei



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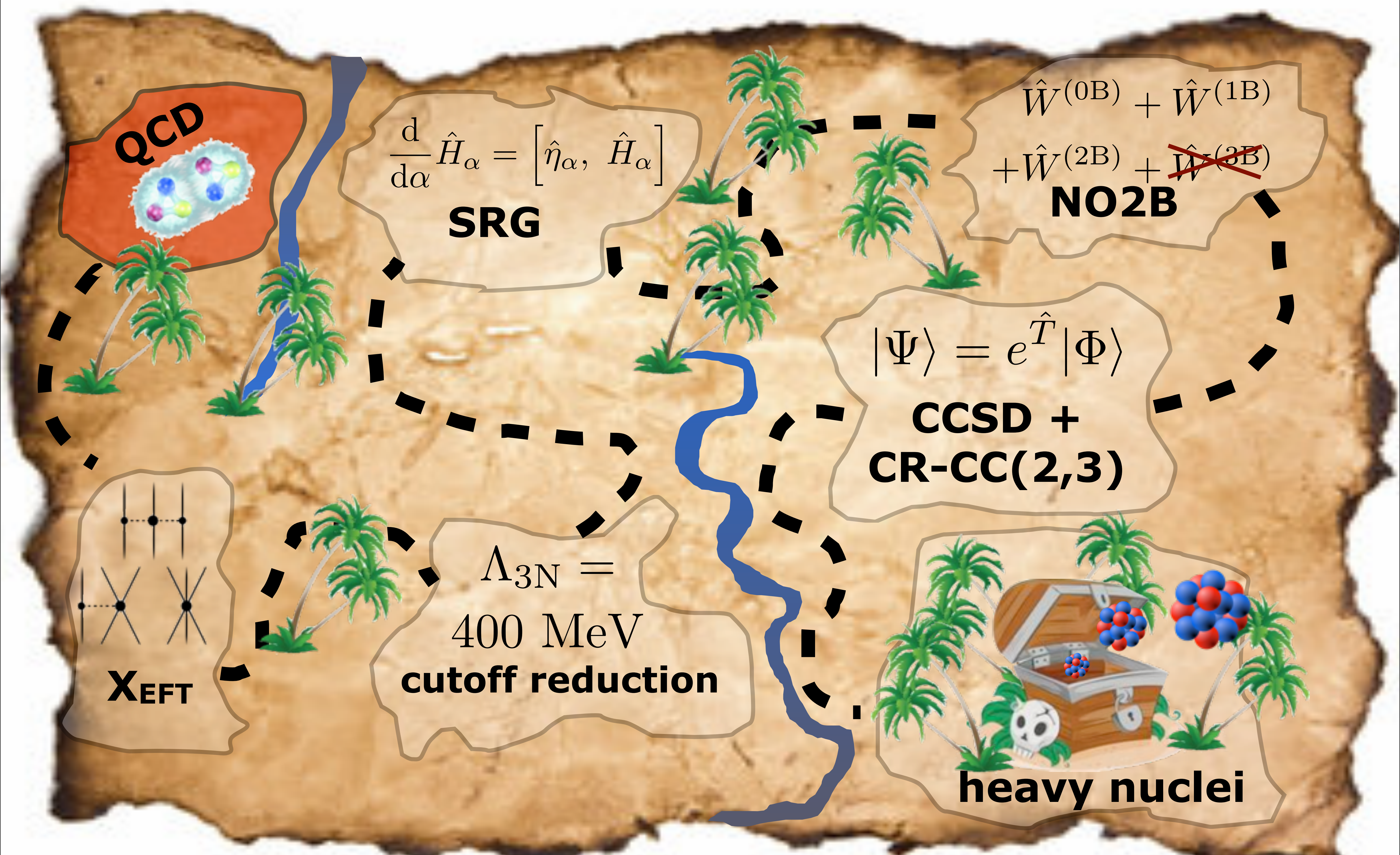

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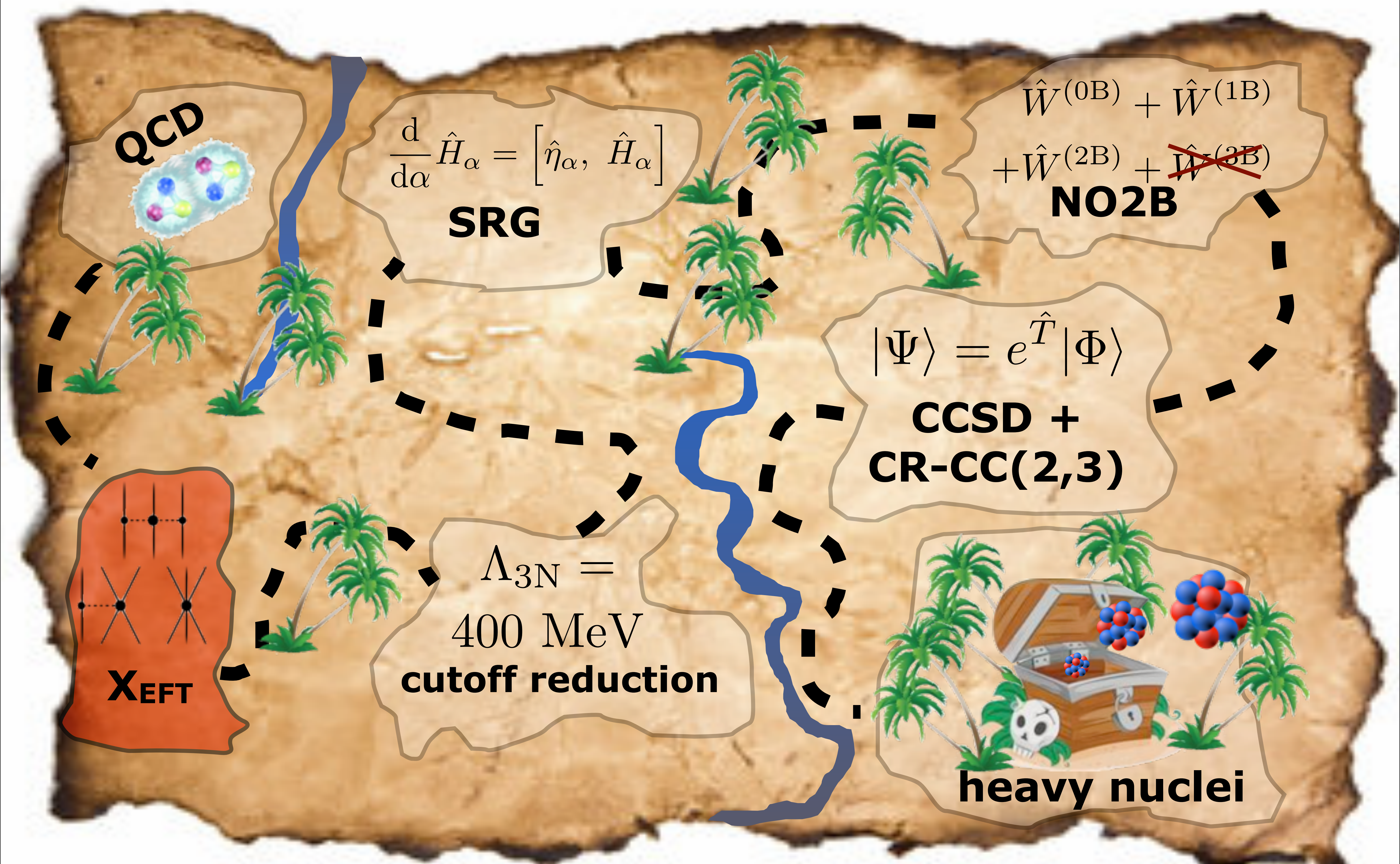

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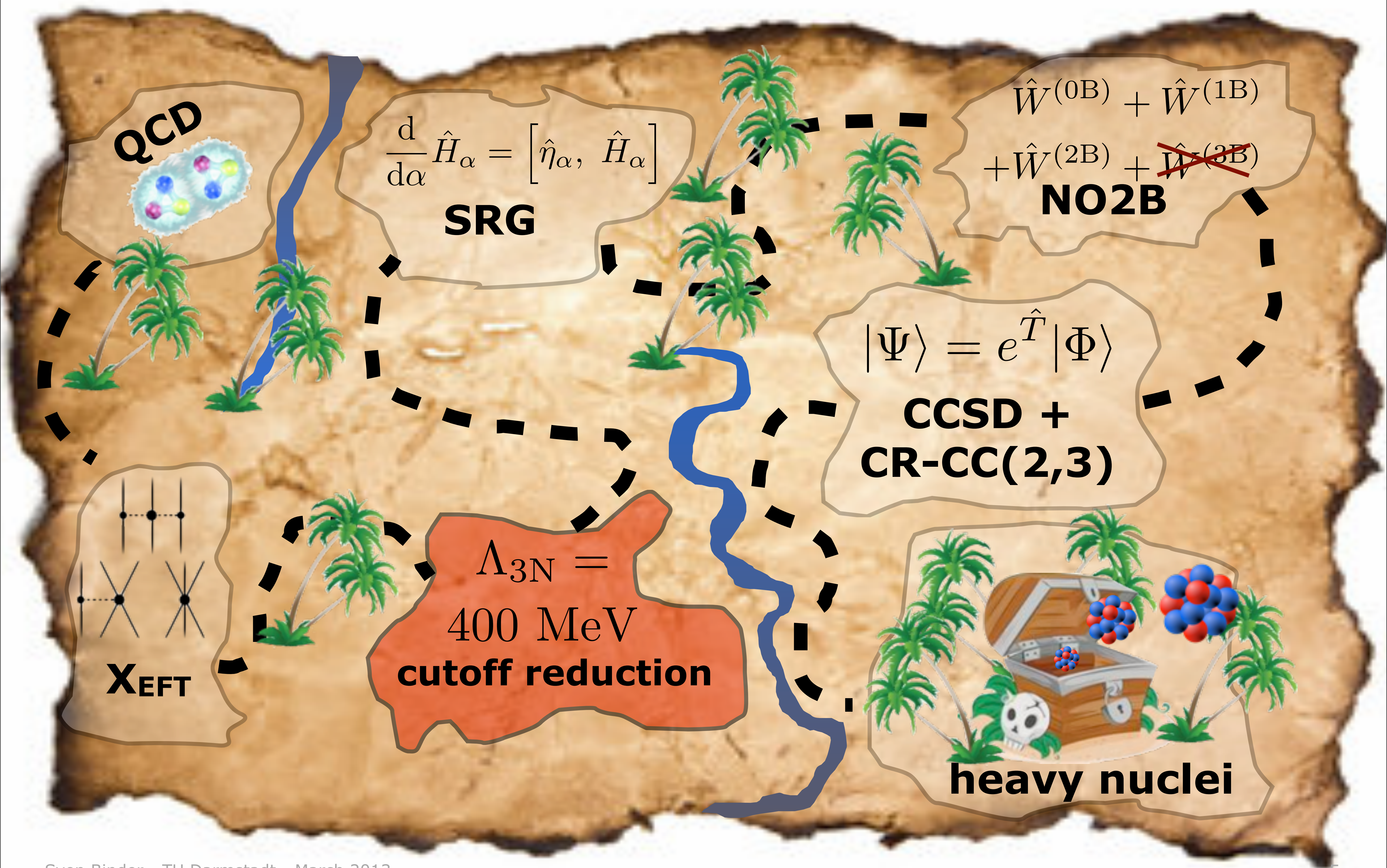

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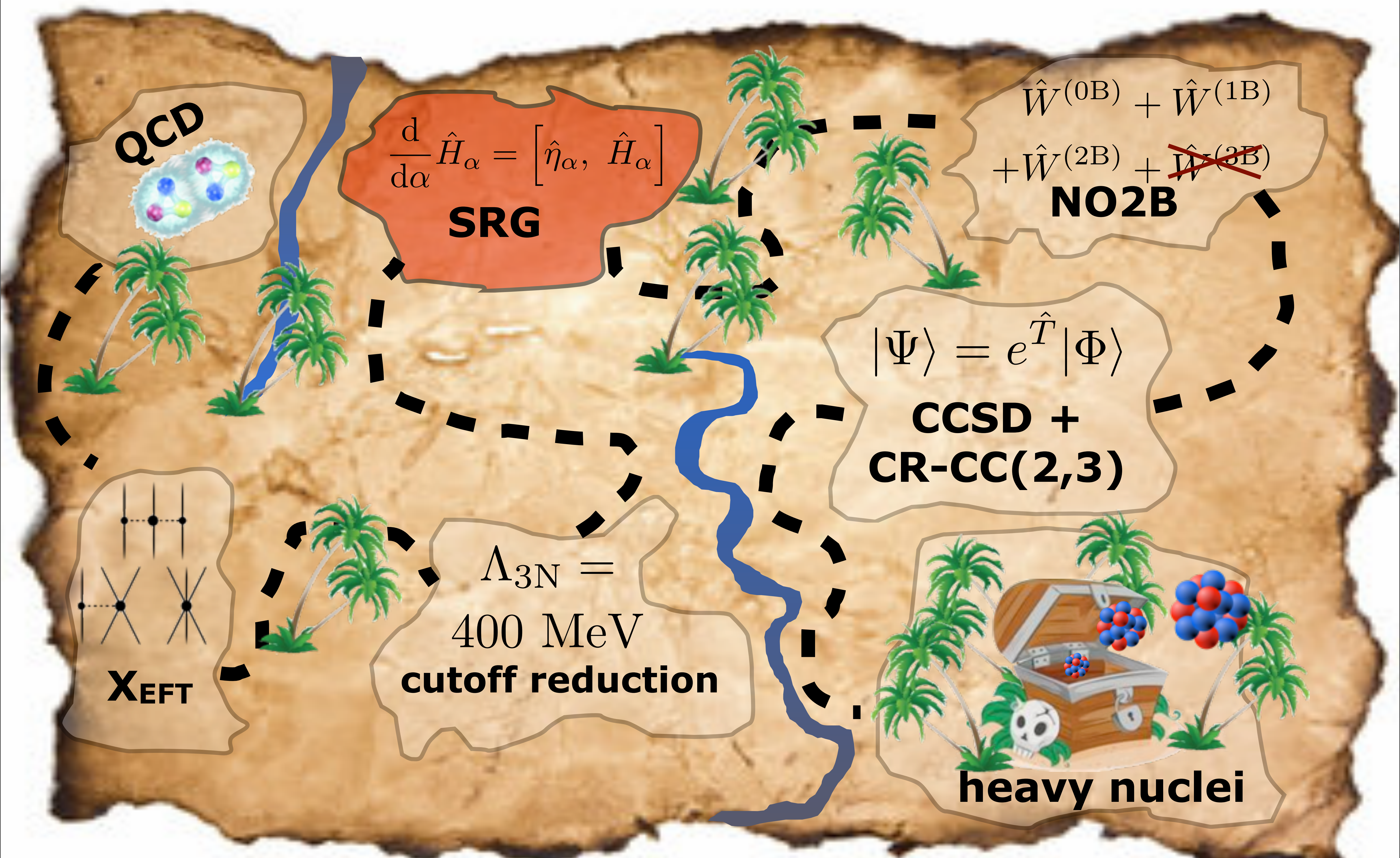

Wednesday, February 19, 14

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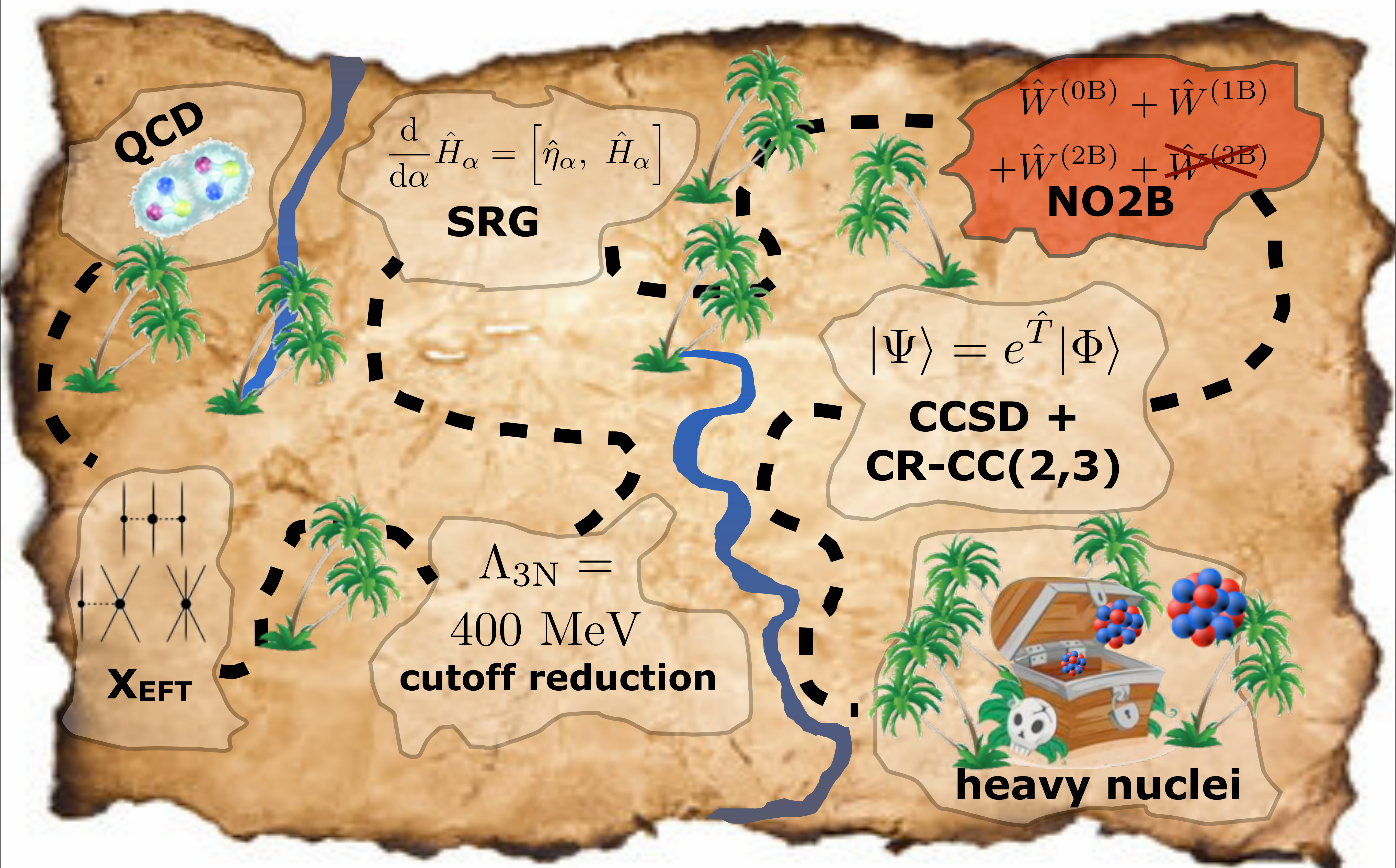

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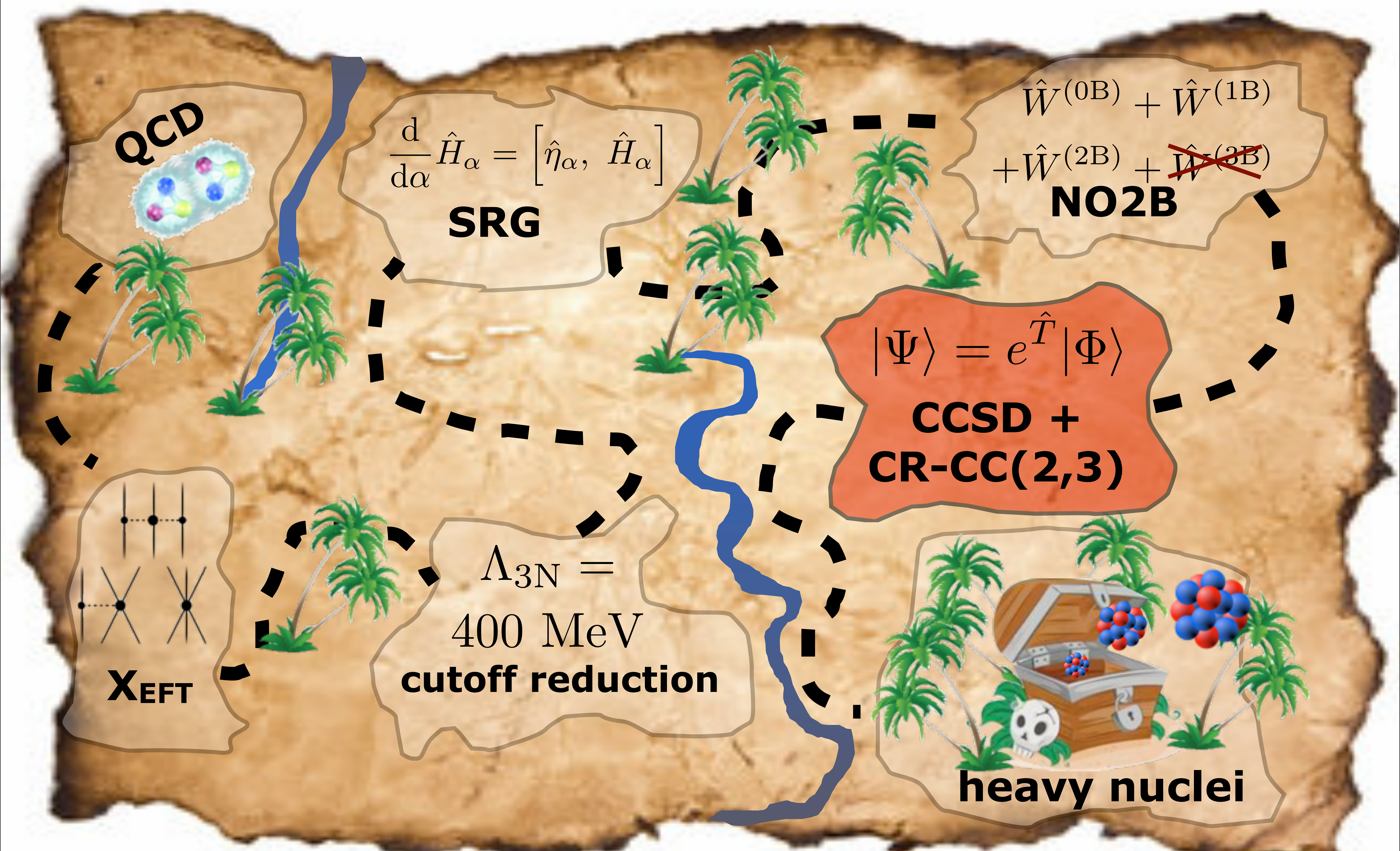

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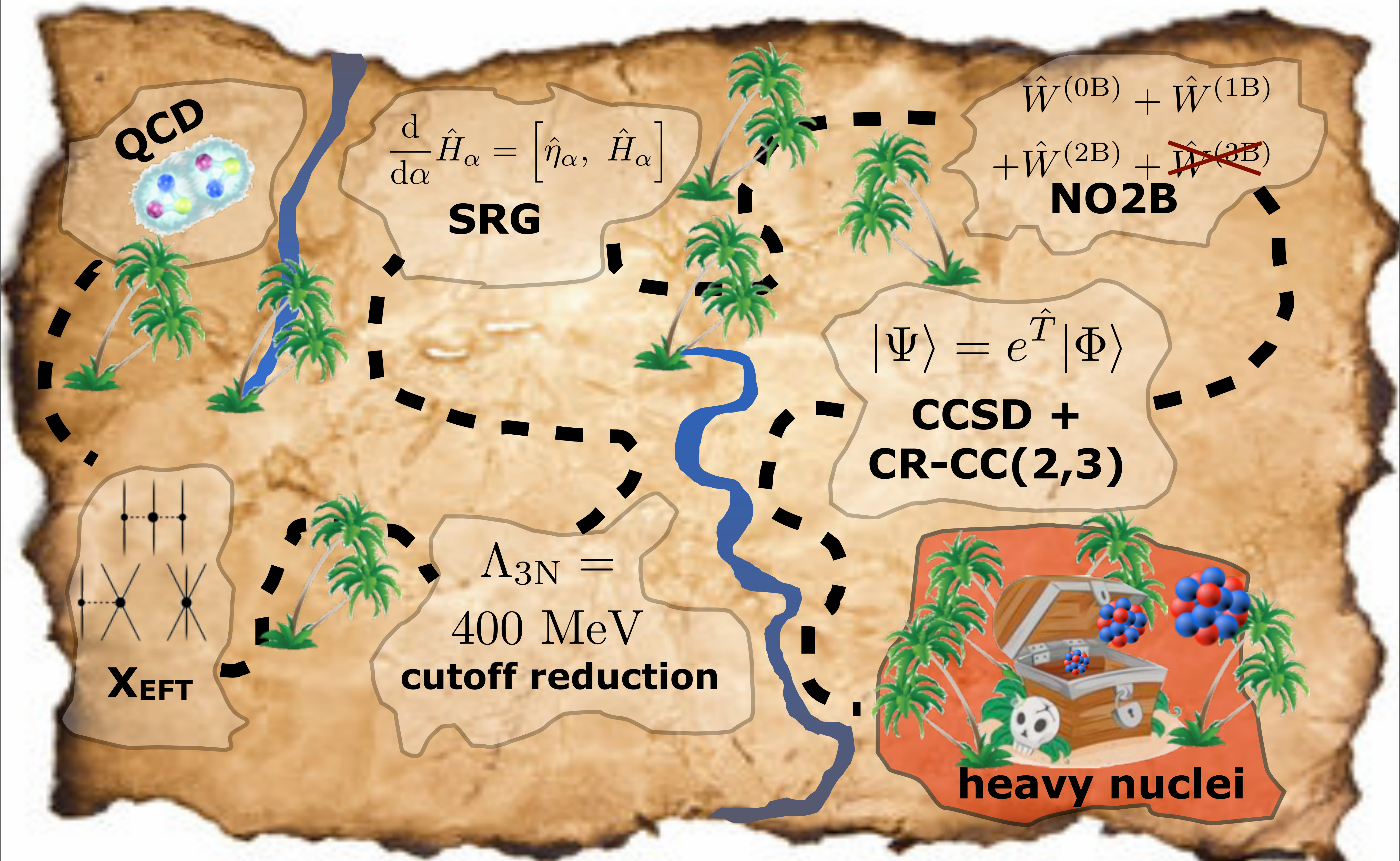
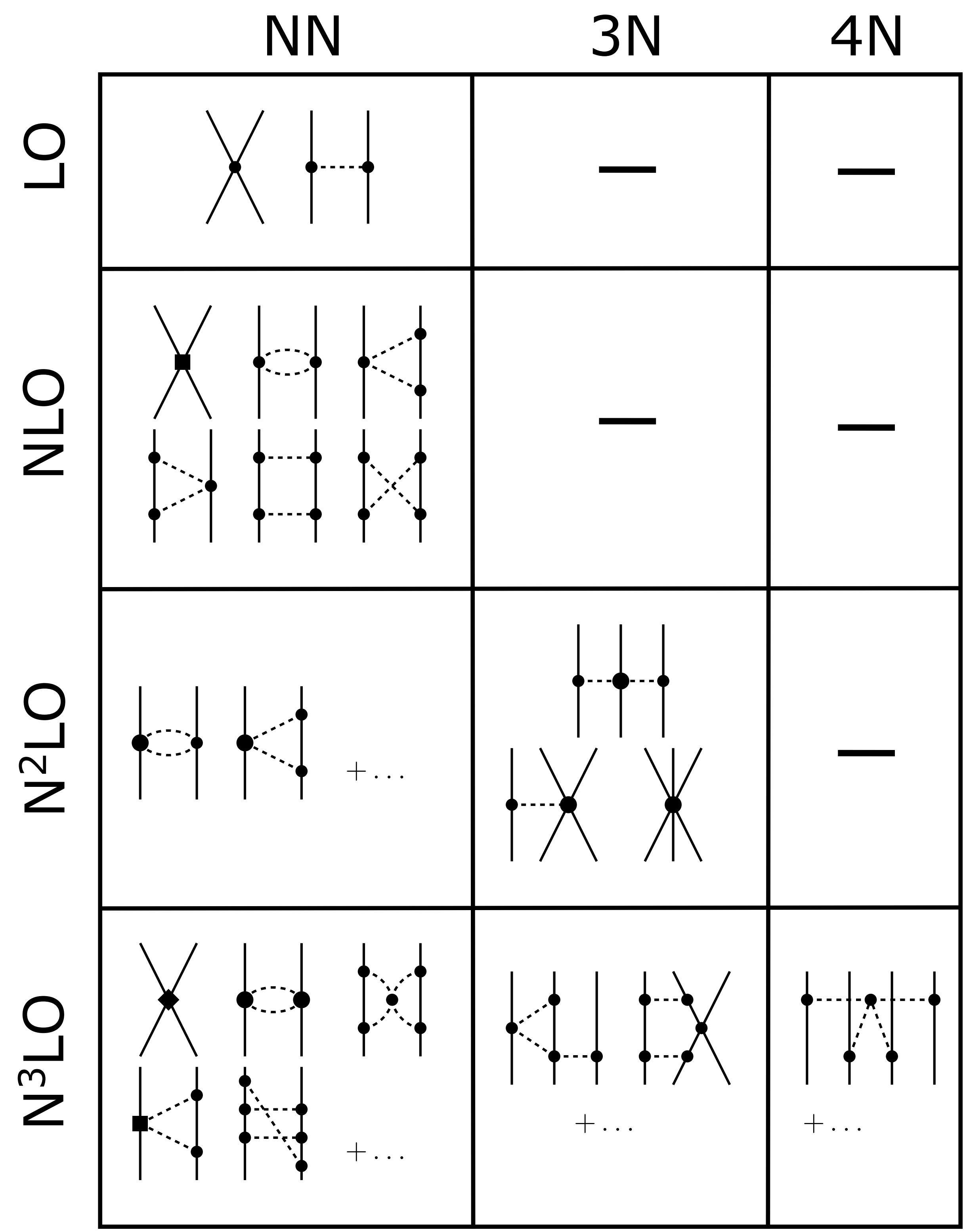


Nuclear Interactions from Chiral EFT



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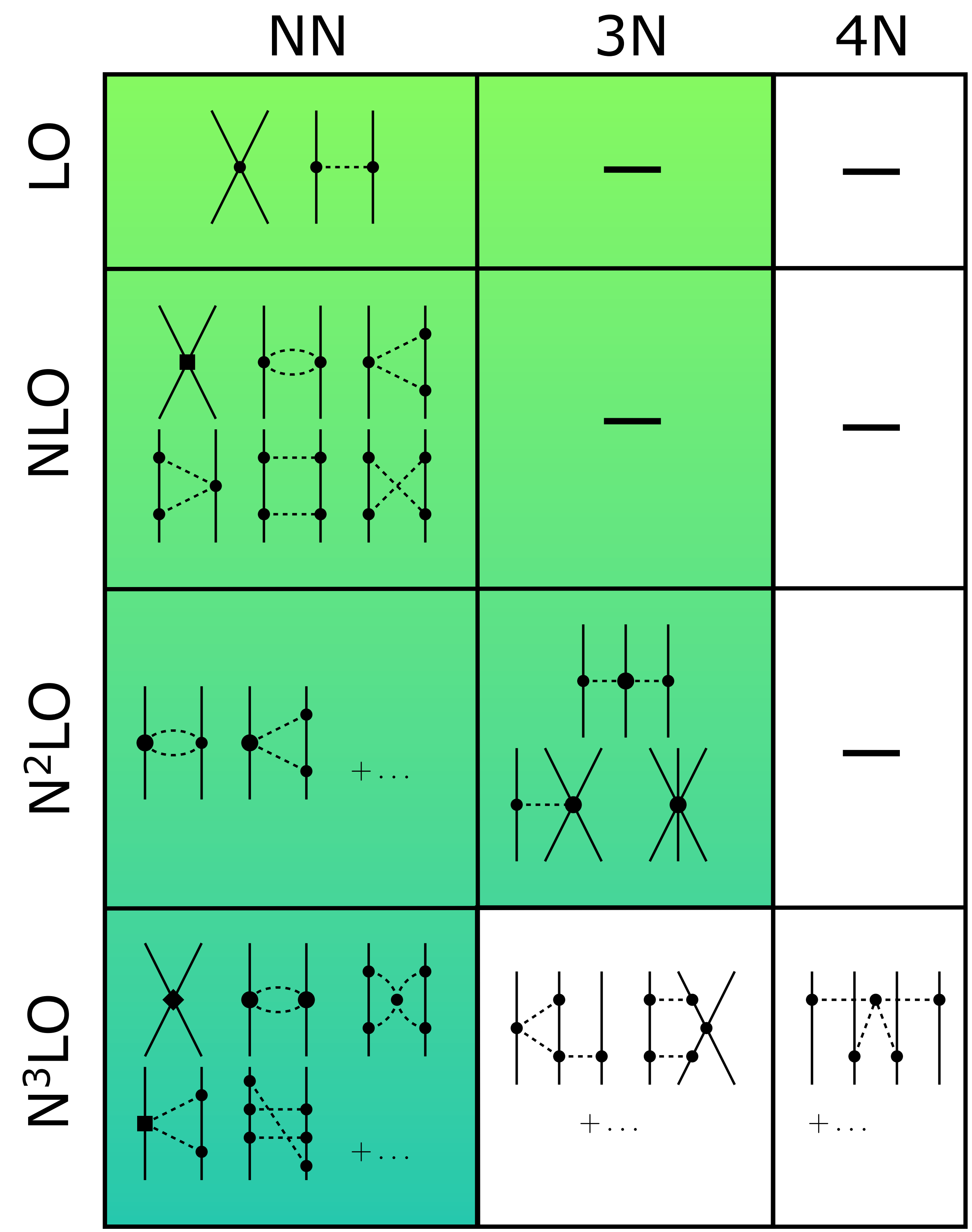

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NN interaction

- **N³LO**: Entem and Machleidt, Λ_{NN} = 500 MeV
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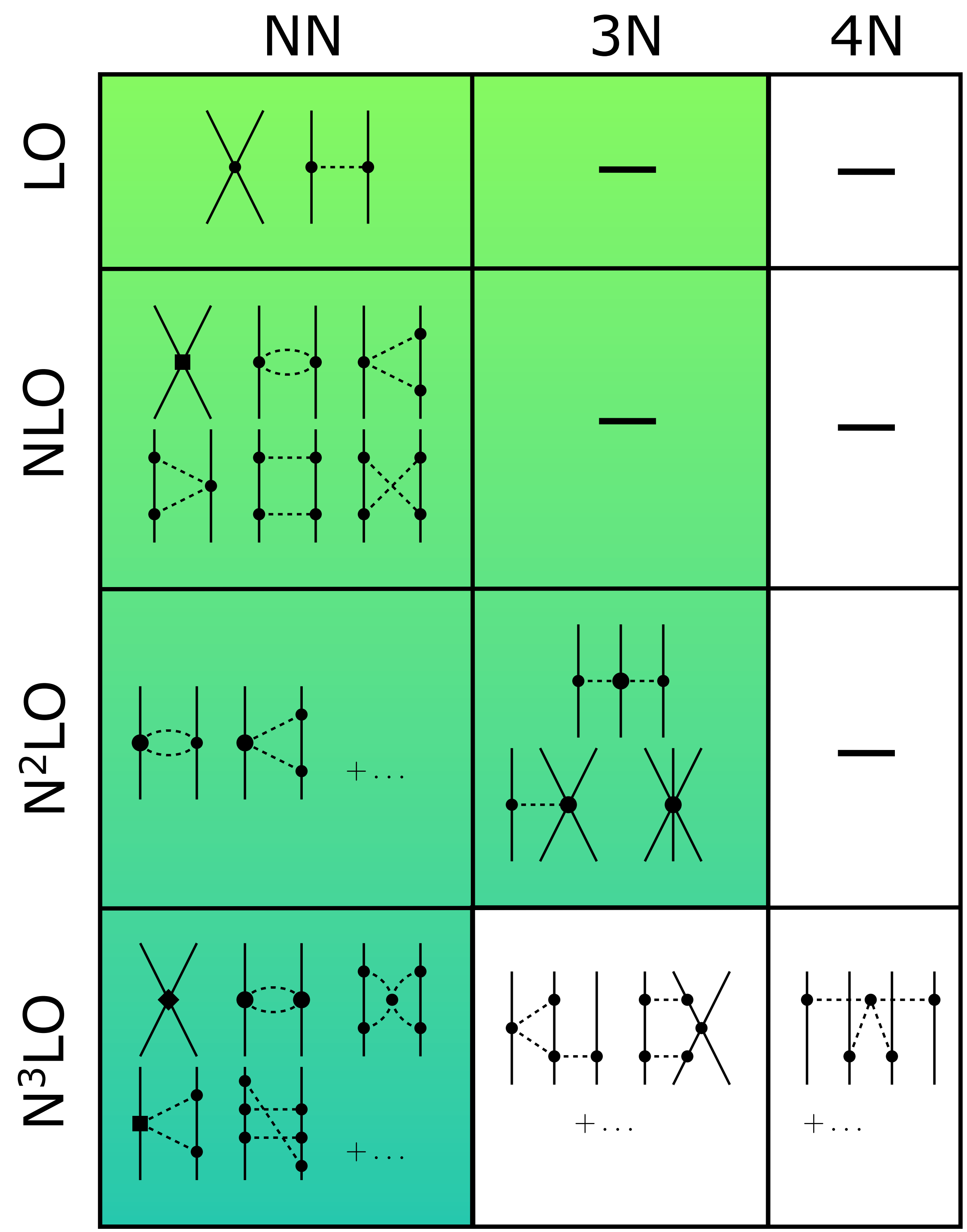

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3N interaction

- **N^2LO**: Navrátil
  - Λ_{3N} = 500 MeV, ^3H fit
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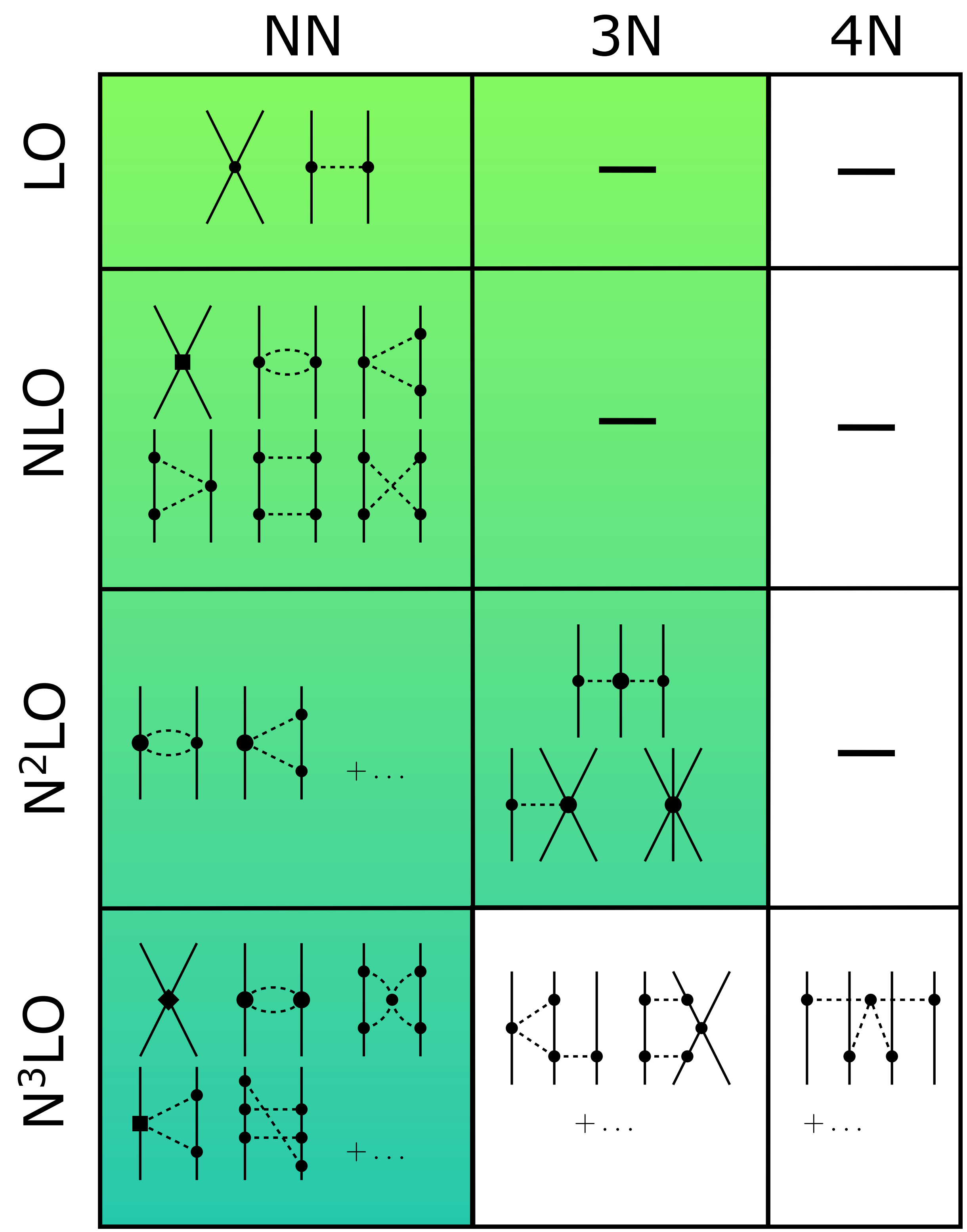

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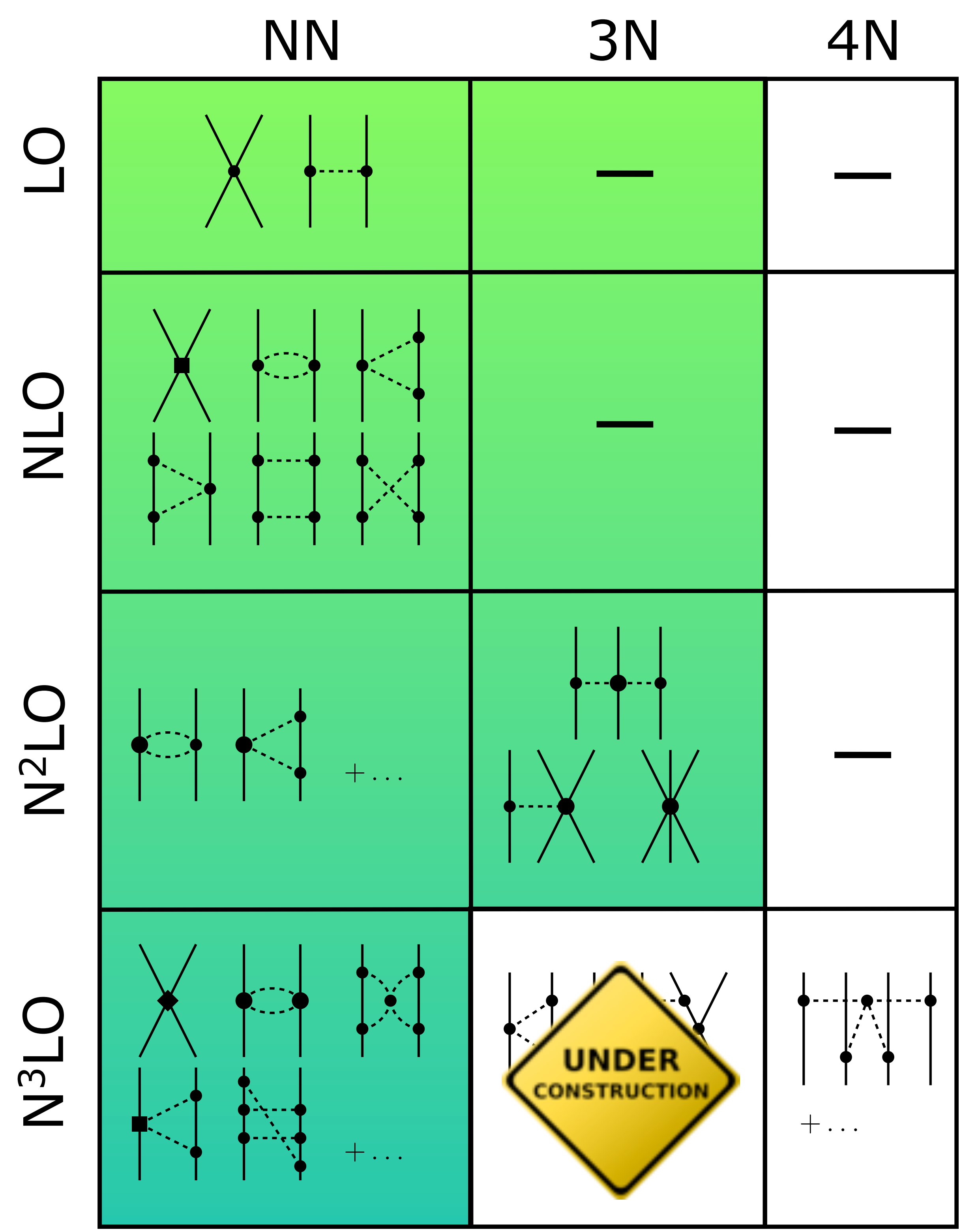

Coupled-Cluster Method

G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D.J. Dean --- arXiv:1312.7872 [nucl-th] (2013)

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

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- **exponential Ansatz** for wave operator

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

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

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

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- **similarity-transformed** Schroedinger equation

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

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

Singles and Doubles Excitations: CCSD

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

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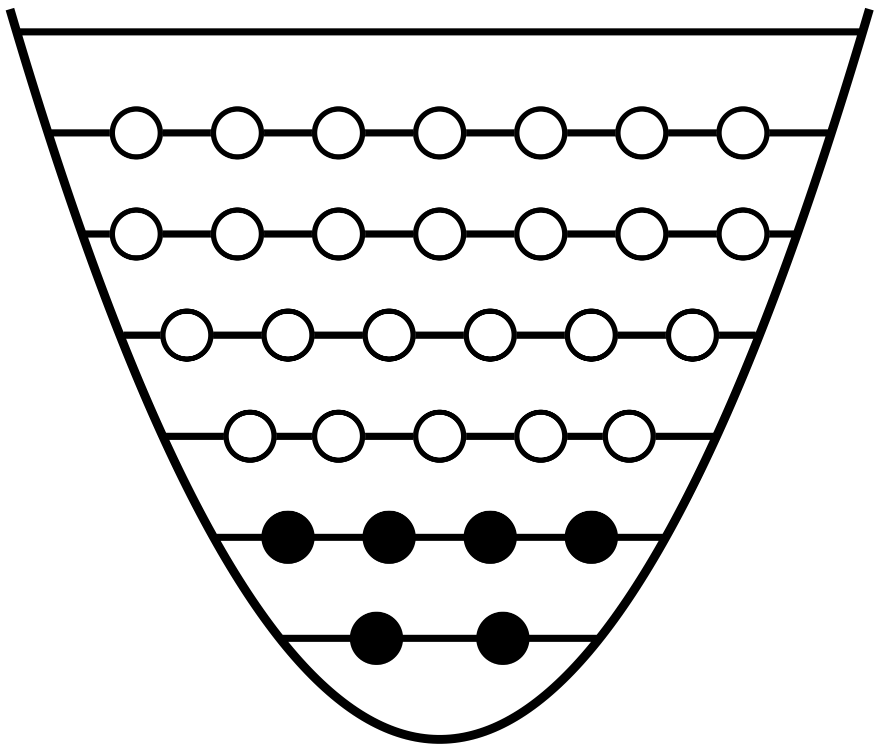

$|\Phi_0\rangle$

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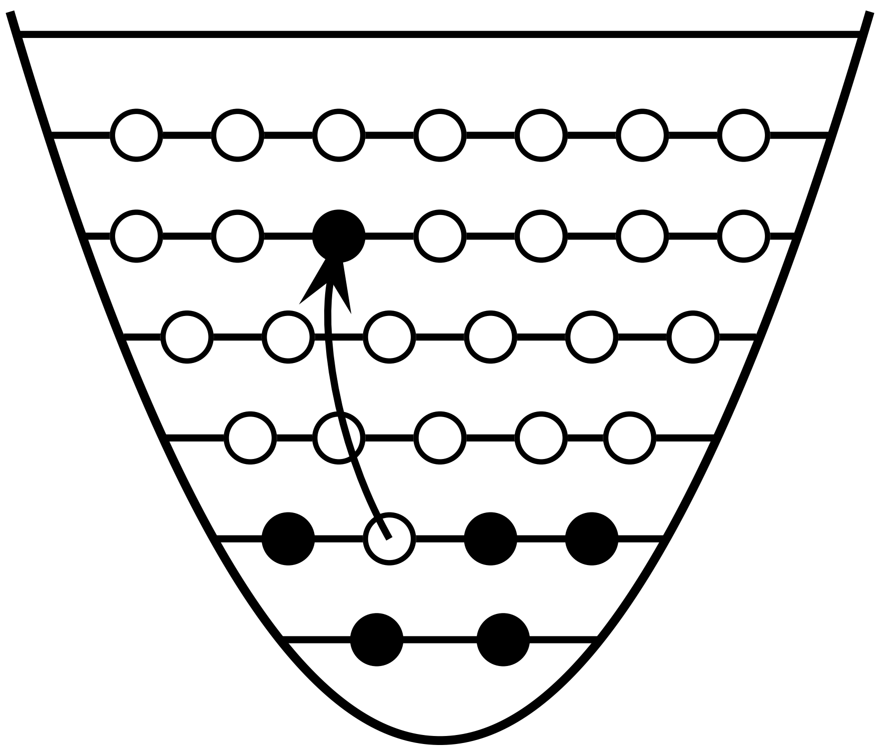

$\hat{T}_1 \, |\Phi_0\rangle$

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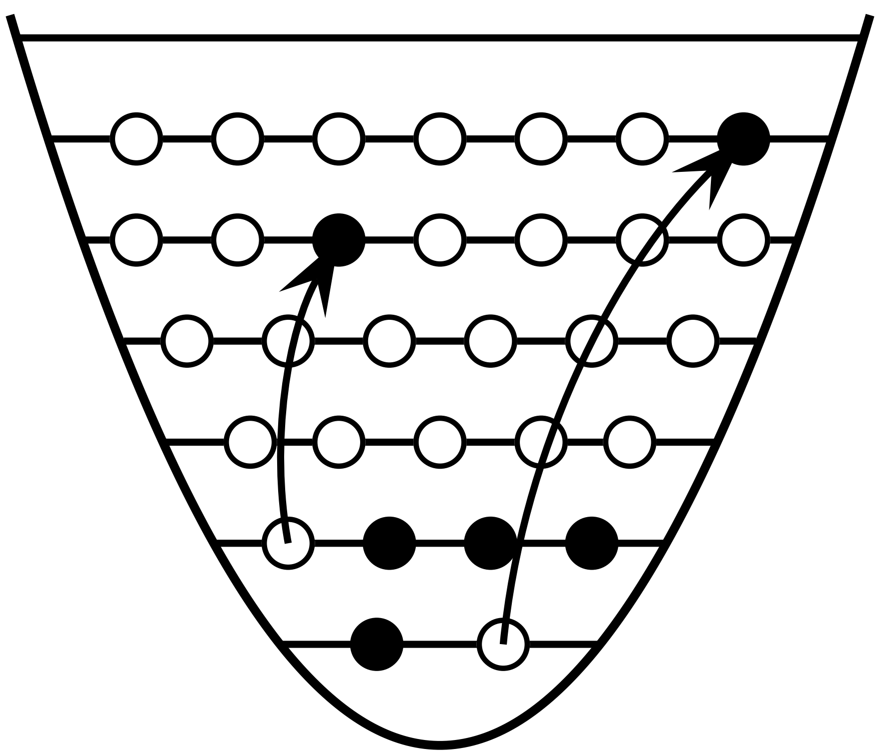

$$\hat{T}_2 \, |\Phi_0\rangle$$

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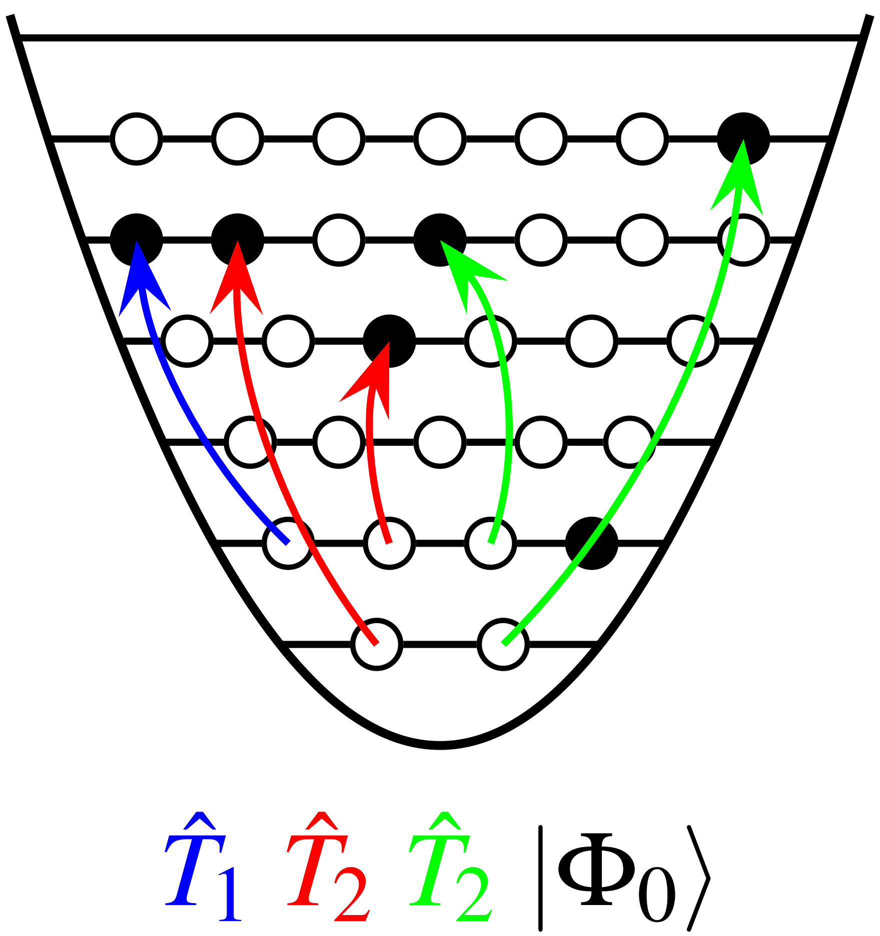

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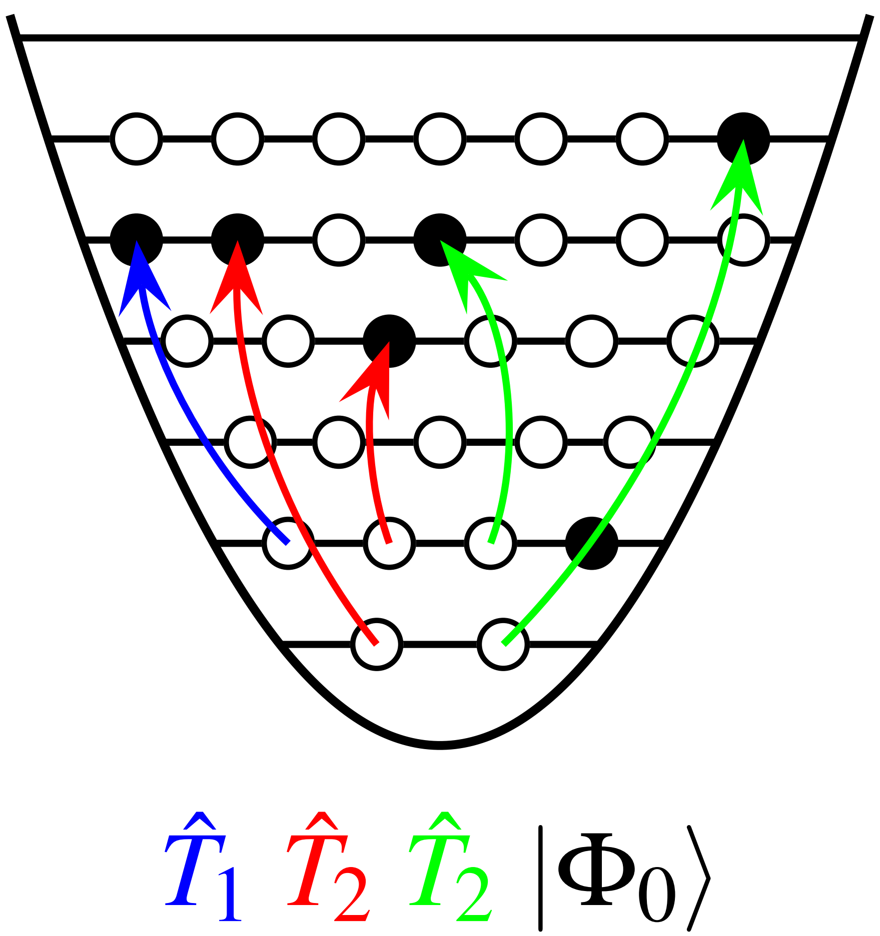

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- CCSD equations

$$
\begin{aligned}
\Delta E^{(\mathrm{CCSD})} &= \langle \Phi_0 | \hat{\mathcal{H}} | \Phi_0 \rangle \\
0 &= \langle \Phi_i^a | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall \ a, i \\
0 &= \langle \Phi_{ij}^{ab} | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall \ a, b, i, j
\end{aligned}
$$

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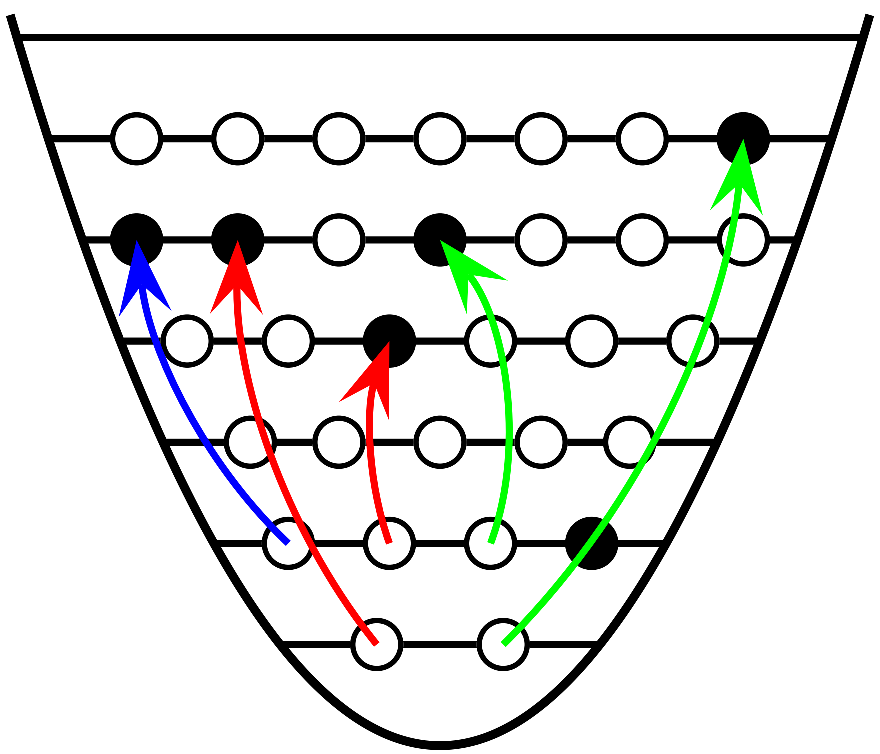

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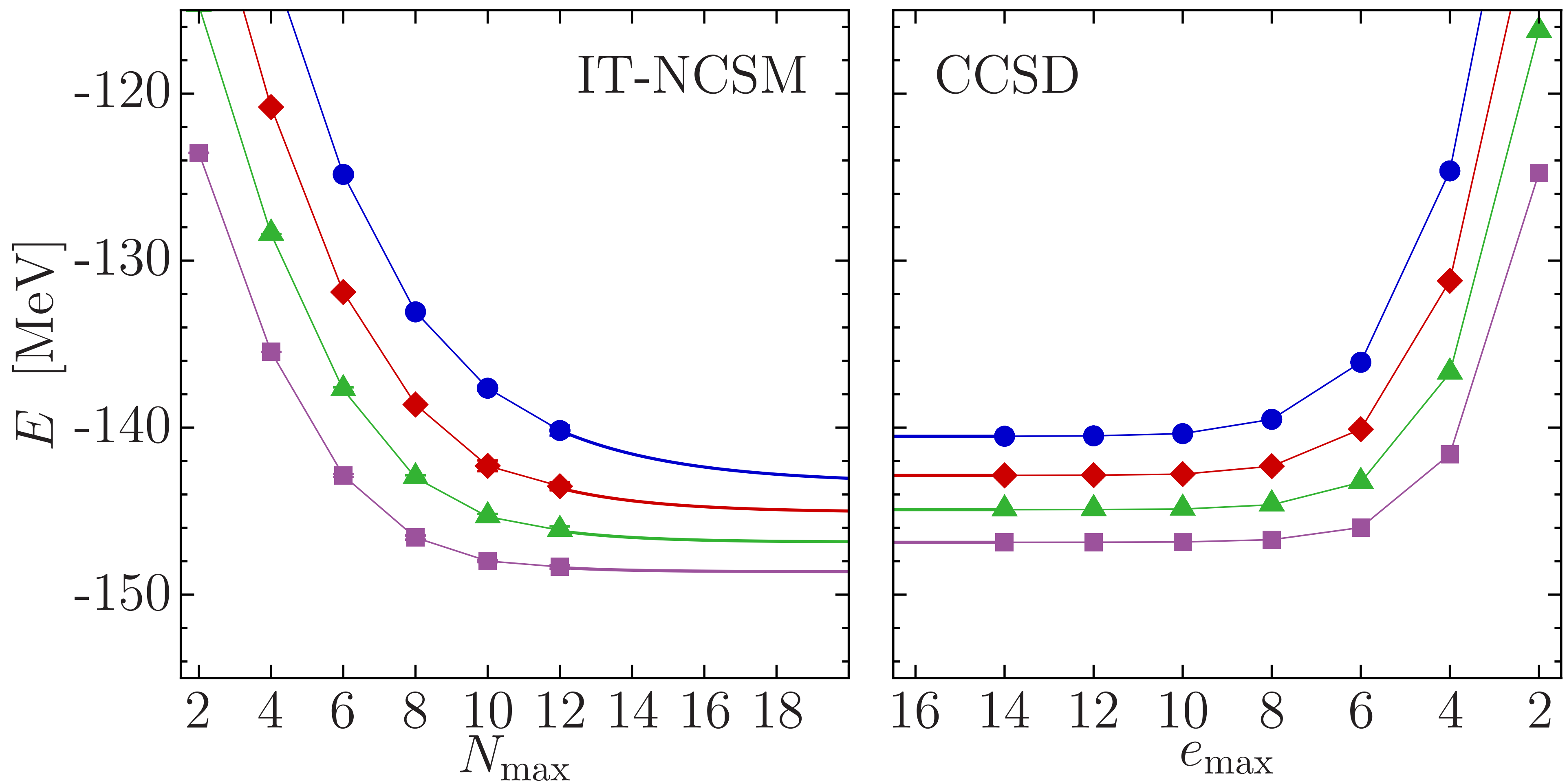
$$0 = \langle \Phi_{ij}^{ab} | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall \ a, b, i, j$$

- Coupled system of **nonlinear equations**

^{16}O: IT–NCSM vs. CCSD

NN+3N-full (HO)
Λ_{3N} = 500 MeV



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

Reduced-Cutoff 3N Interaction

R. Roth, S. Binder, K. Vobig, A. Calci, J. Langhammer, P. Navrátil --- PRL 109, 052501 (2012)

R. Roth, A. Calci, J. Langhammer, S. Binder --- arXiv:1311.3563

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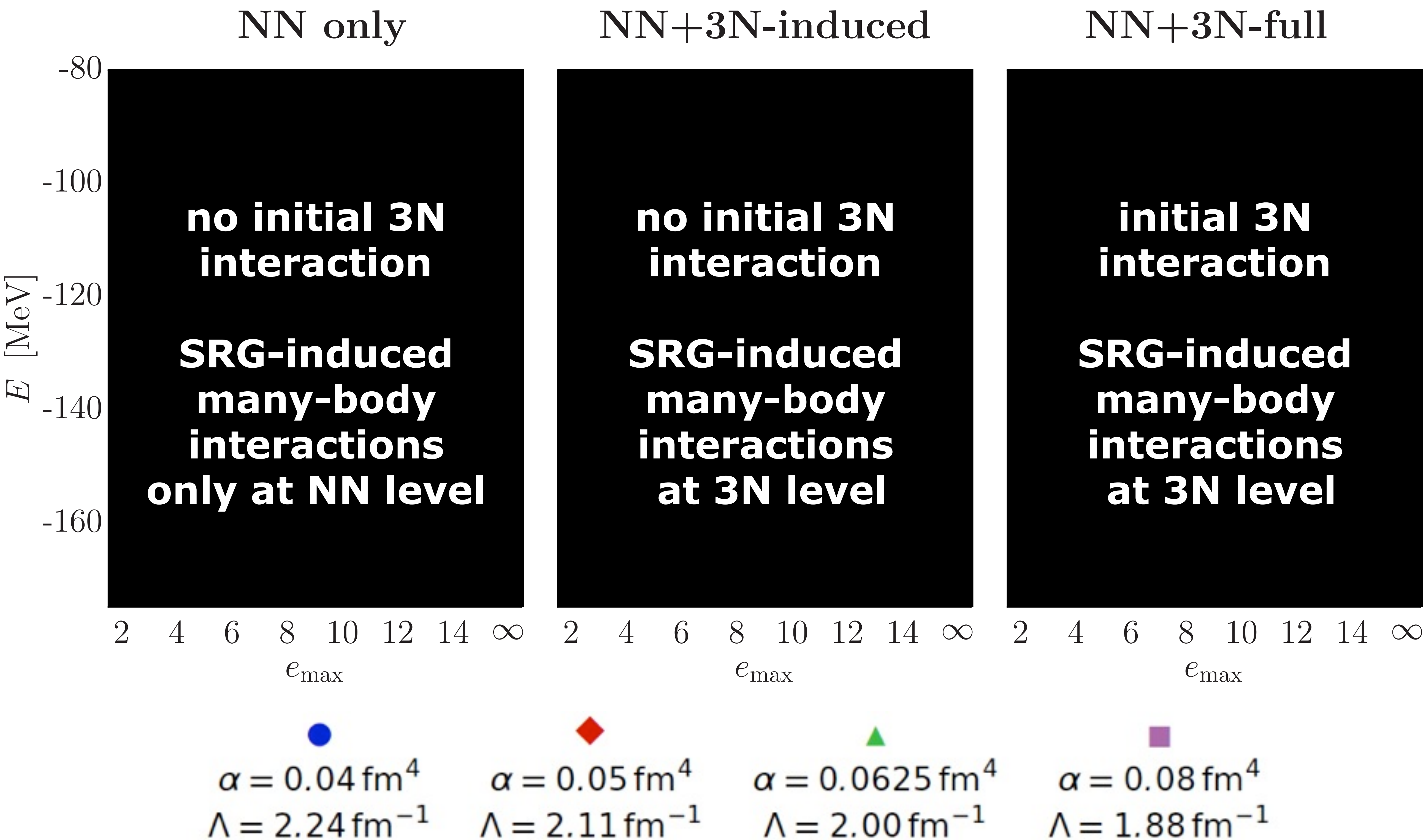

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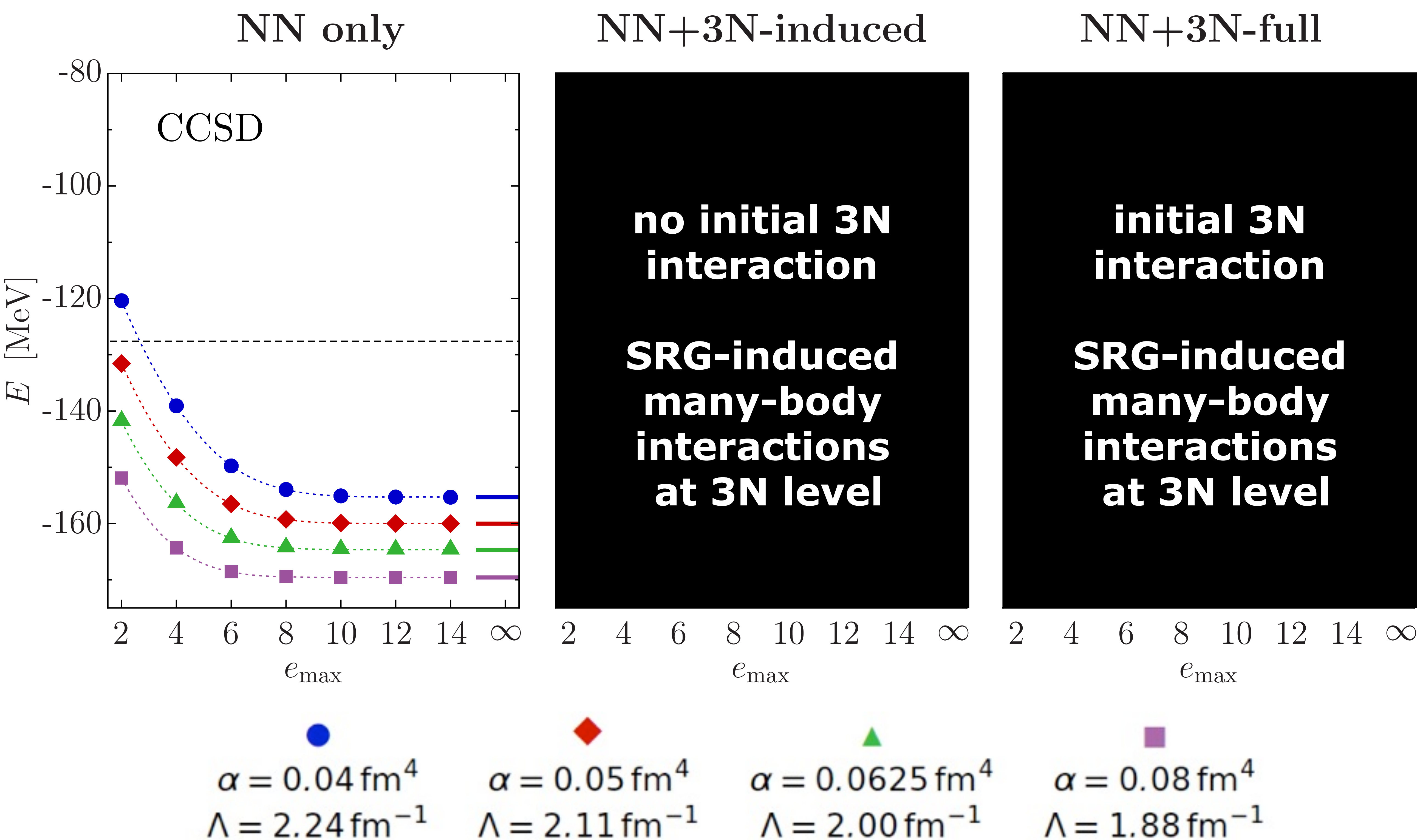

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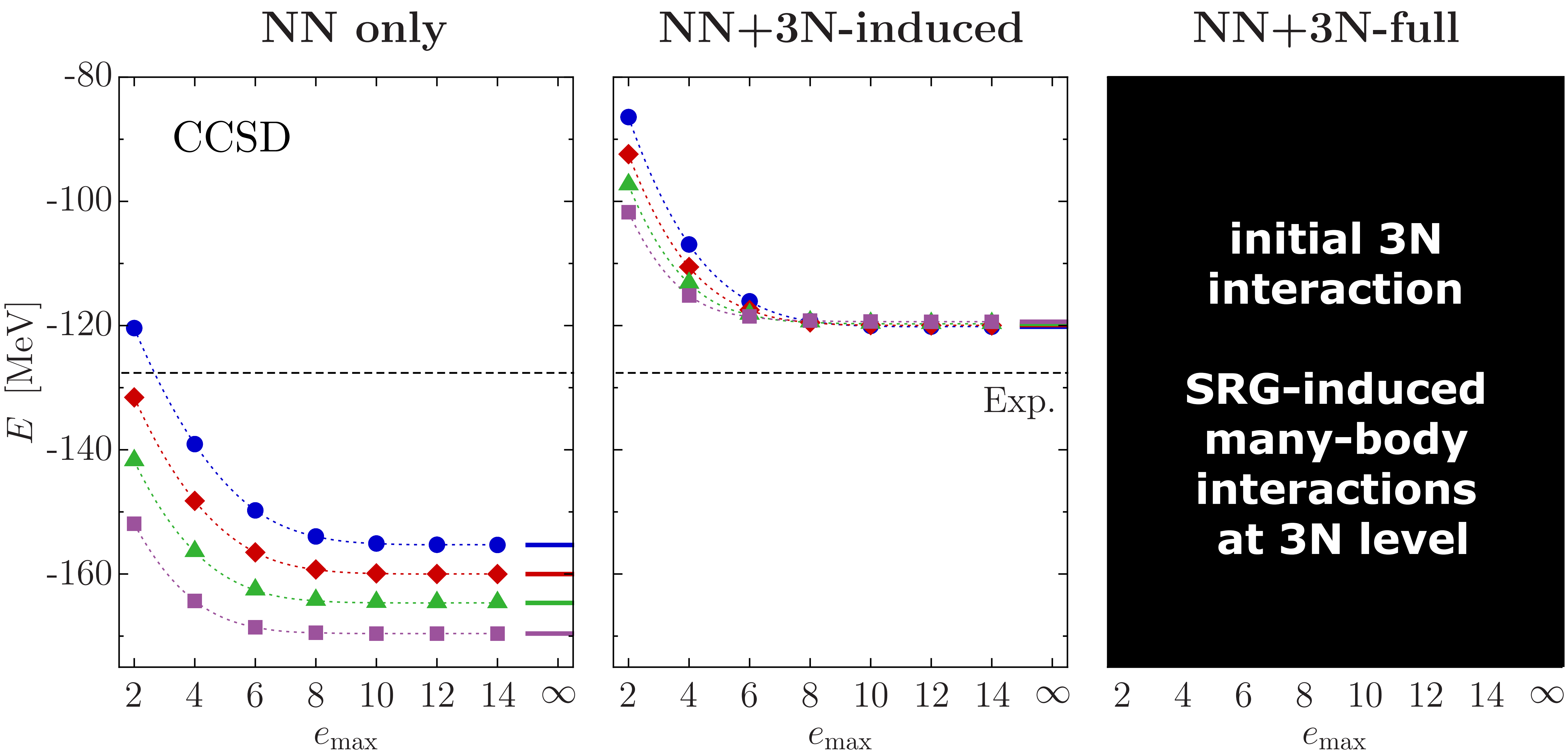

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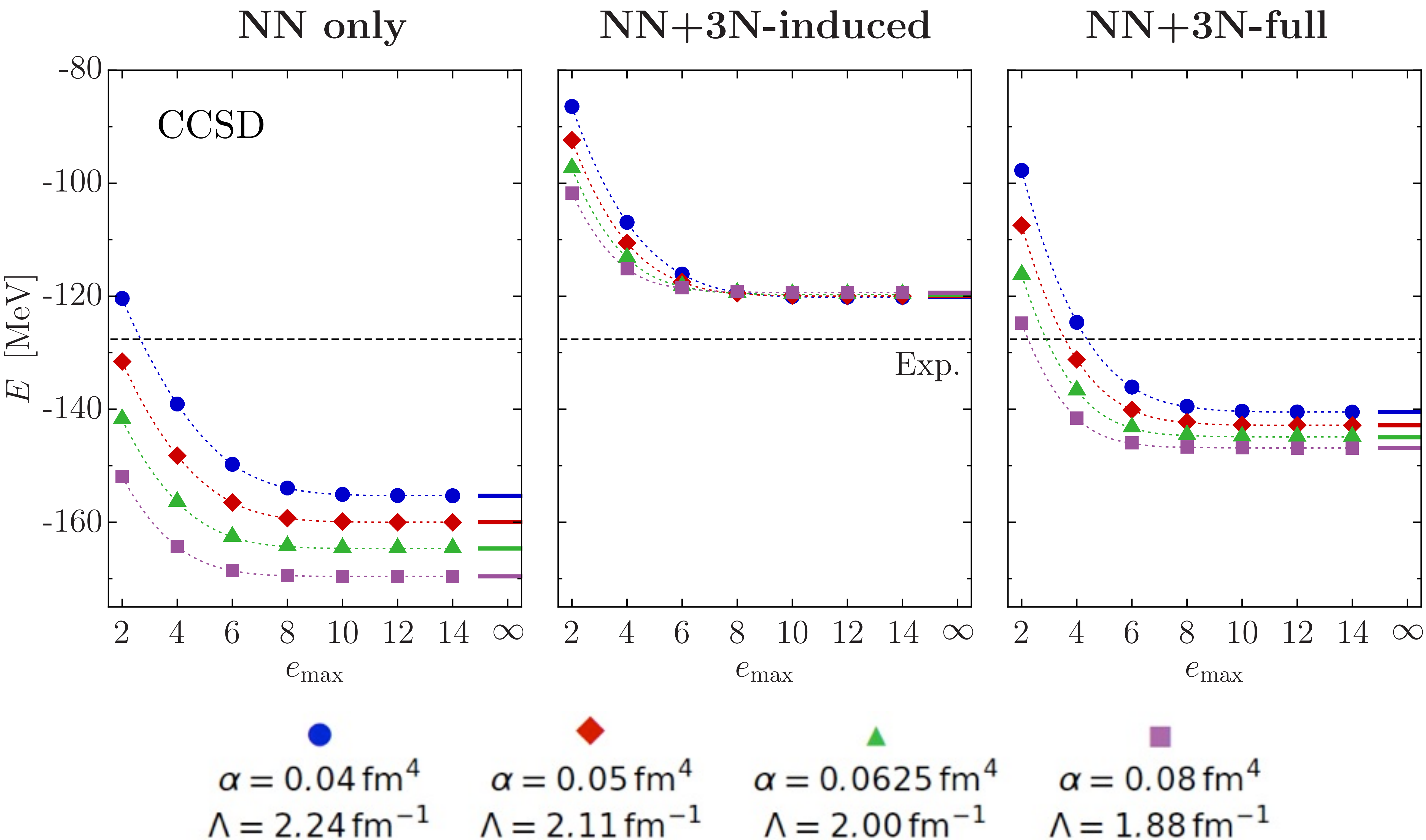

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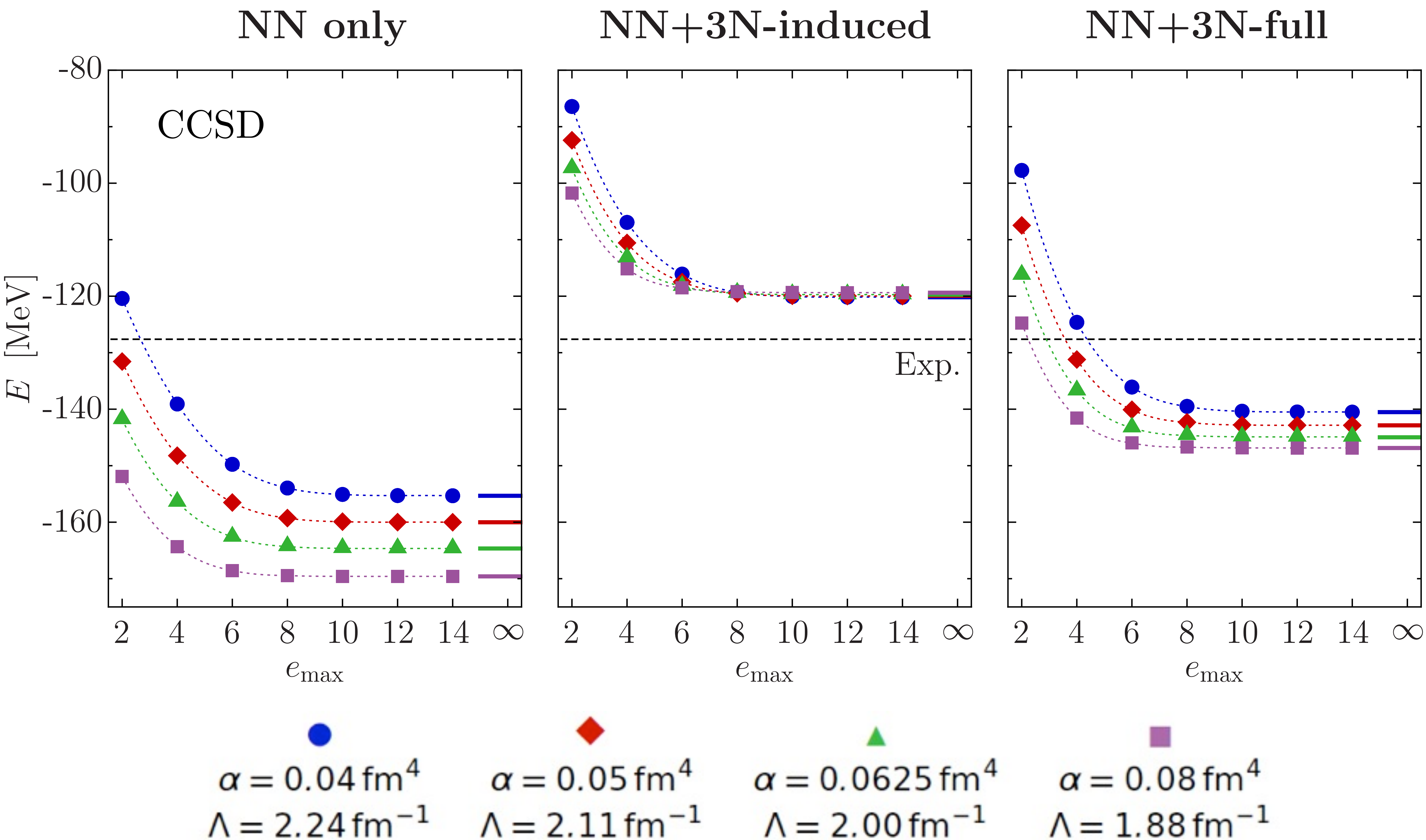

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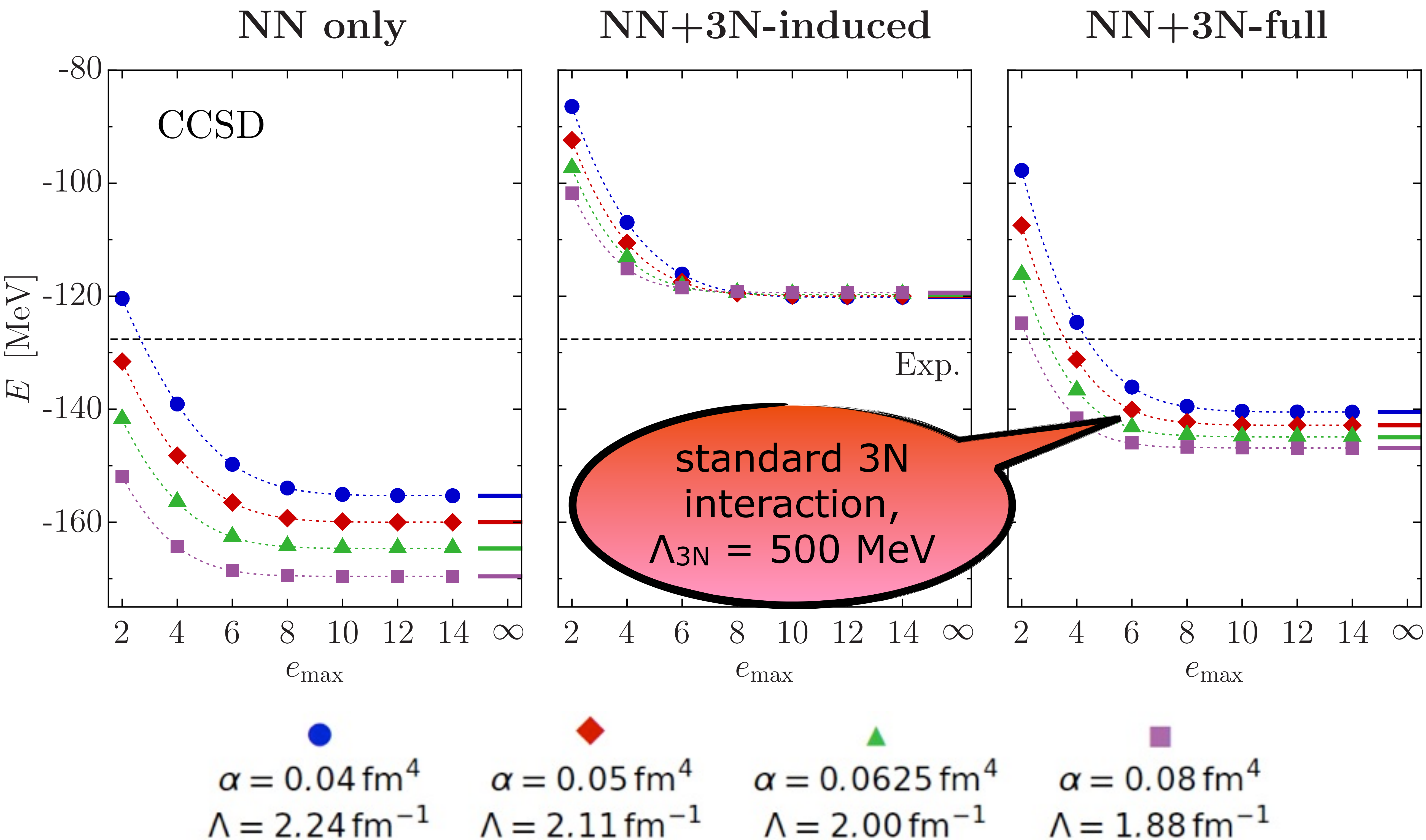

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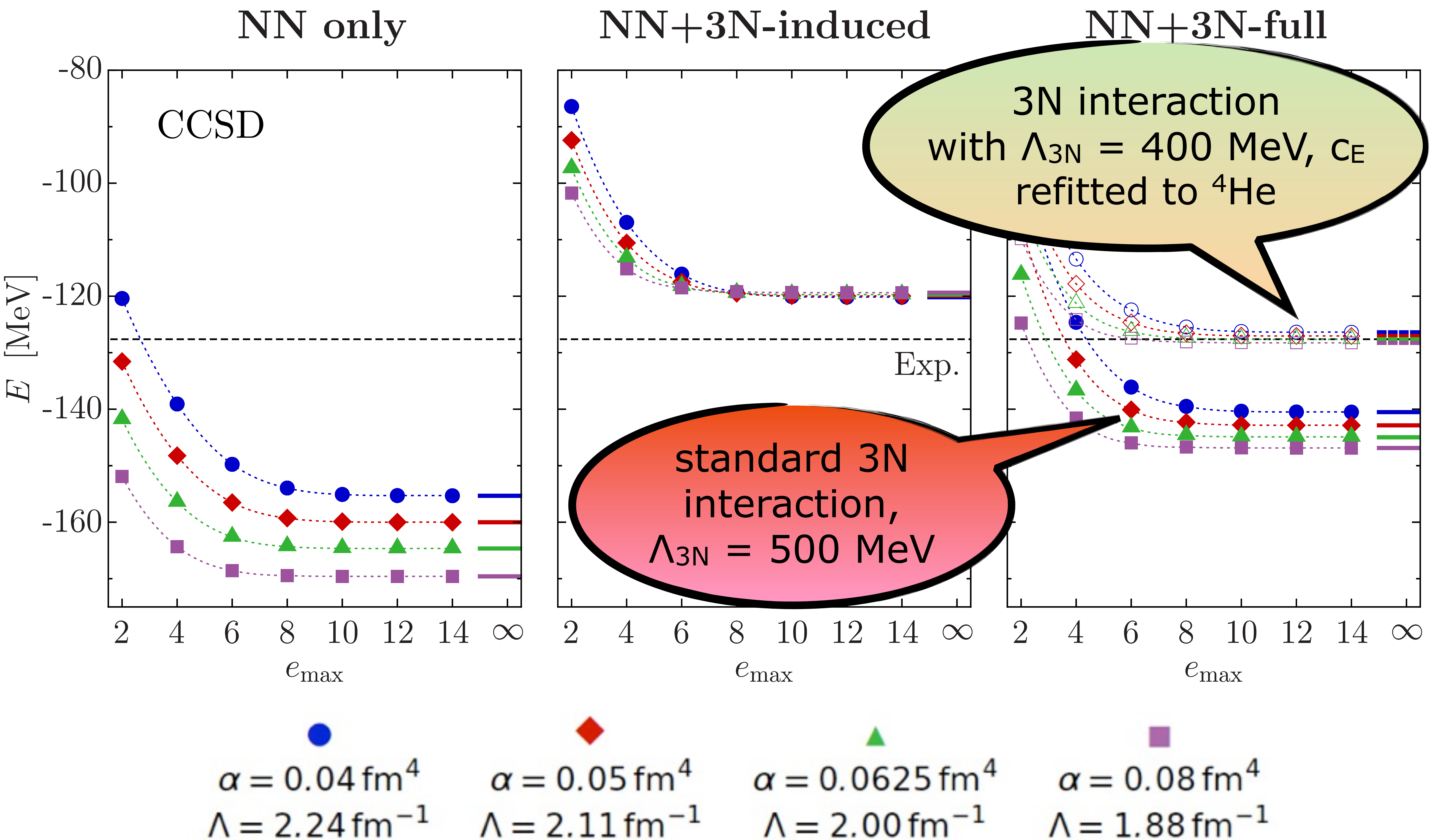
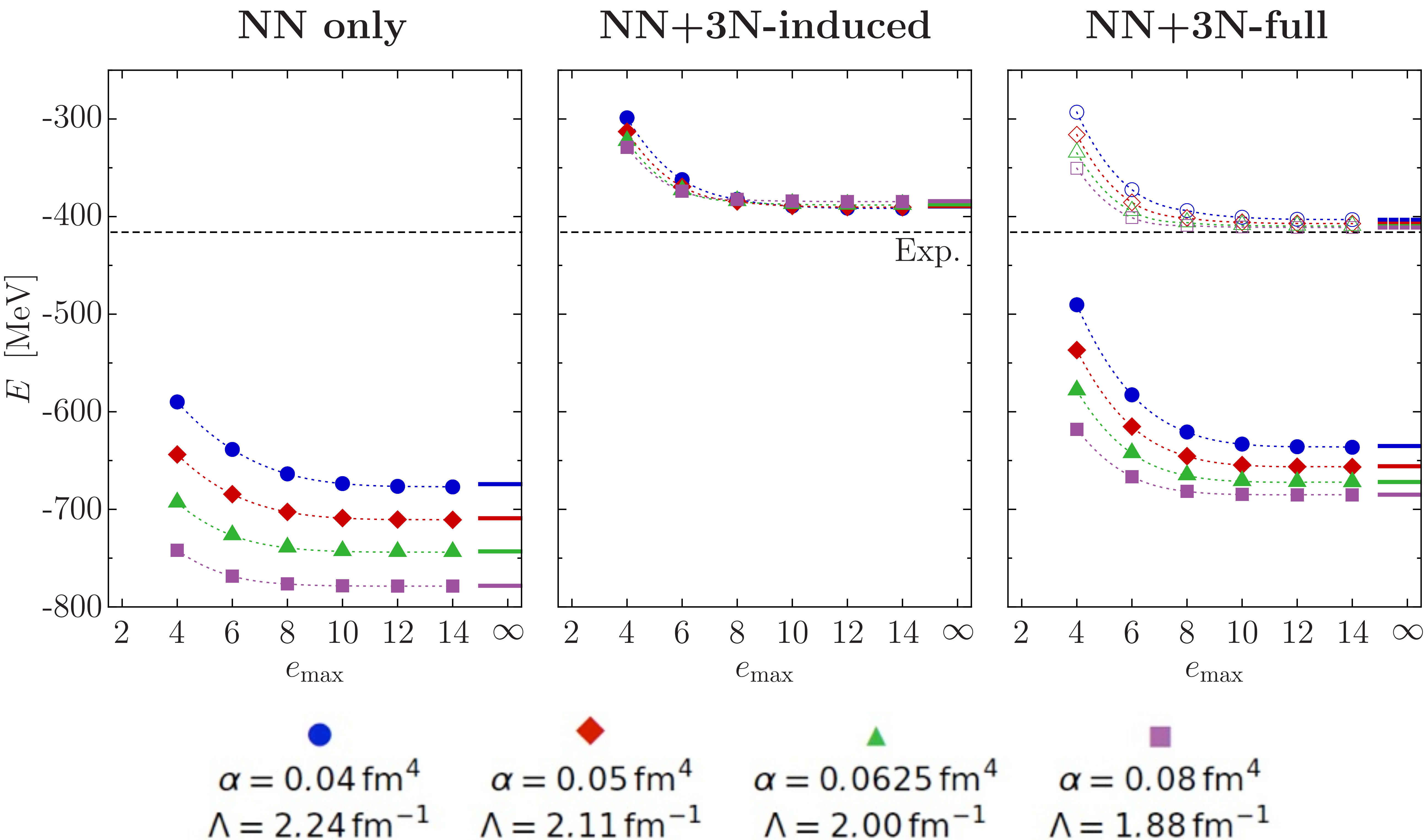


^{48}Ca: Reduced-Cutoff 3N Interaction



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

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

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

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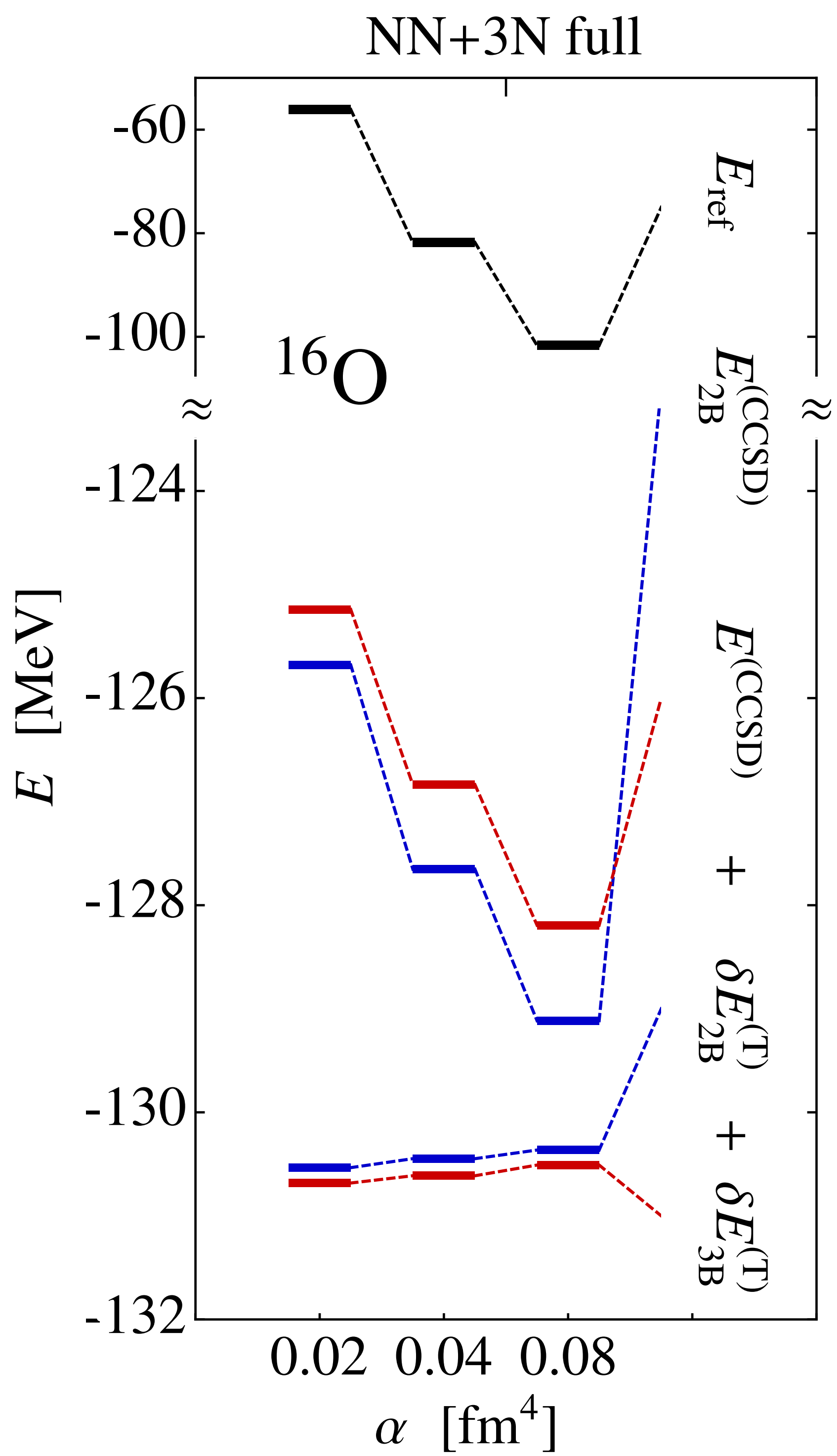
$$\hat{V}_{\mathrm{NO2B}} = W^{0\mathrm{B}} + \sum W^{1\mathrm{B}}_{\circ\circ}\, \hat{a}^{\dagger}_{\circ}\hat{a}_{\circ} + \sum W^{2\mathrm{B}}_{\circ\circ\circ\circ}\, \hat{a}^{\dagger}_{\circ}\hat{a}^{\dagger}_{\circ}\hat{a}_{\circ}\hat{a}_{\circ}$$

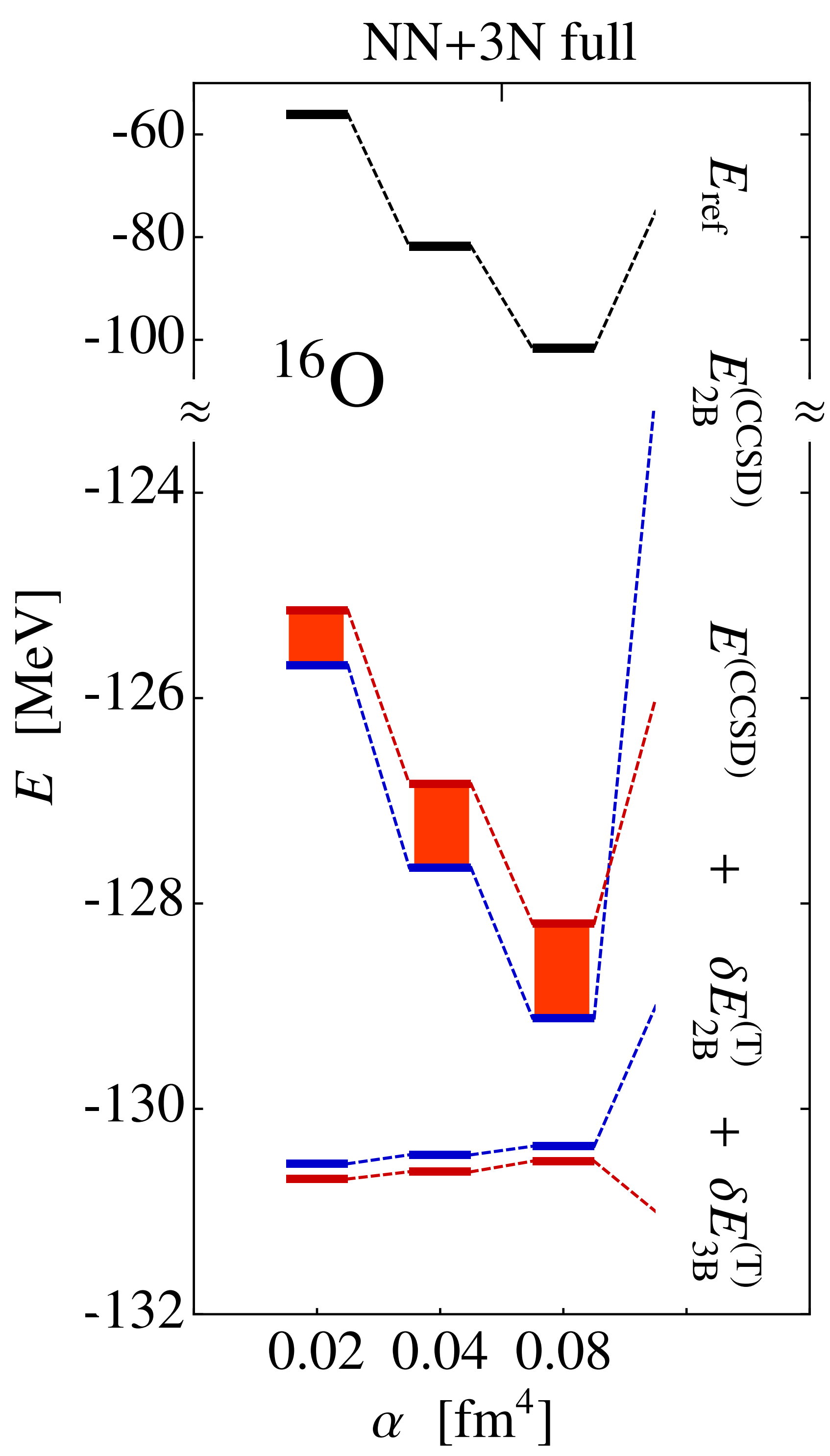
- **Normal-Ordered Two-Body Approximation (NO2B)**: discard residual normal-ordered 3B part $W^{3\mathrm{B}}$

Benchmark NO2B



Wednesday, February 19, 14

Benchmark NO2B



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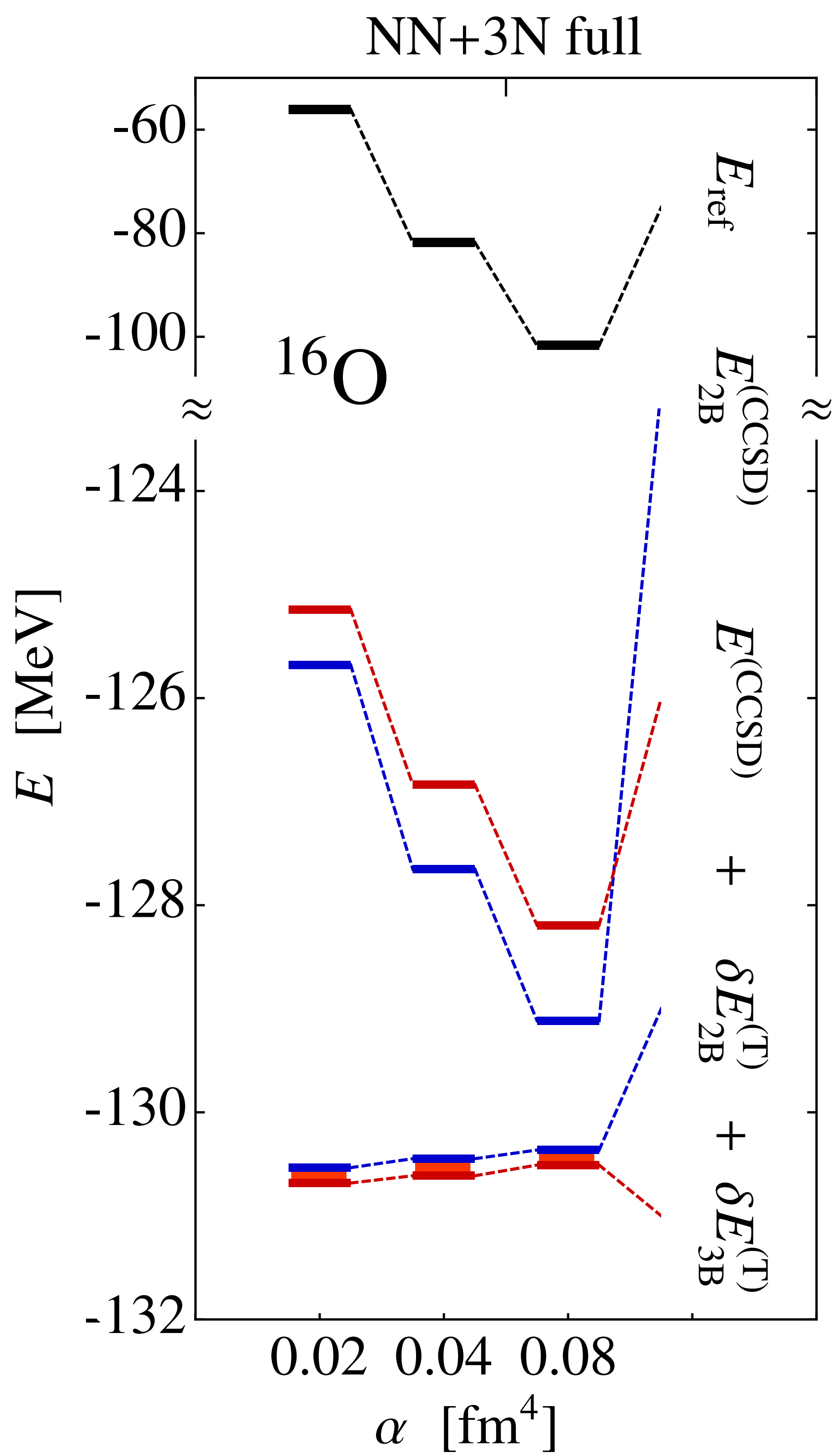

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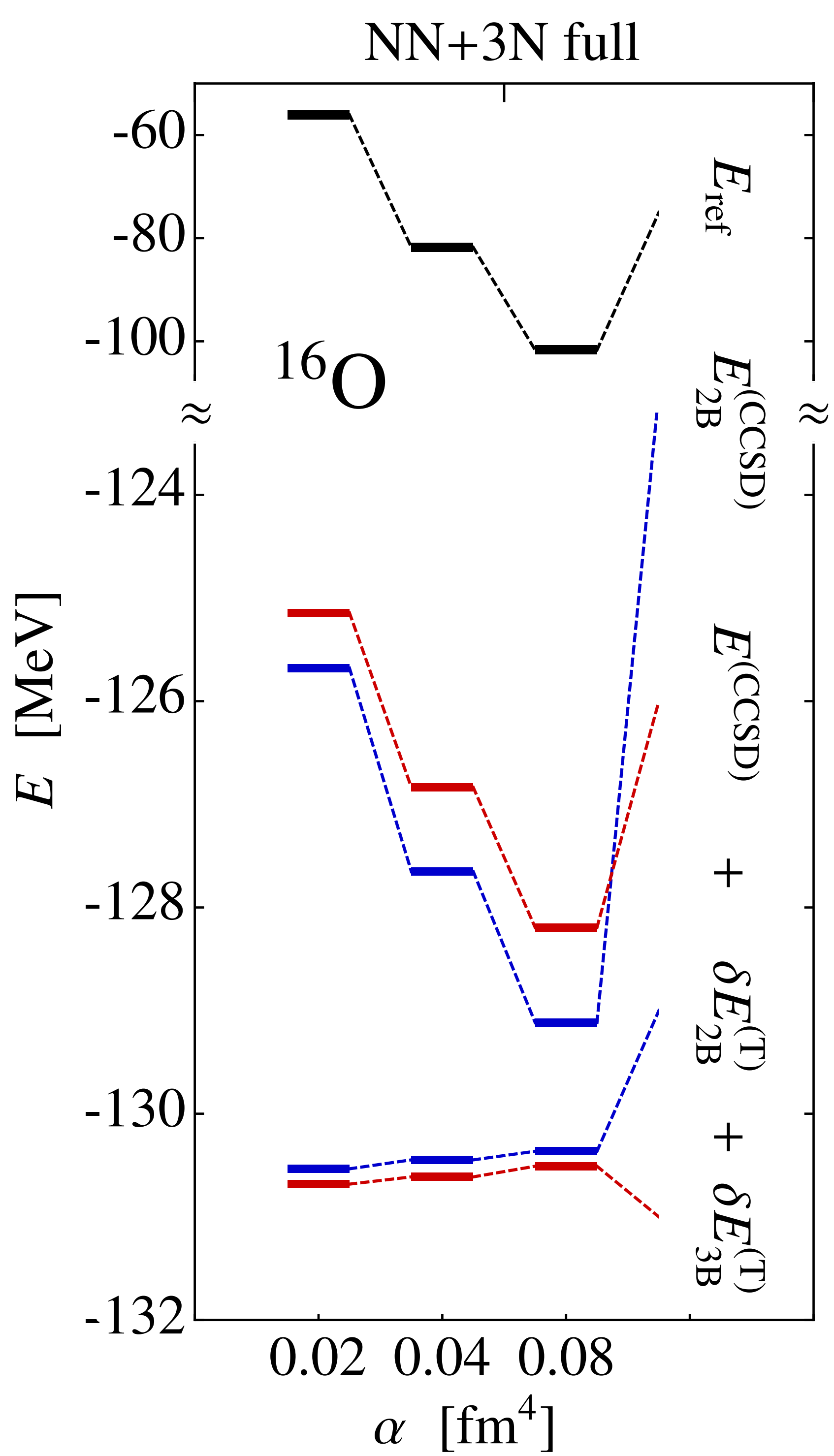

- Residual 3N interaction **relevant** for **CCSD**, **negligible** for additional **triples correction** (ΛCCSD(T))

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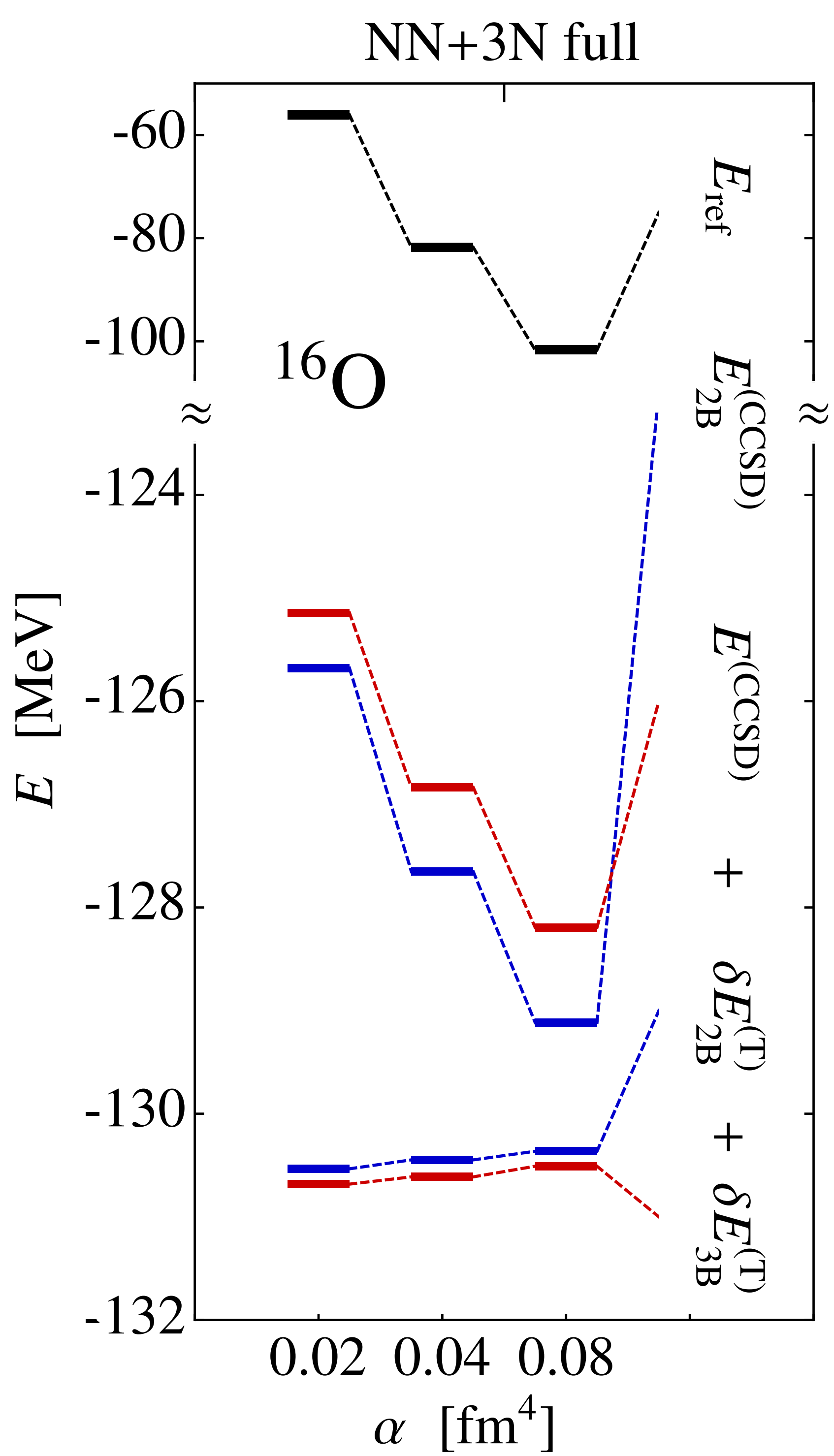
Benchmark NO2B



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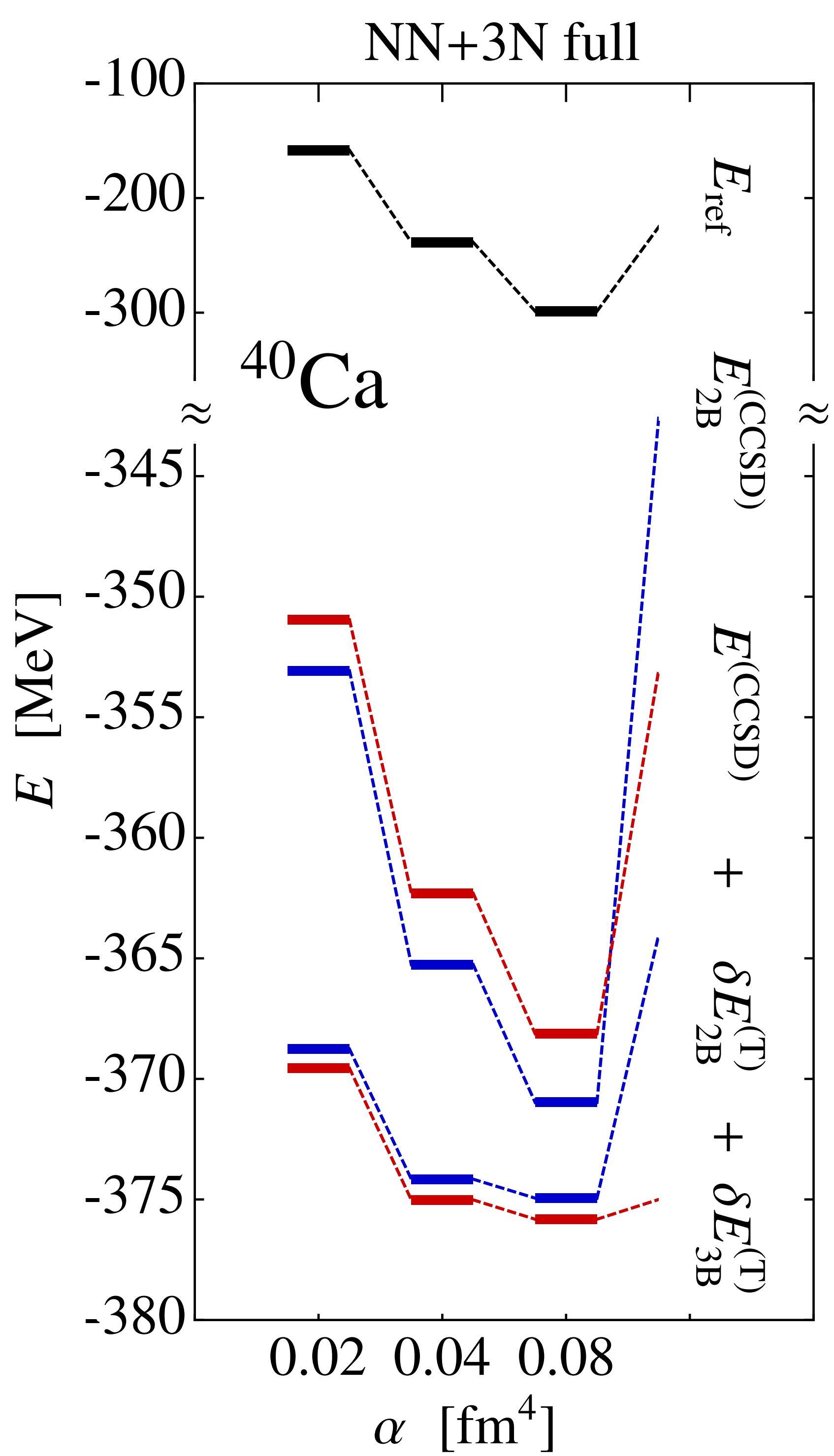
- Errors due to NO2B **< 1%**

Benchmark NO2B



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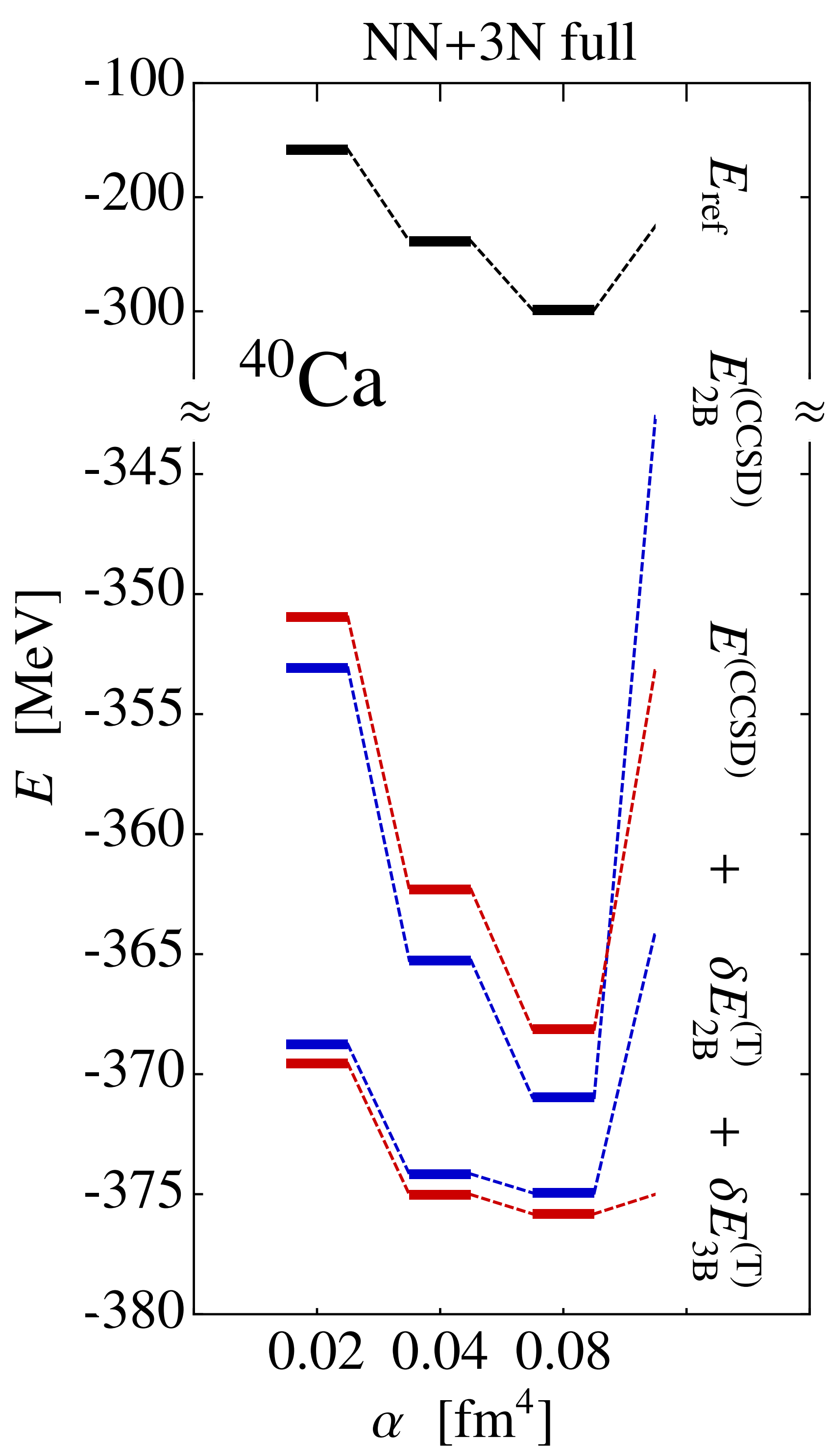
Benchmark NO2B



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- ⇒ NO2B is **efficient** and **accurate** way to include 3N interaction

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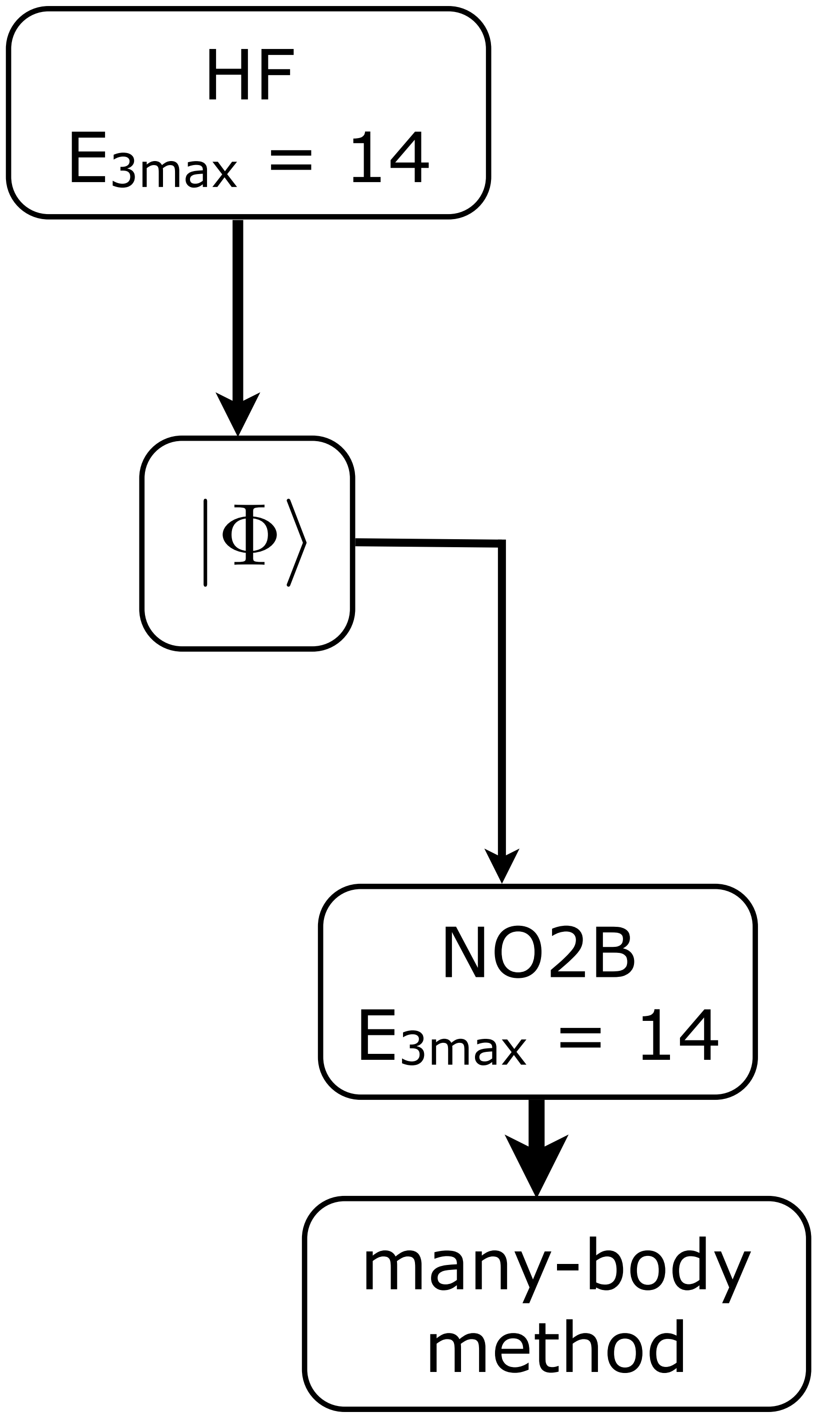
Normal-Ordering Procedure



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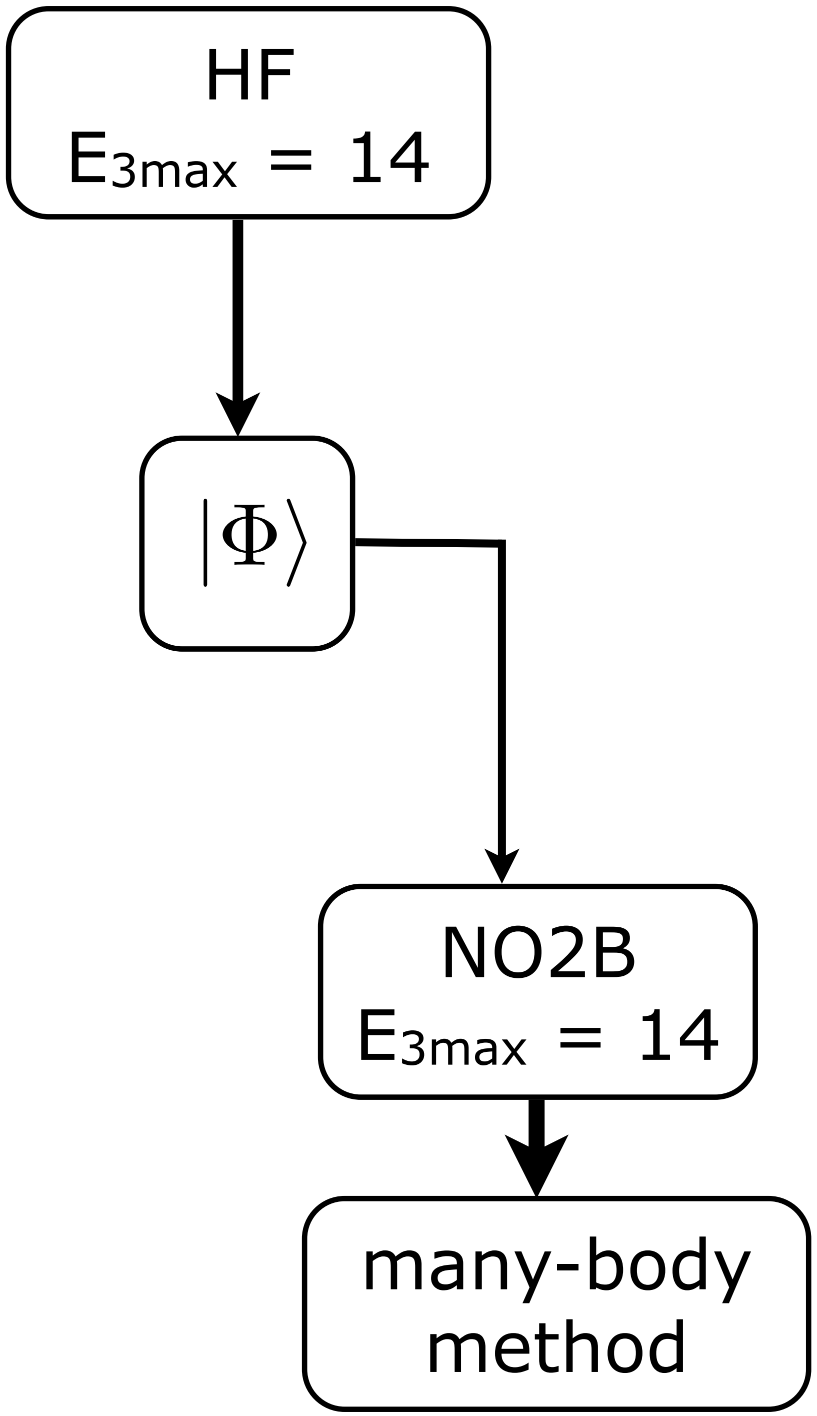

$E_{3\mathrm{max}}$:

restrict principal HO quantum numbers e_i in

$$\langle pqr|\hat{W}|stu\rangle$$

according to

$$\left.\begin{matrix} e_p + e_q + e_r \\ e_s + e_t + e_u \end{matrix}\right\} \leq E_{3\mathrm{max}}$$

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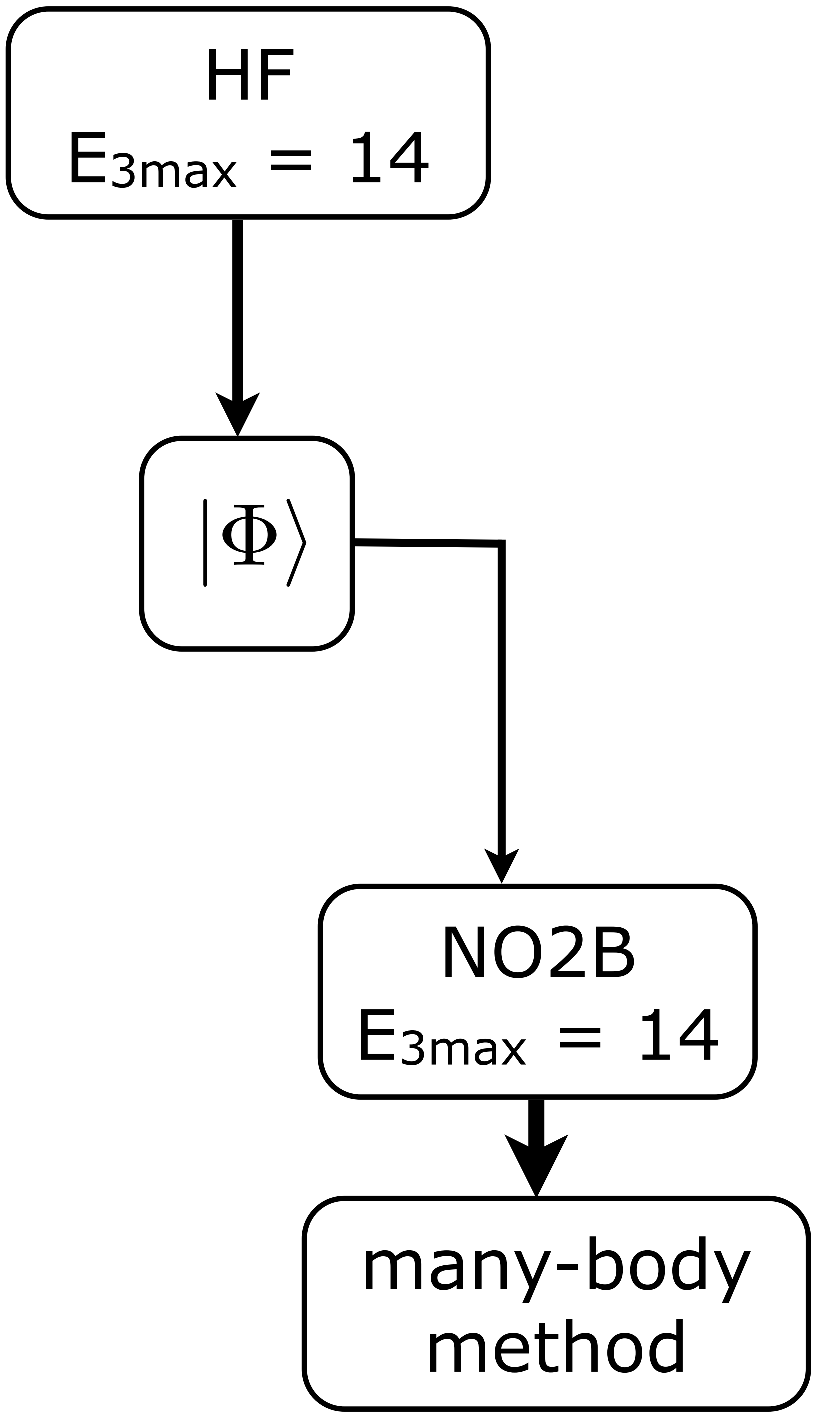
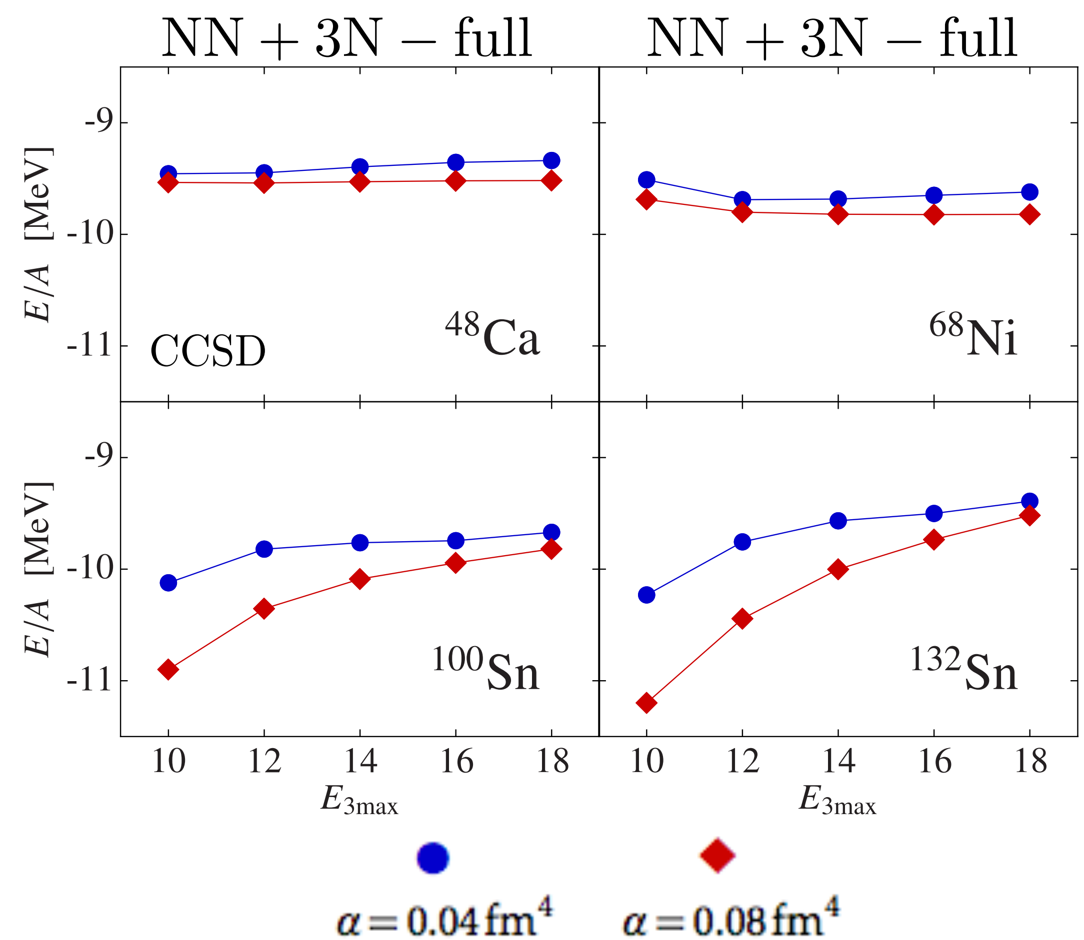


- heavy nuclei require **large E3max**



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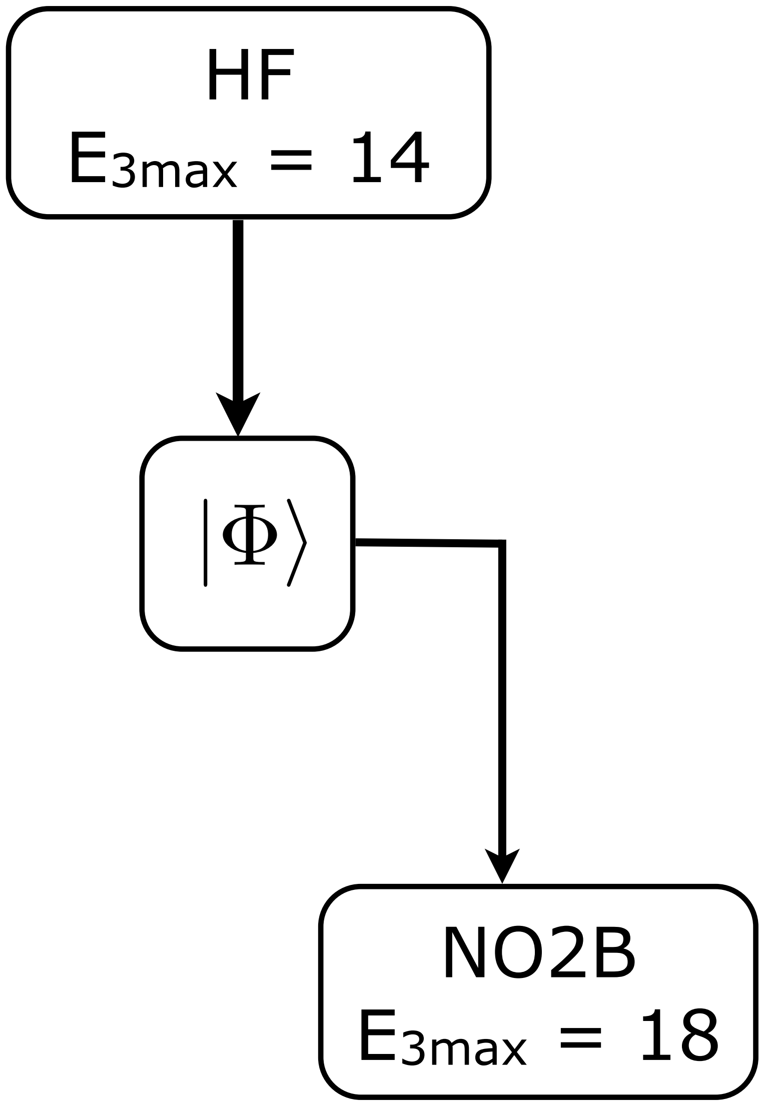

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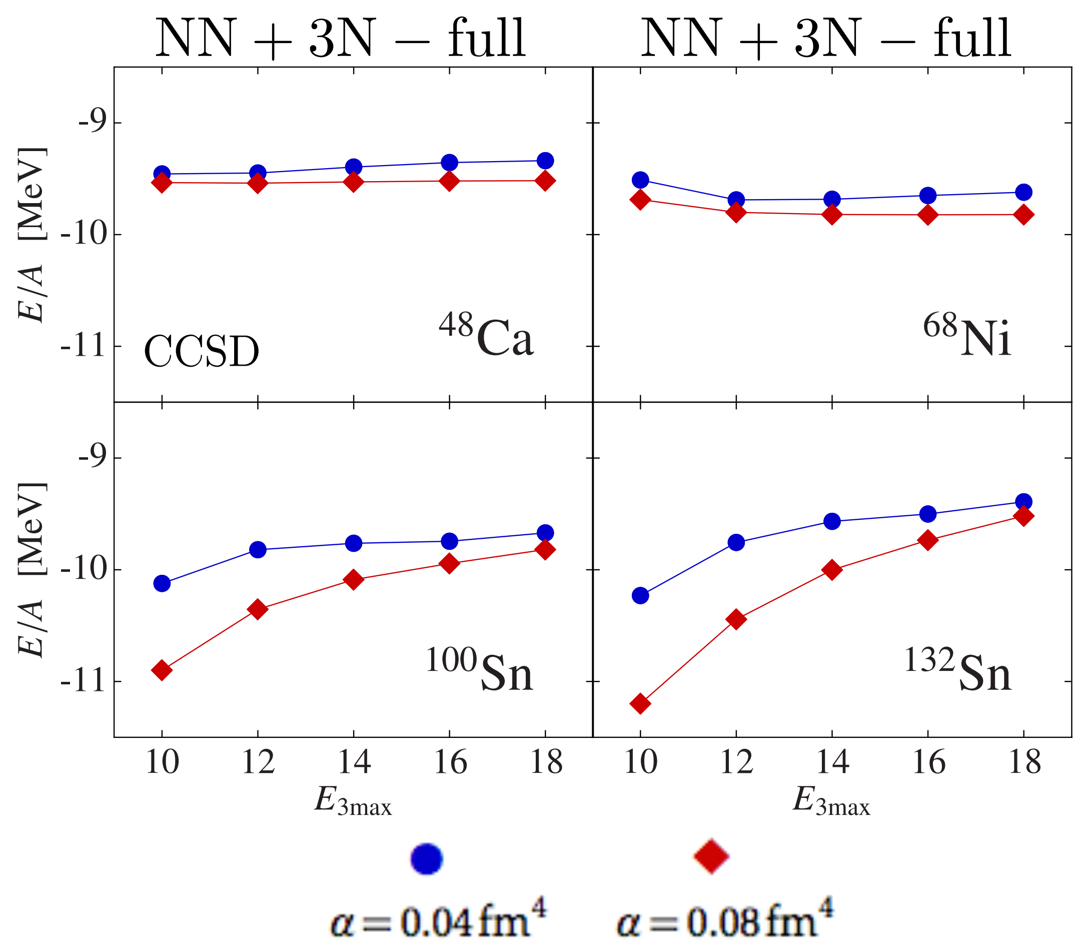

- simple protocol to **avoid using full sets** of large-E_{3max} matrix elements

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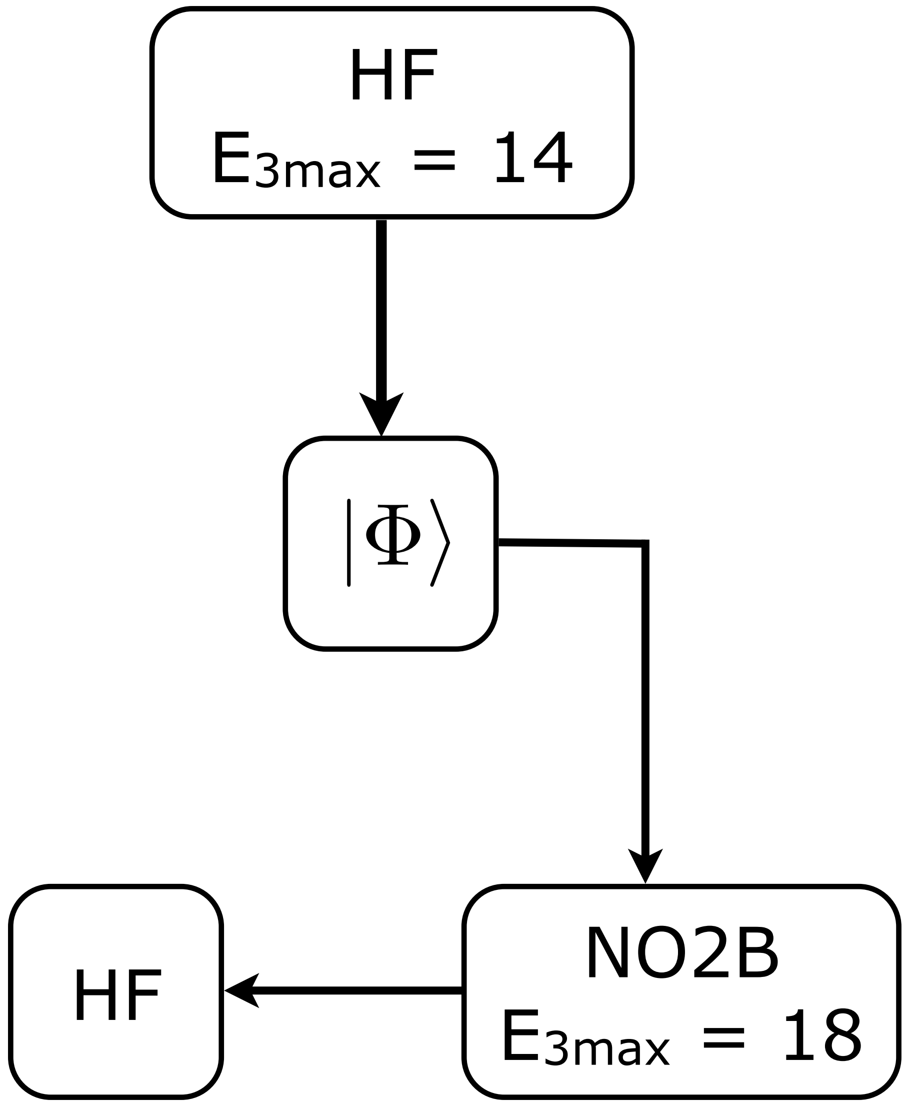

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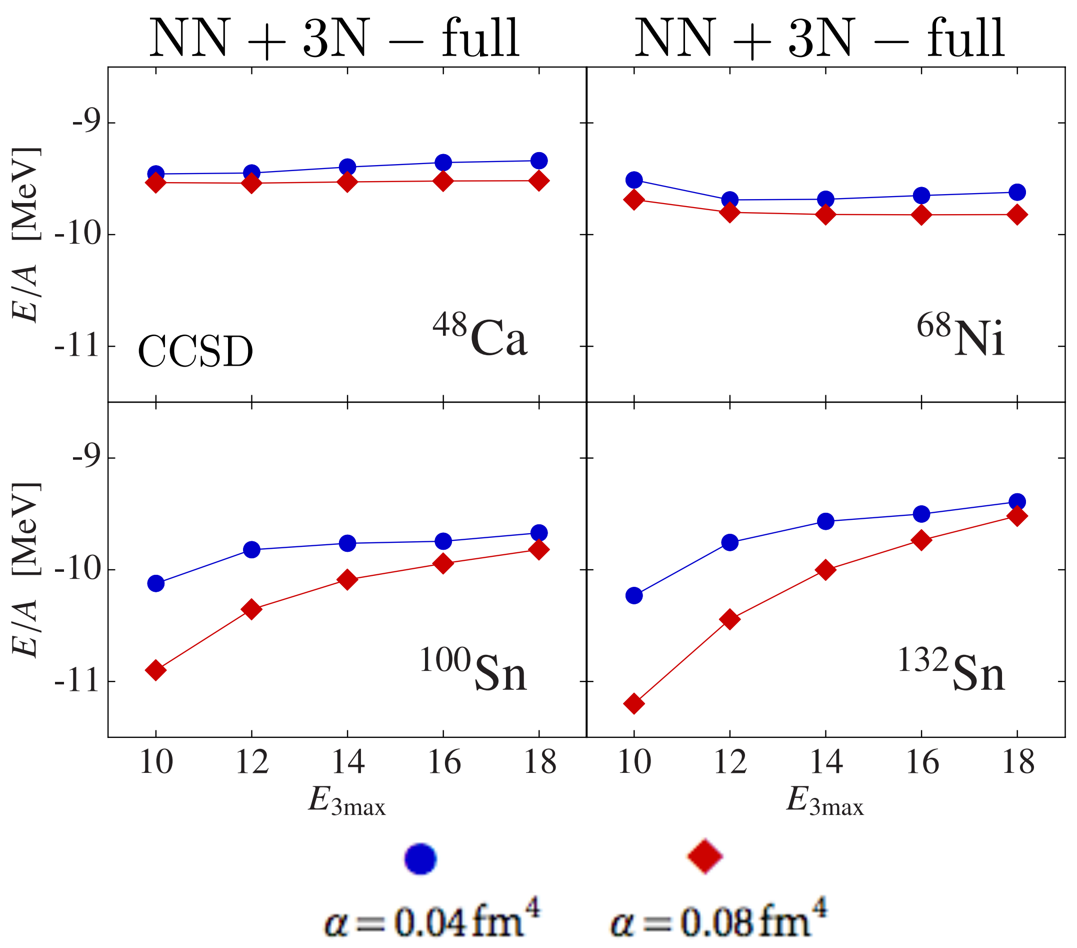

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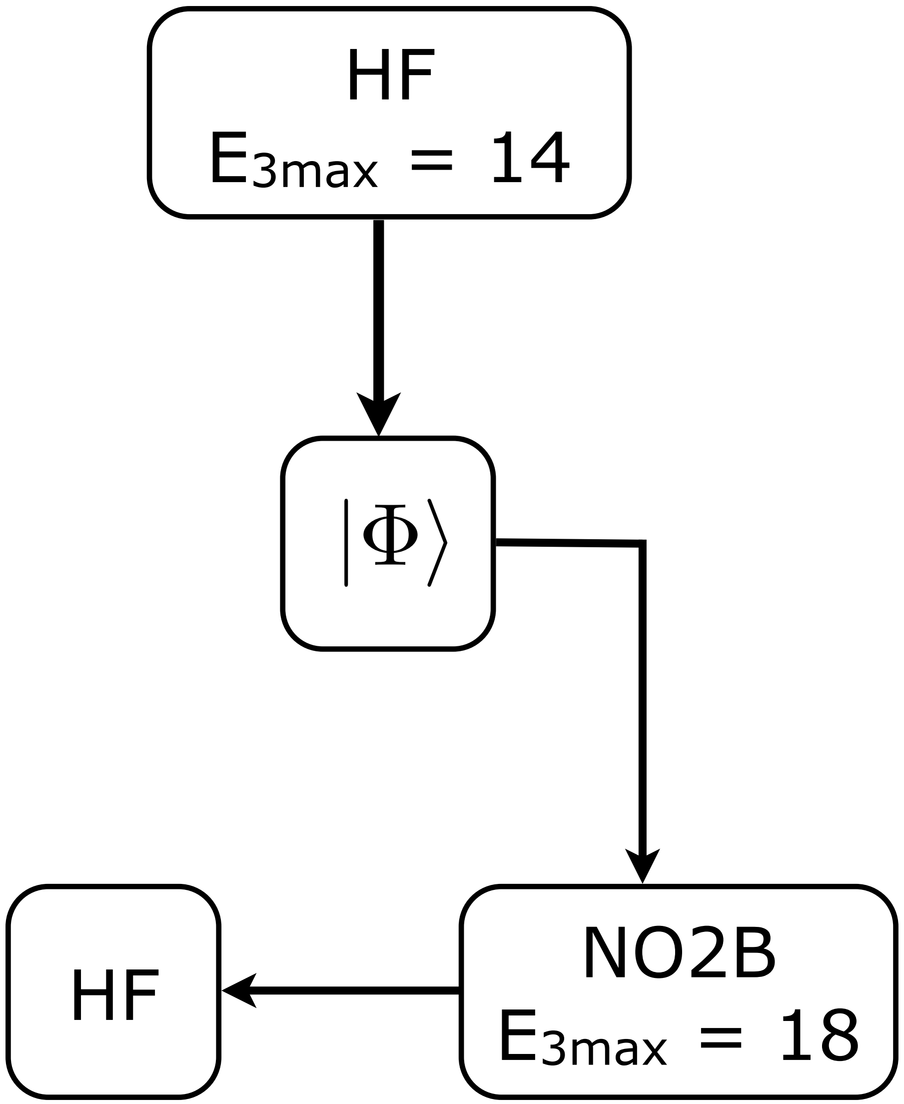

need only a **small subset** of normal-ordered matrix elements!

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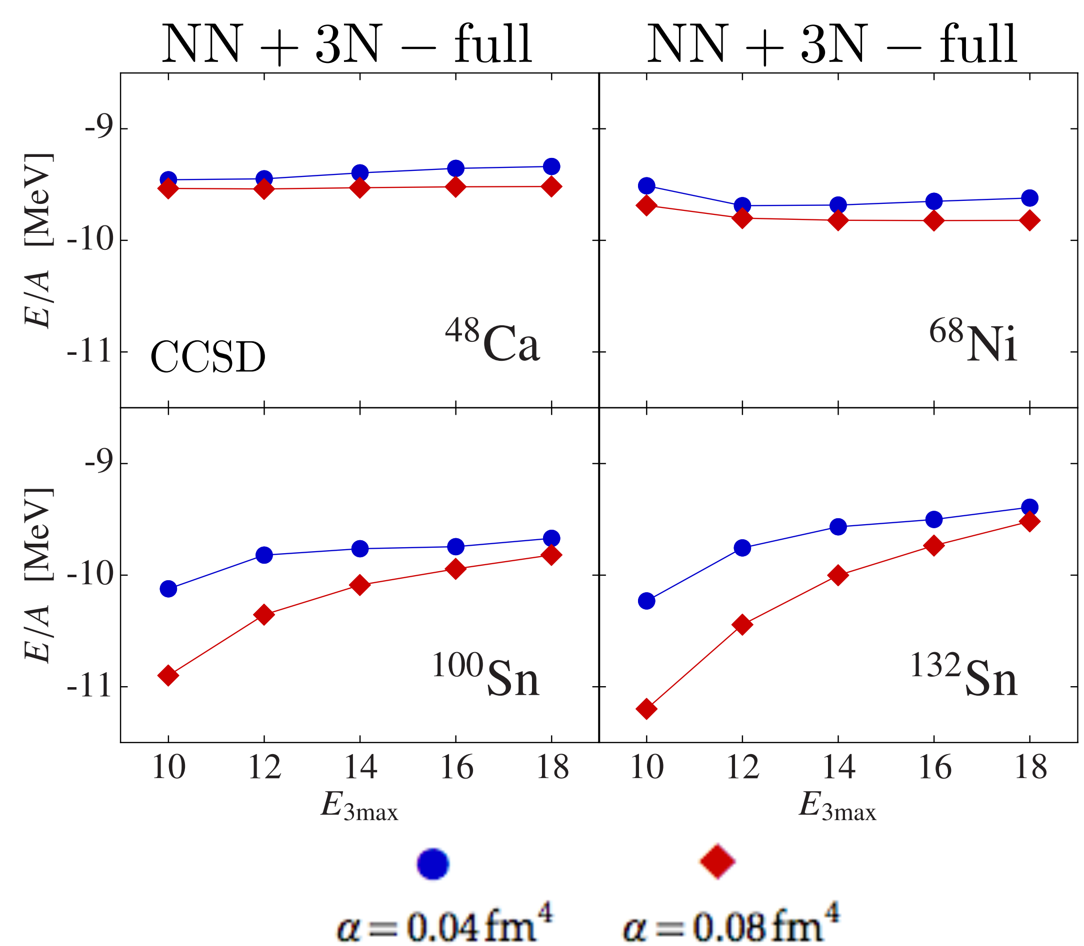

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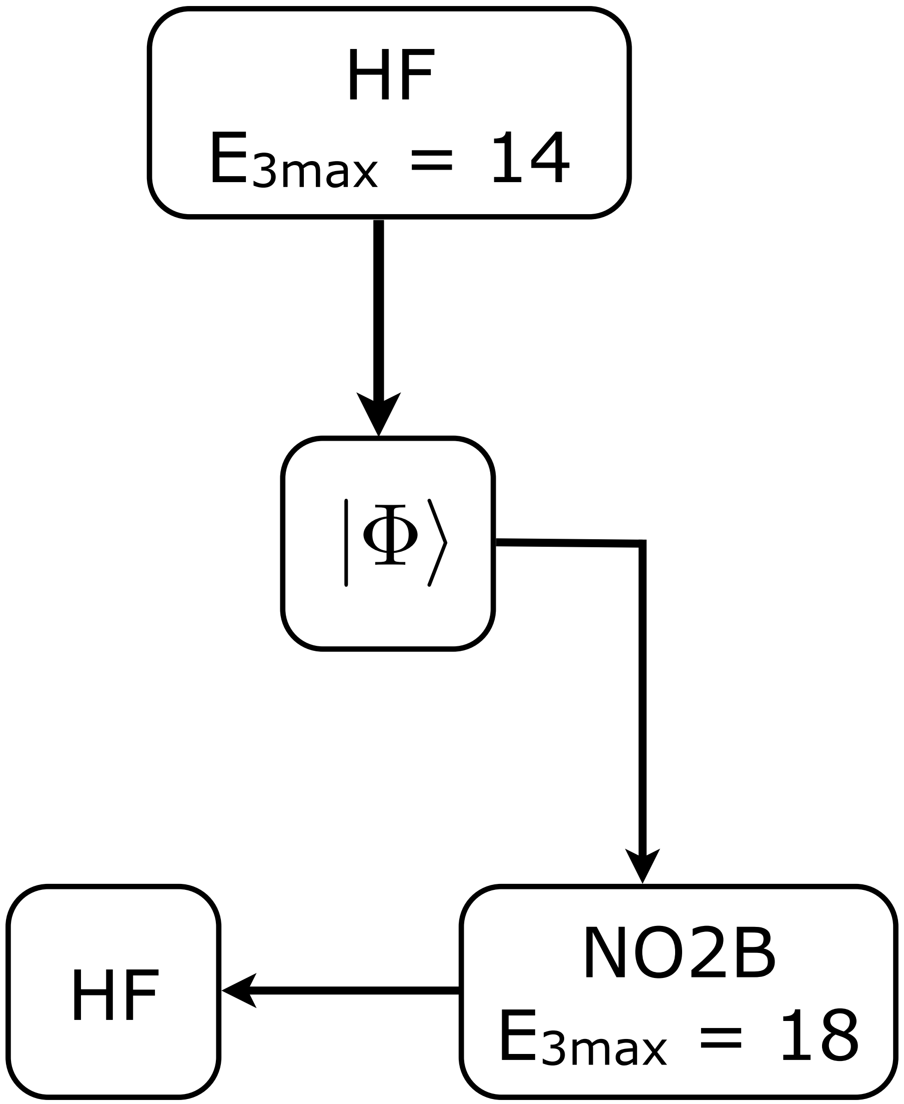

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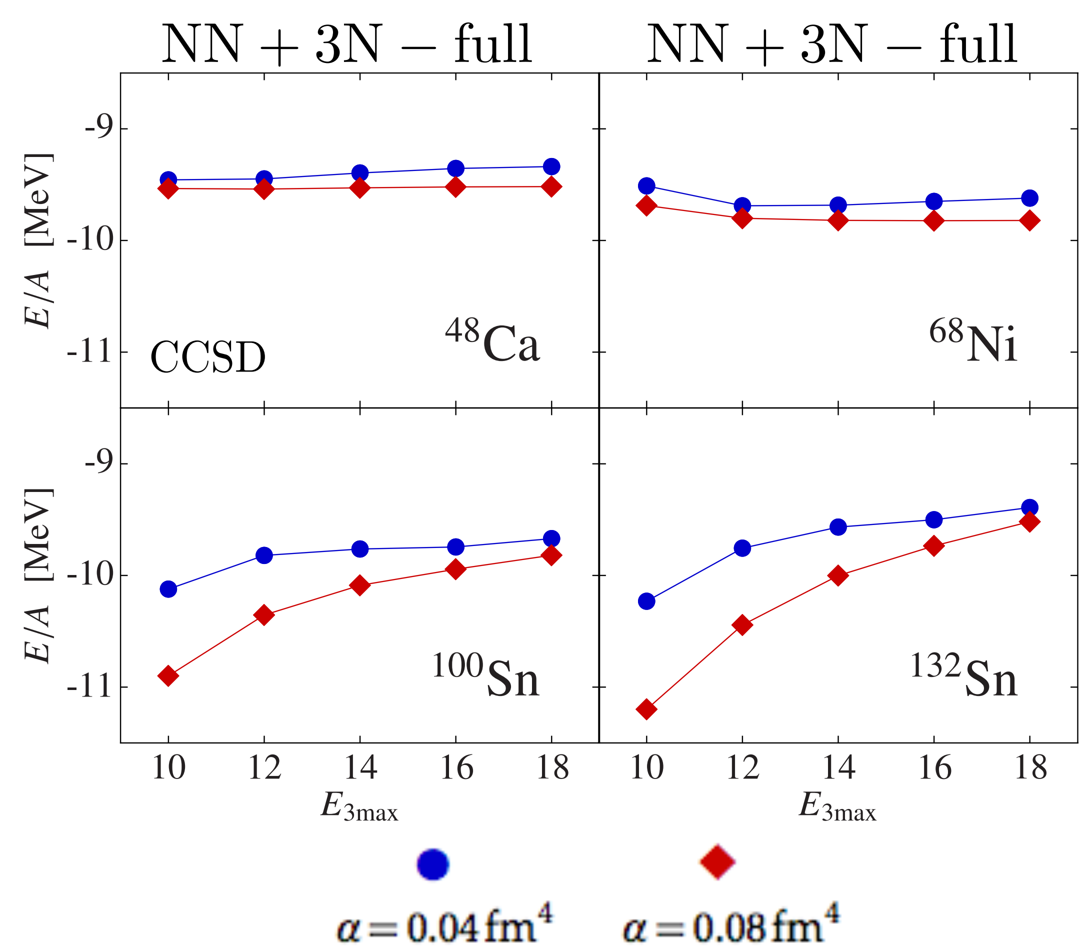

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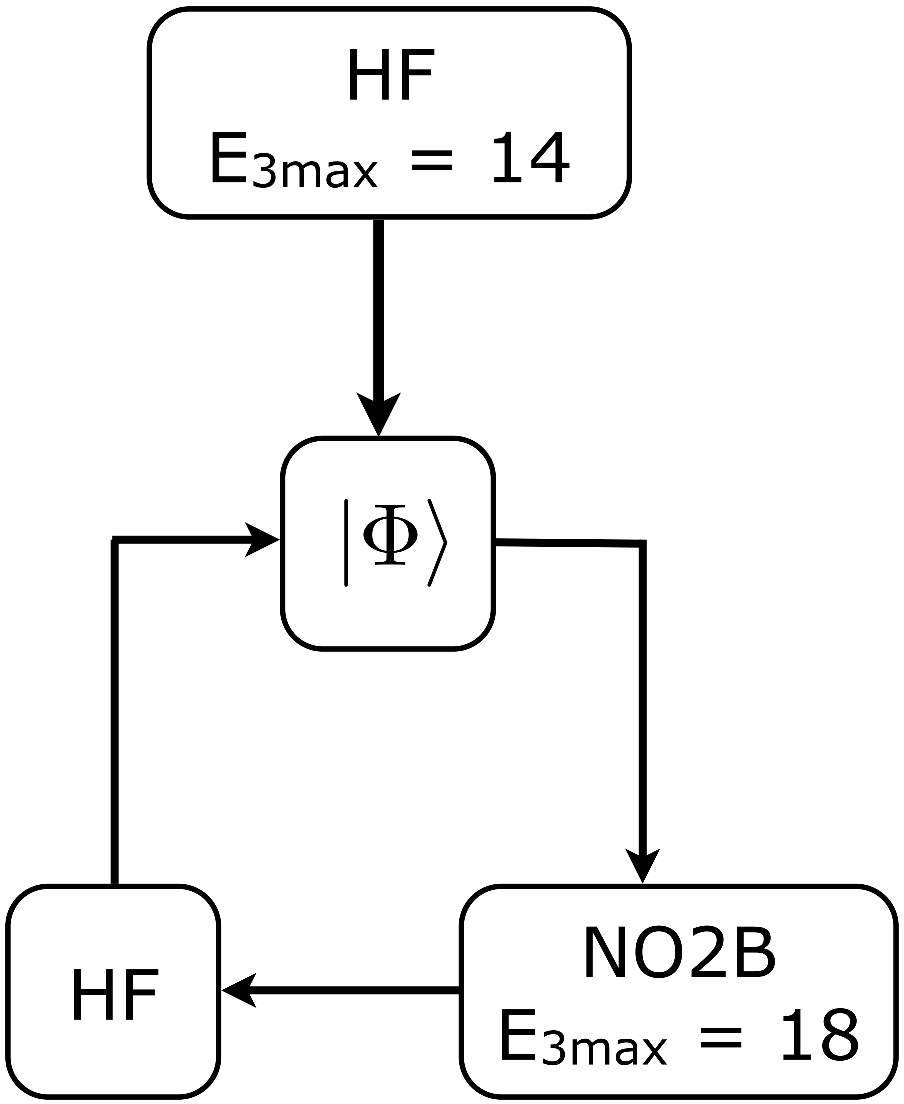

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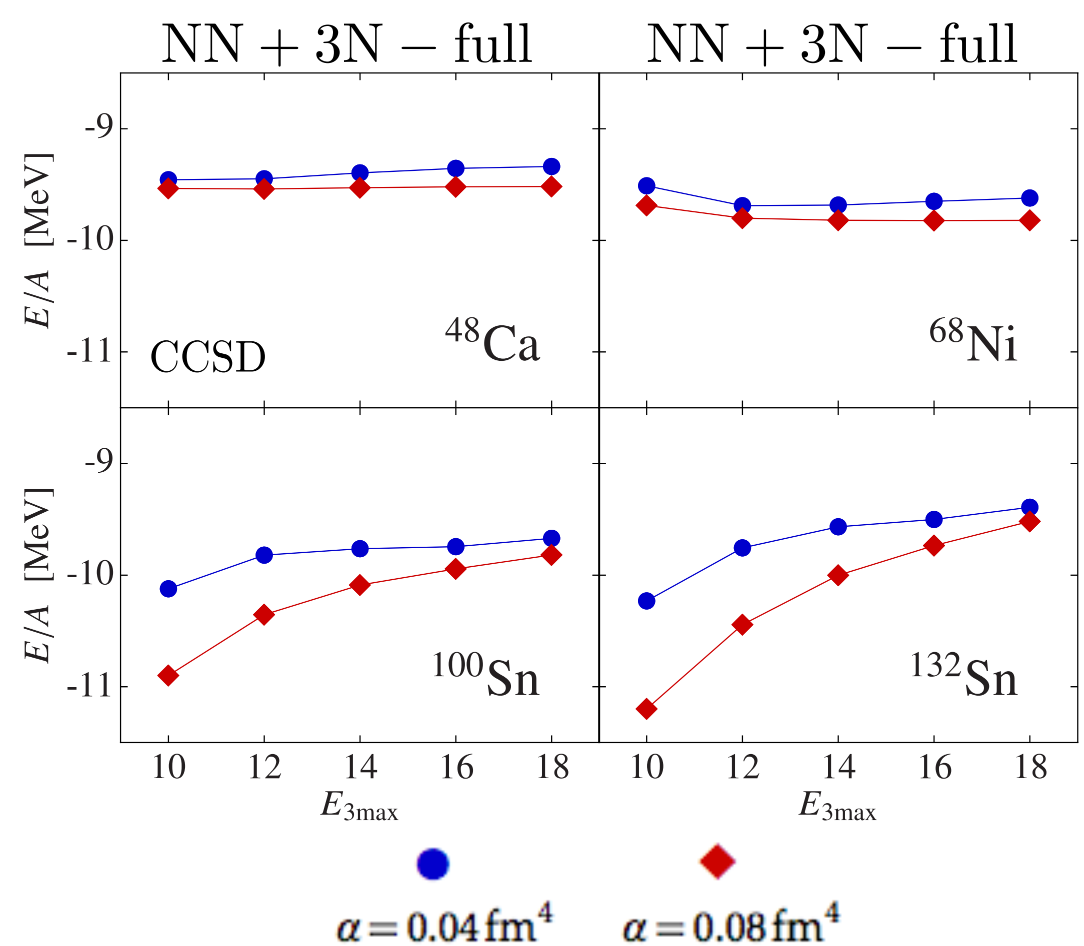

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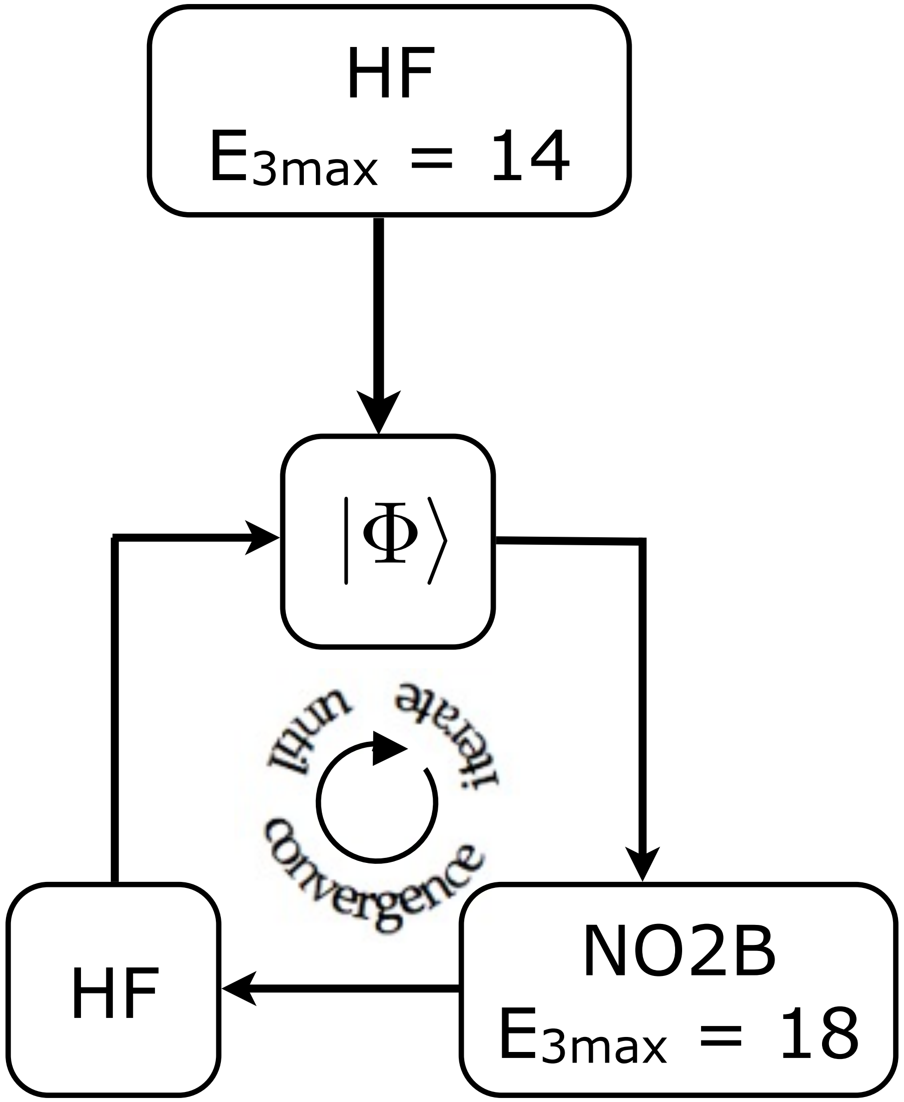

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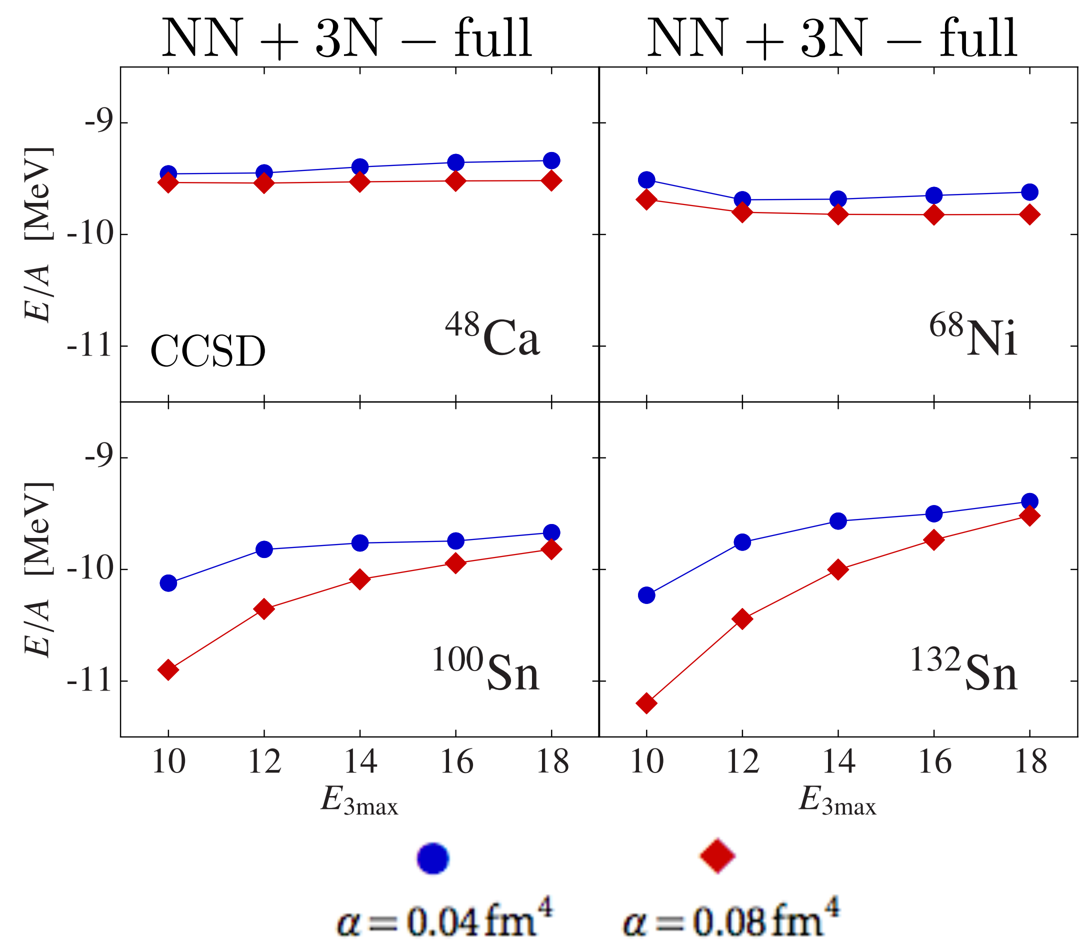

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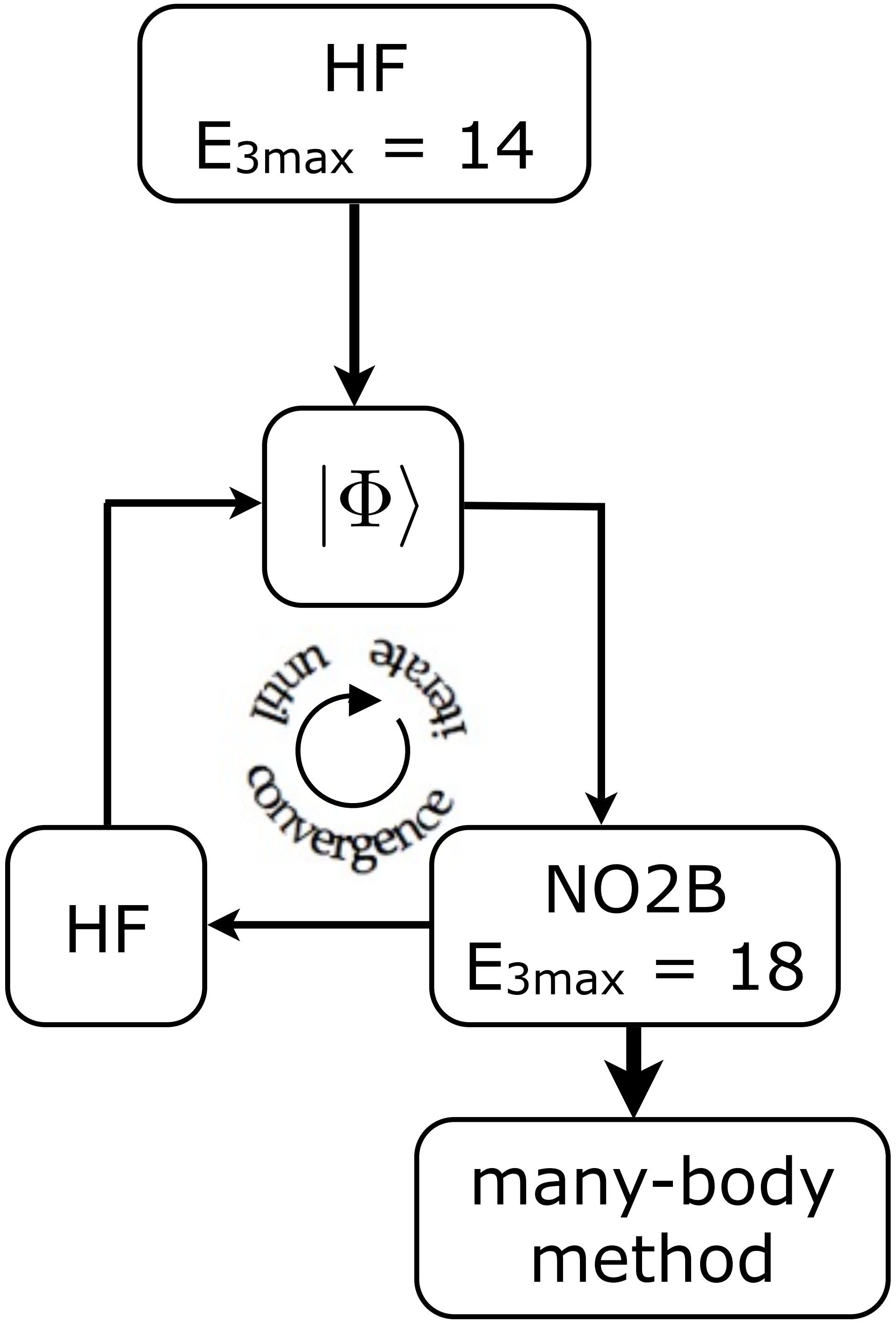

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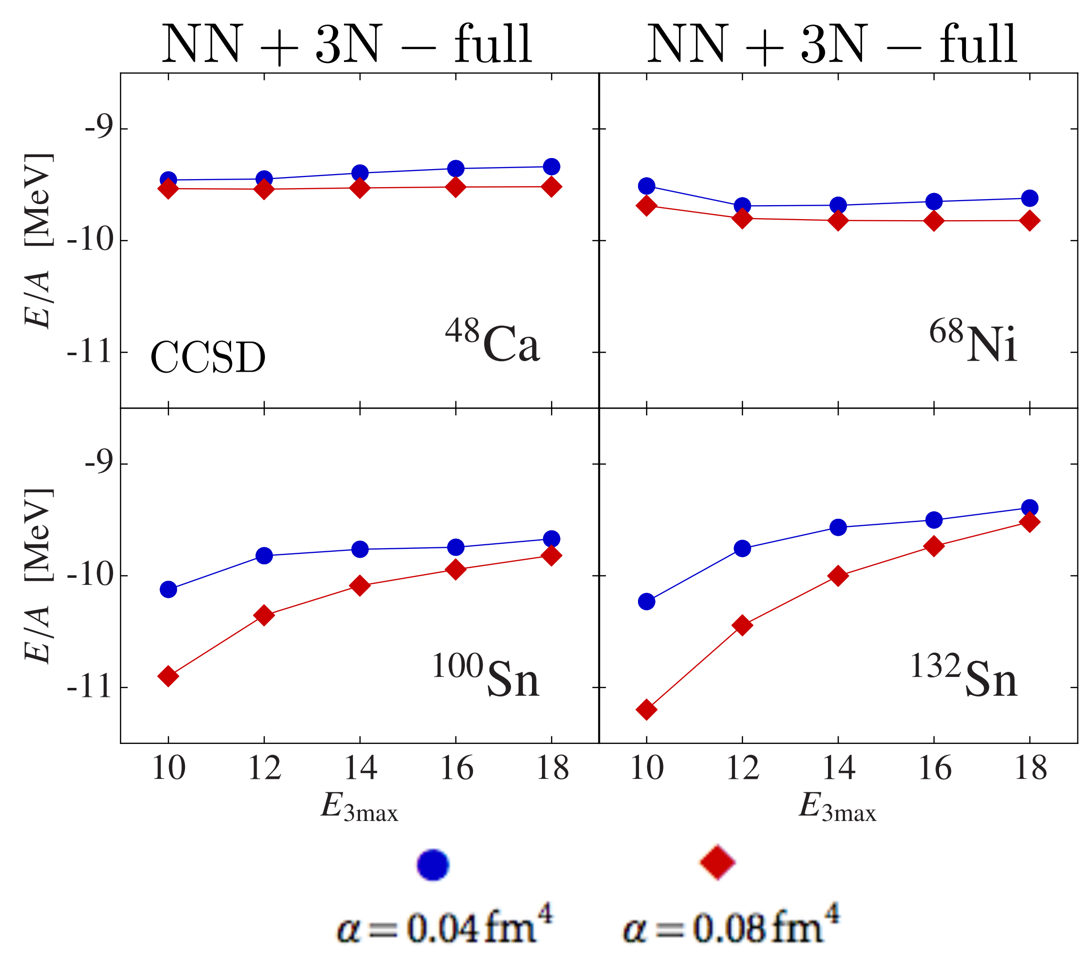

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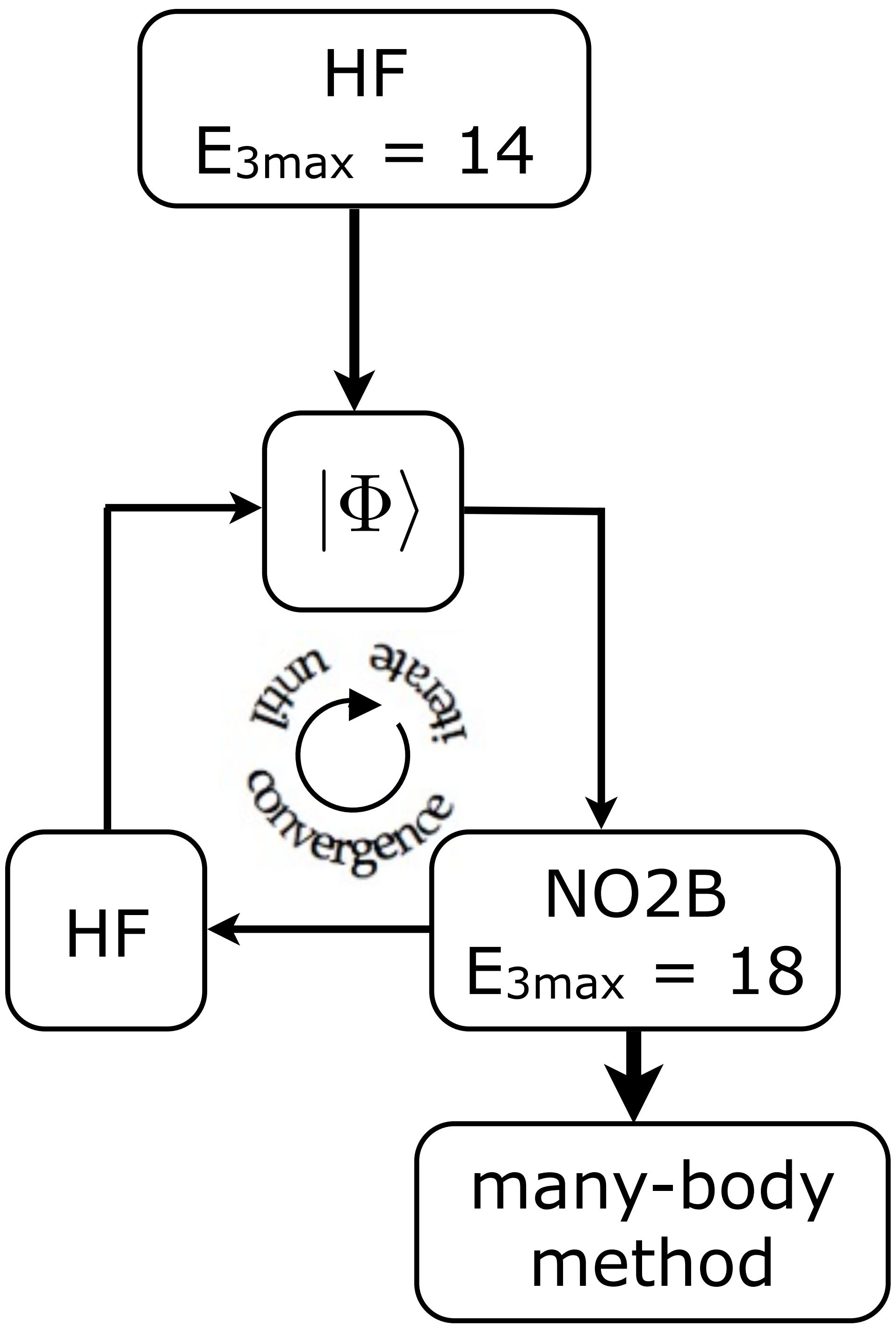

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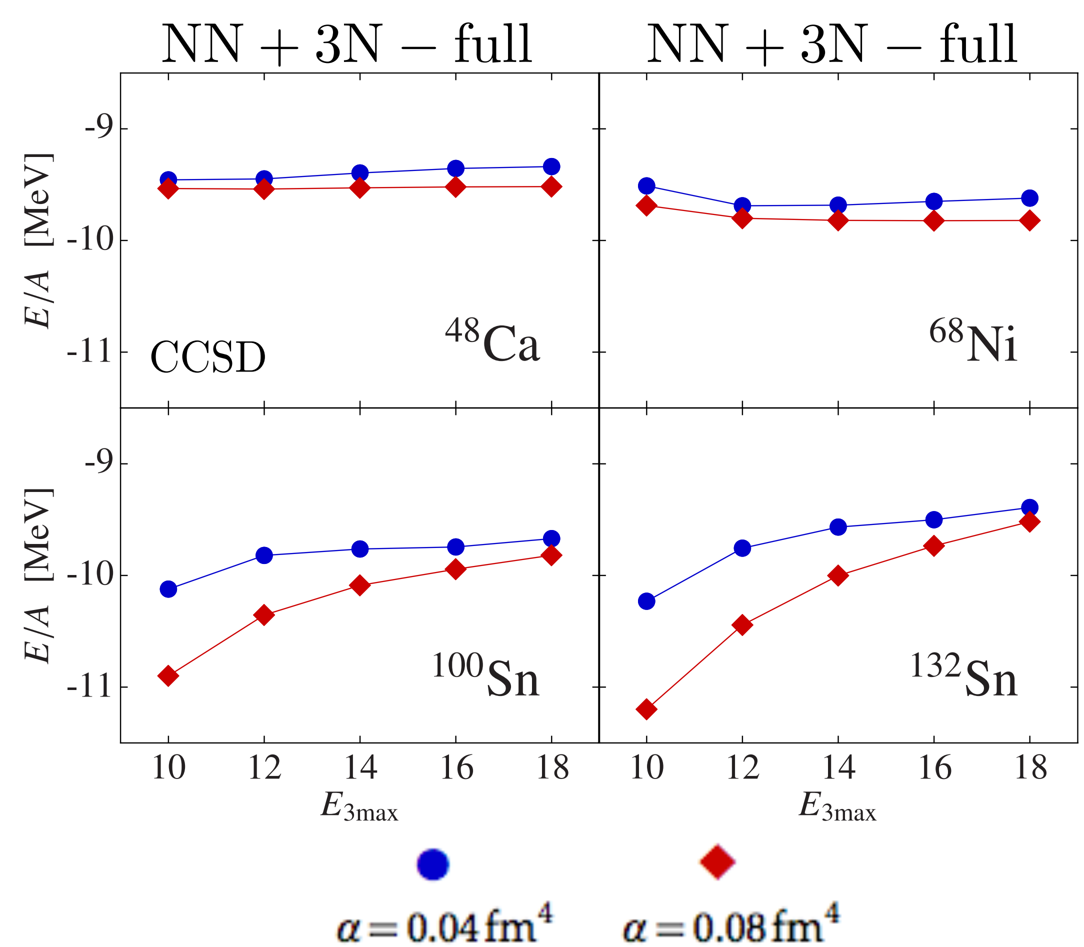
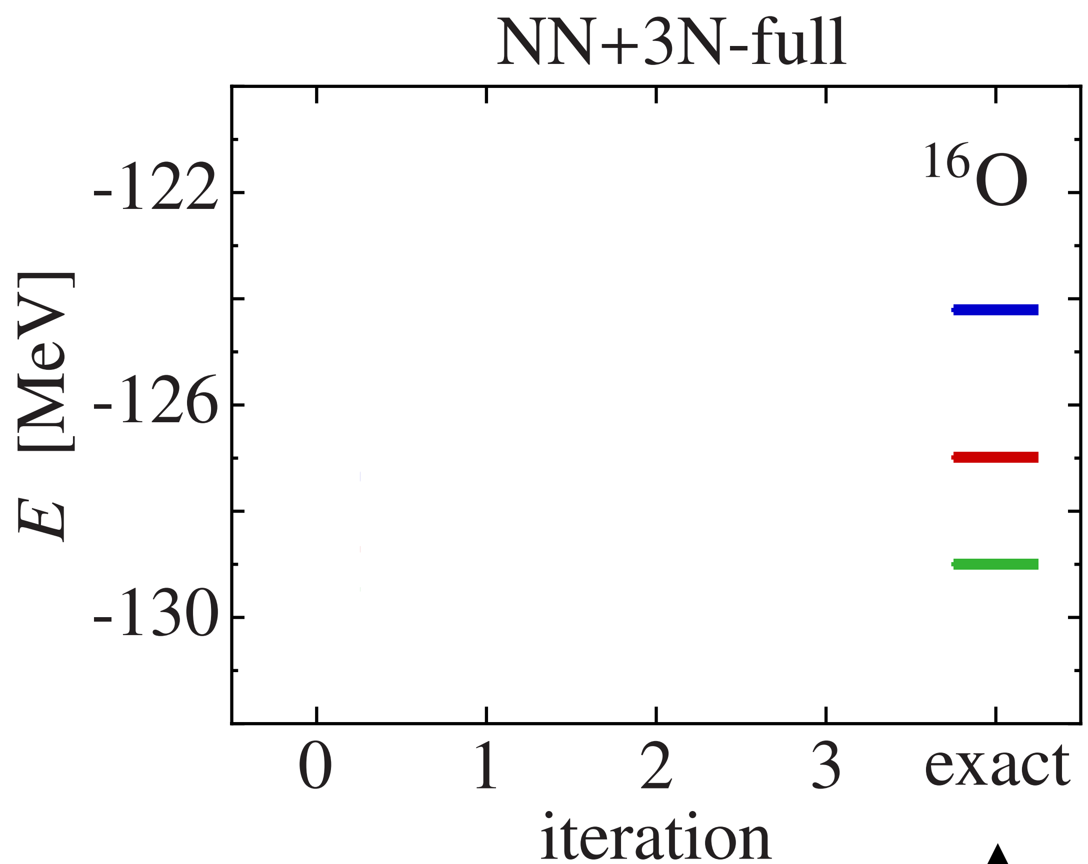


- simple protocol to **avoid using full sets** of large-E_{3max} matrix elements
- large-E_{3max} information enters via **NO2B**

Normal–Ordering Procedure

- **Example**: normal ordering for E_{3max} = 14



$|\Phi(E_{3\text{max}} = 14)\rangle$

CCSD

$\alpha = 0.02\,\text{fm}^4$ $\alpha = 0.04\,\text{fm}^4$ $\alpha = 0.08\,\text{fm}^4$

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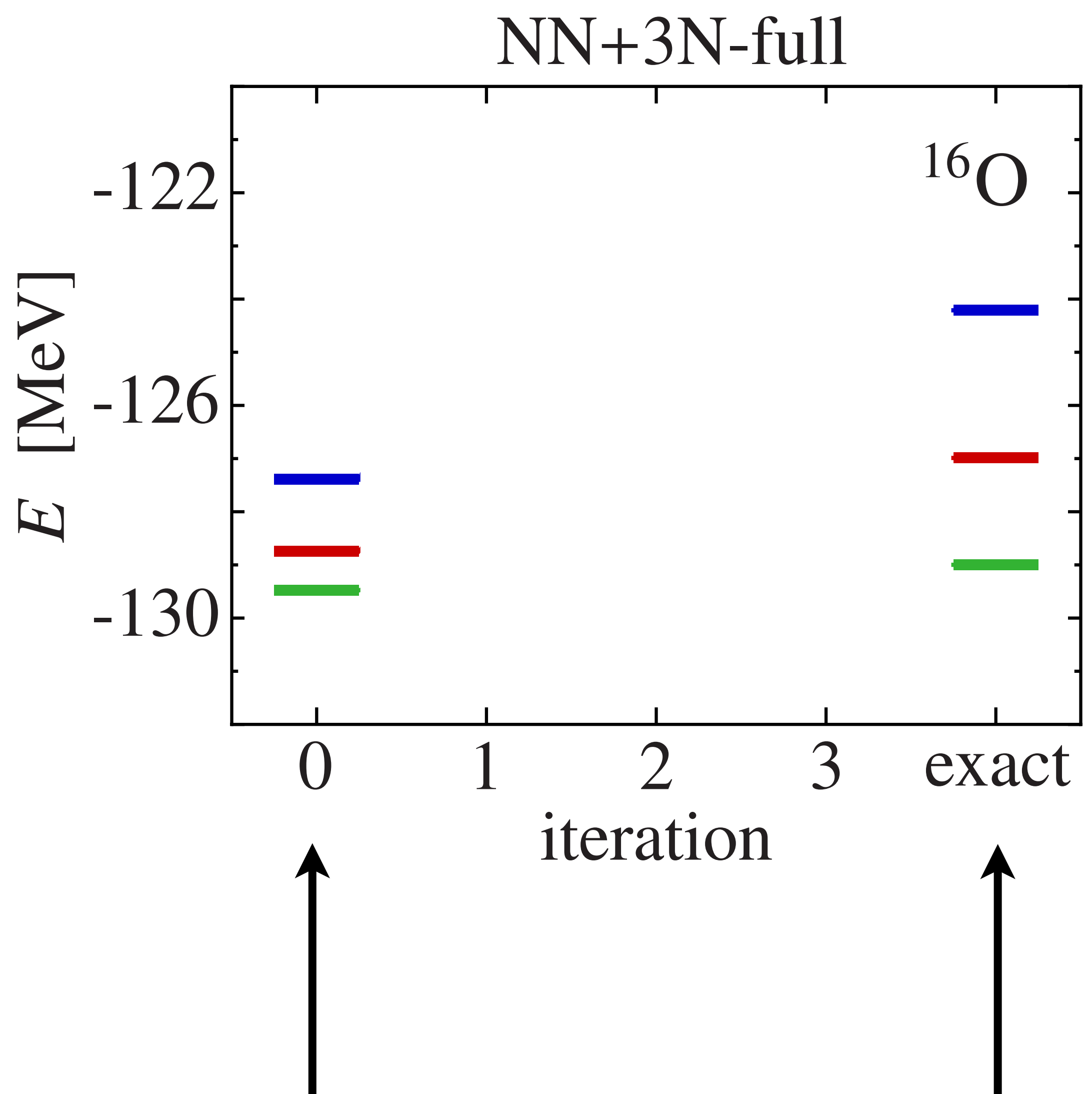

$|\Phi(E_{3\max} = 8)\rangle$

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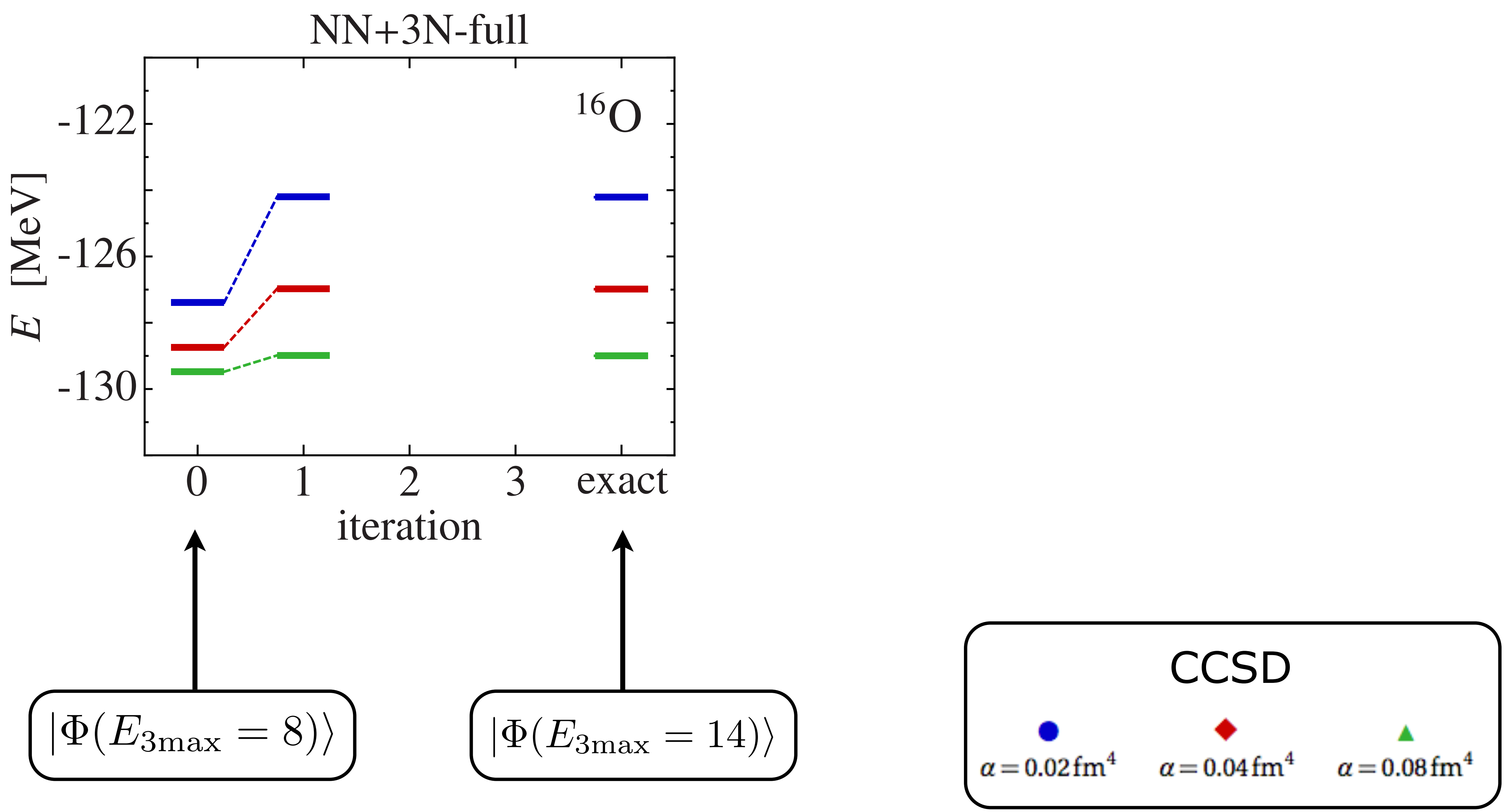

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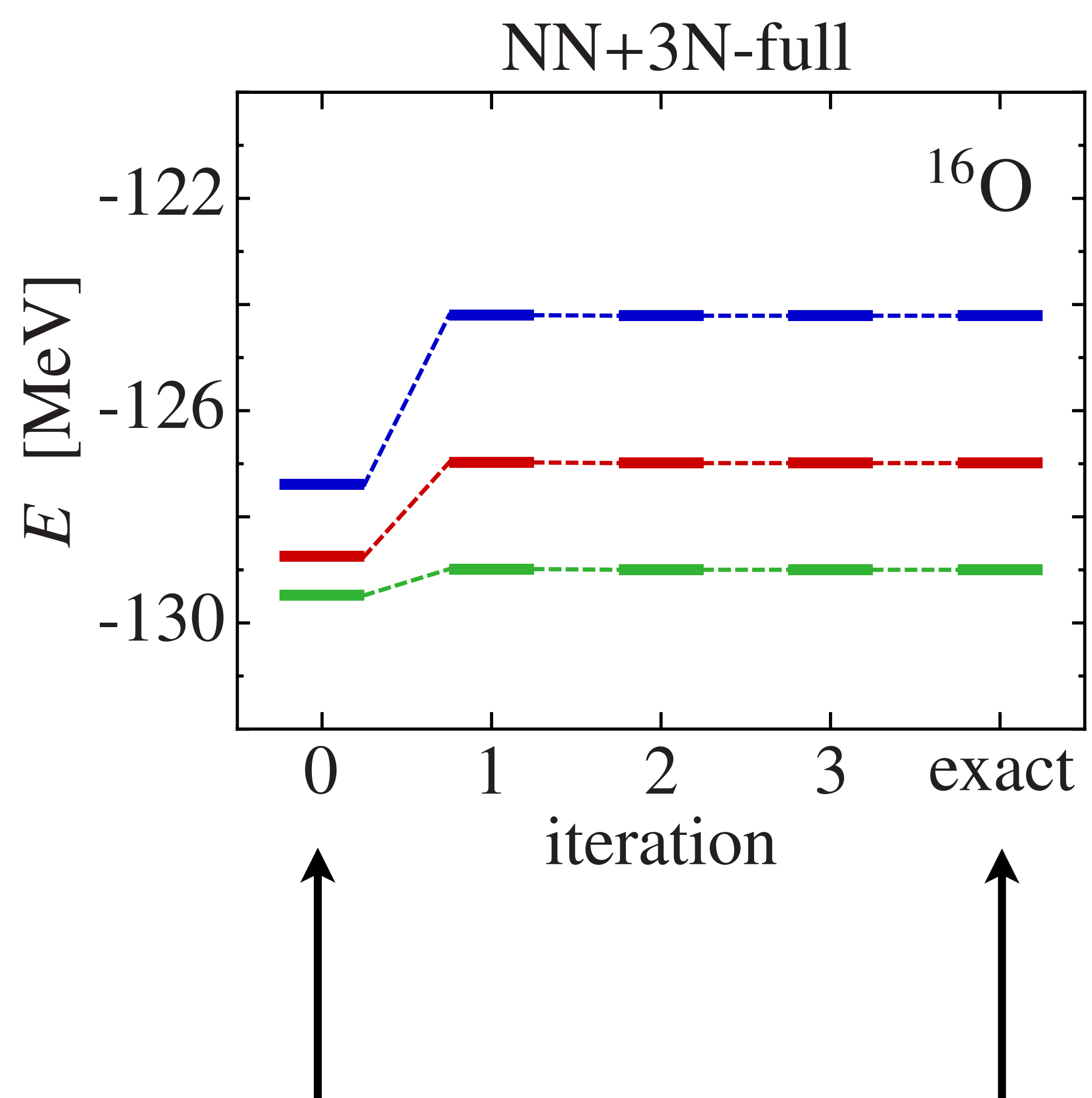

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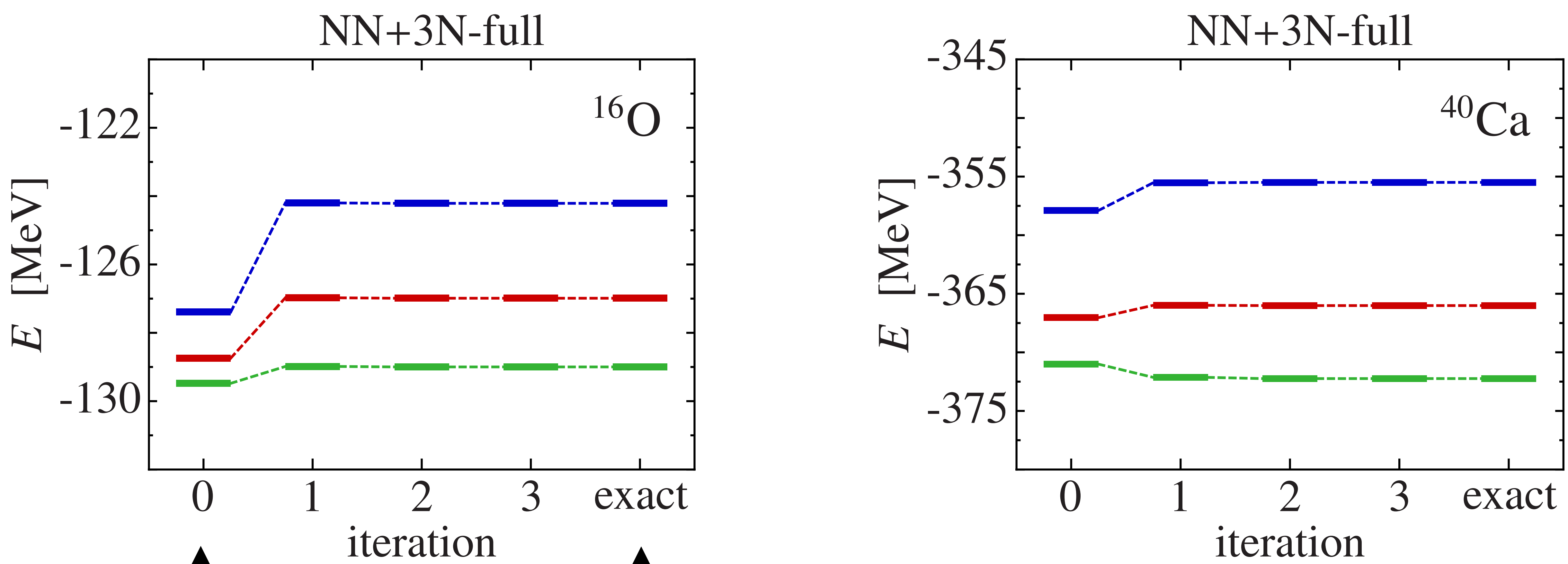

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Coupled-Cluster Triples Corrections

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

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

S. Binder, P. Piecuch, A. Calci, J. Langhammer, R. Roth --- Phys. Rev. C 88, 054319 (2013)

P. Piecuch, M. Wloch --- J. Chem. Phys. 123, 224105 (2005)

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perturbation theory

$$\Lambda\mathrm{CCSD(T)}$$

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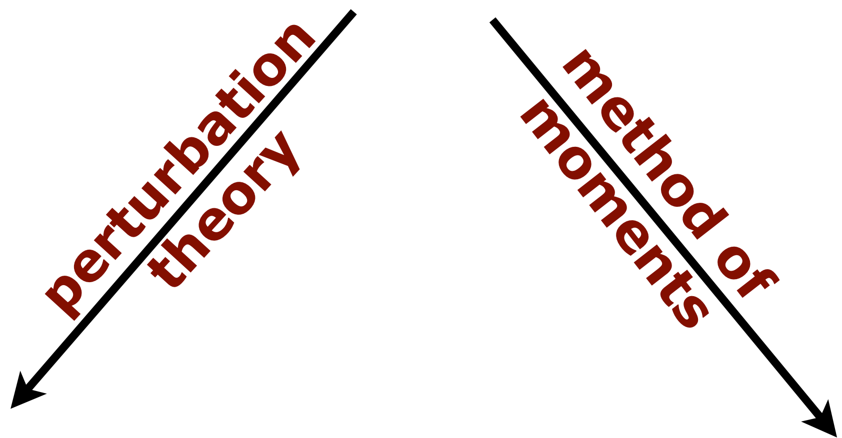

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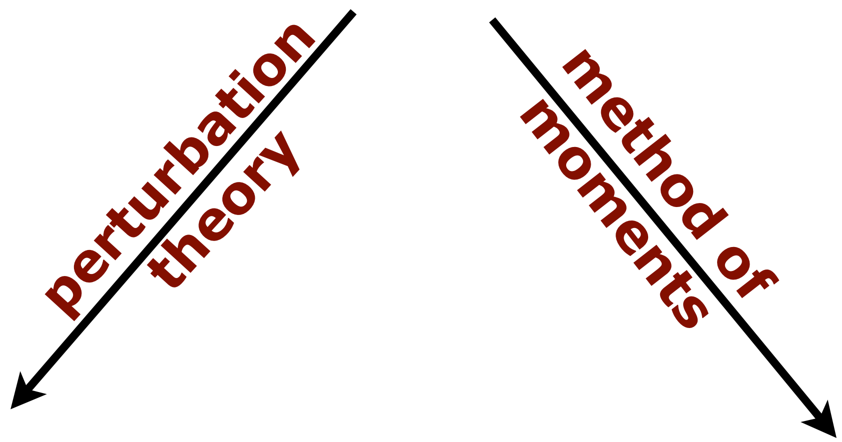

$$\Lambda\mathrm{CCSD(T)} \qquad\qquad \mathrm{CR-CC(2,3)}$$

- Non-iterative **triples corrections**

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ΛCCSD(T) and CR-CC(2,3) in Chemistry

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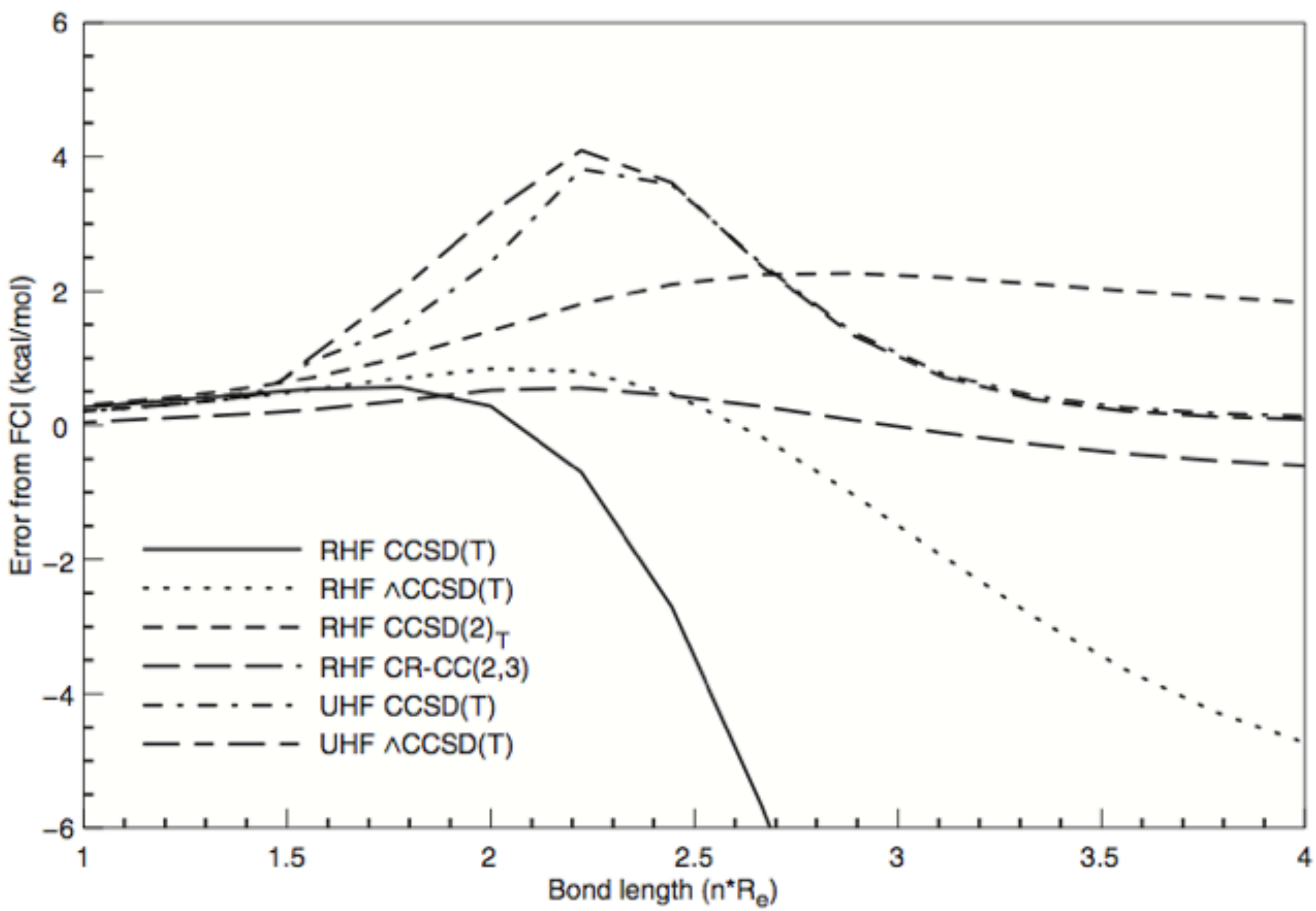
Alternative perturbation theories for triple excitations in coupled-cluster theory

Andrew G. Taube*†



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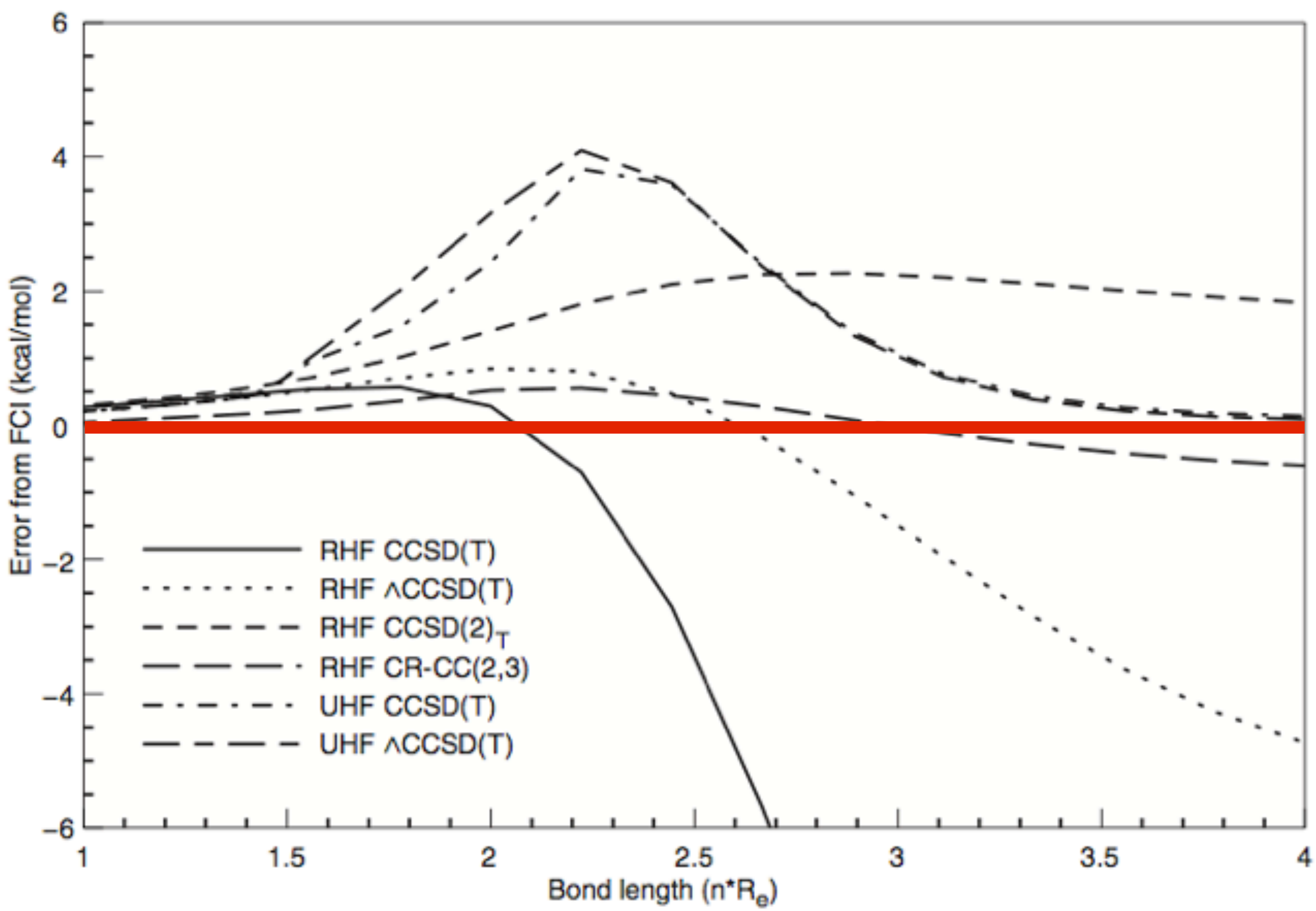

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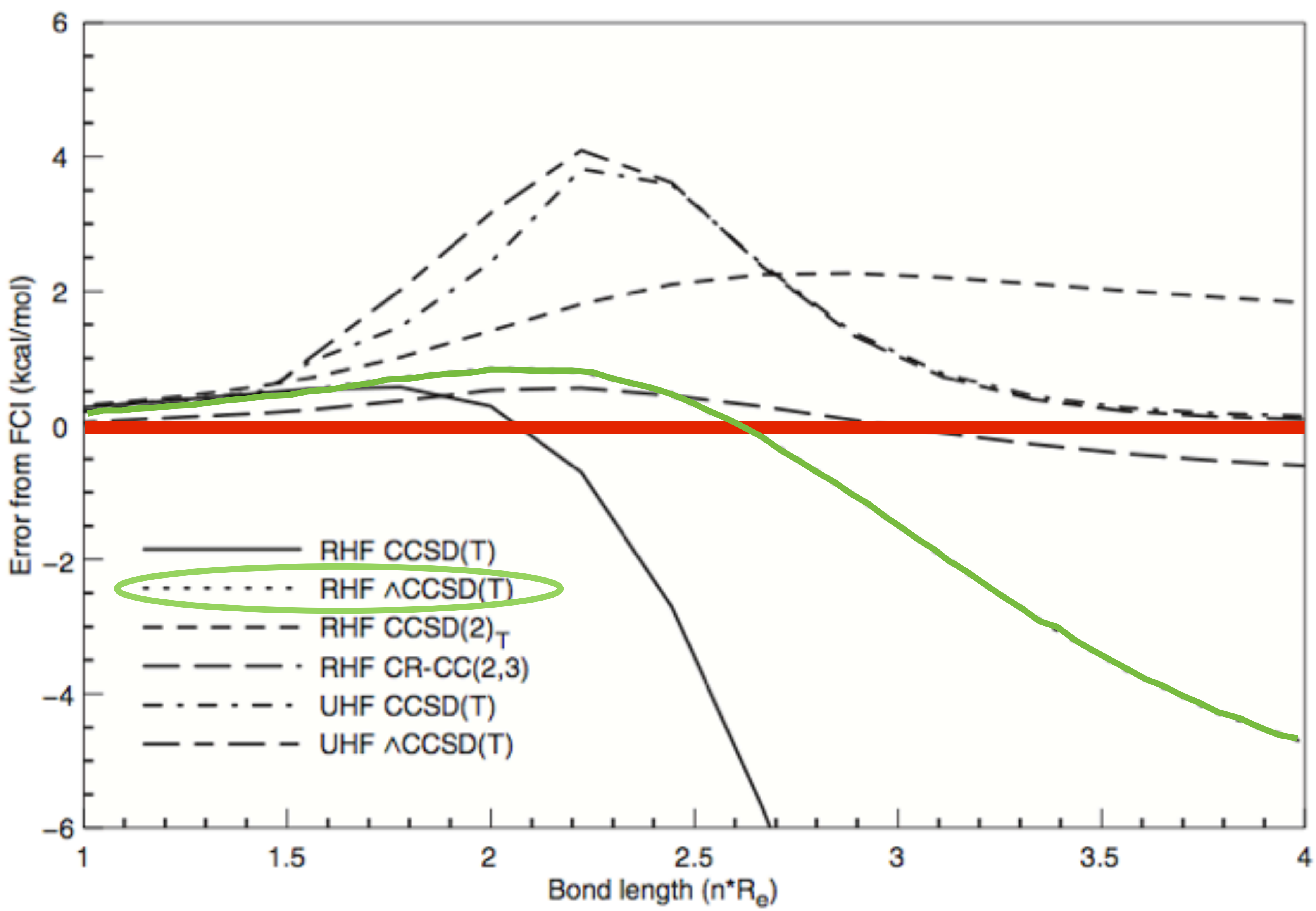

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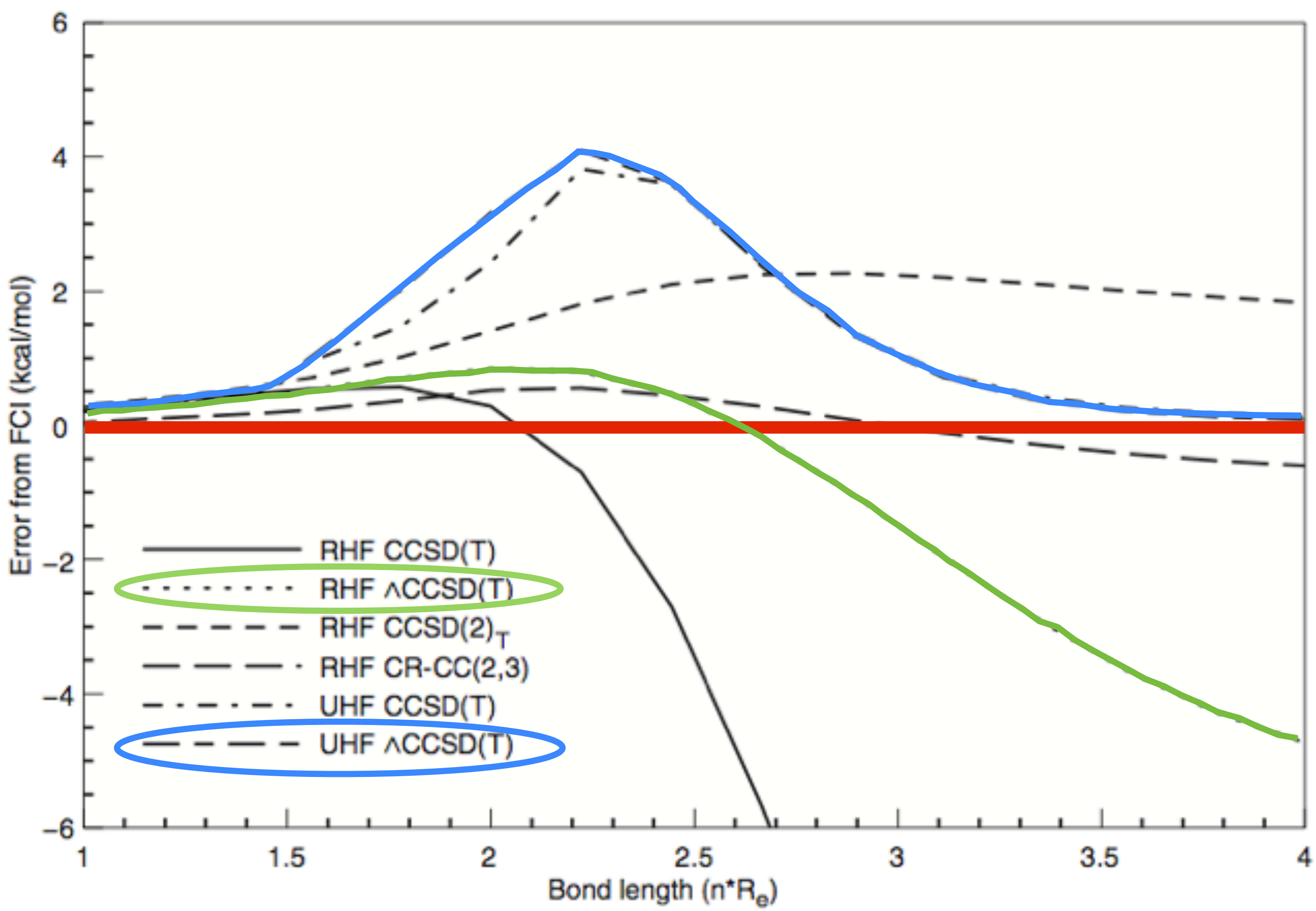

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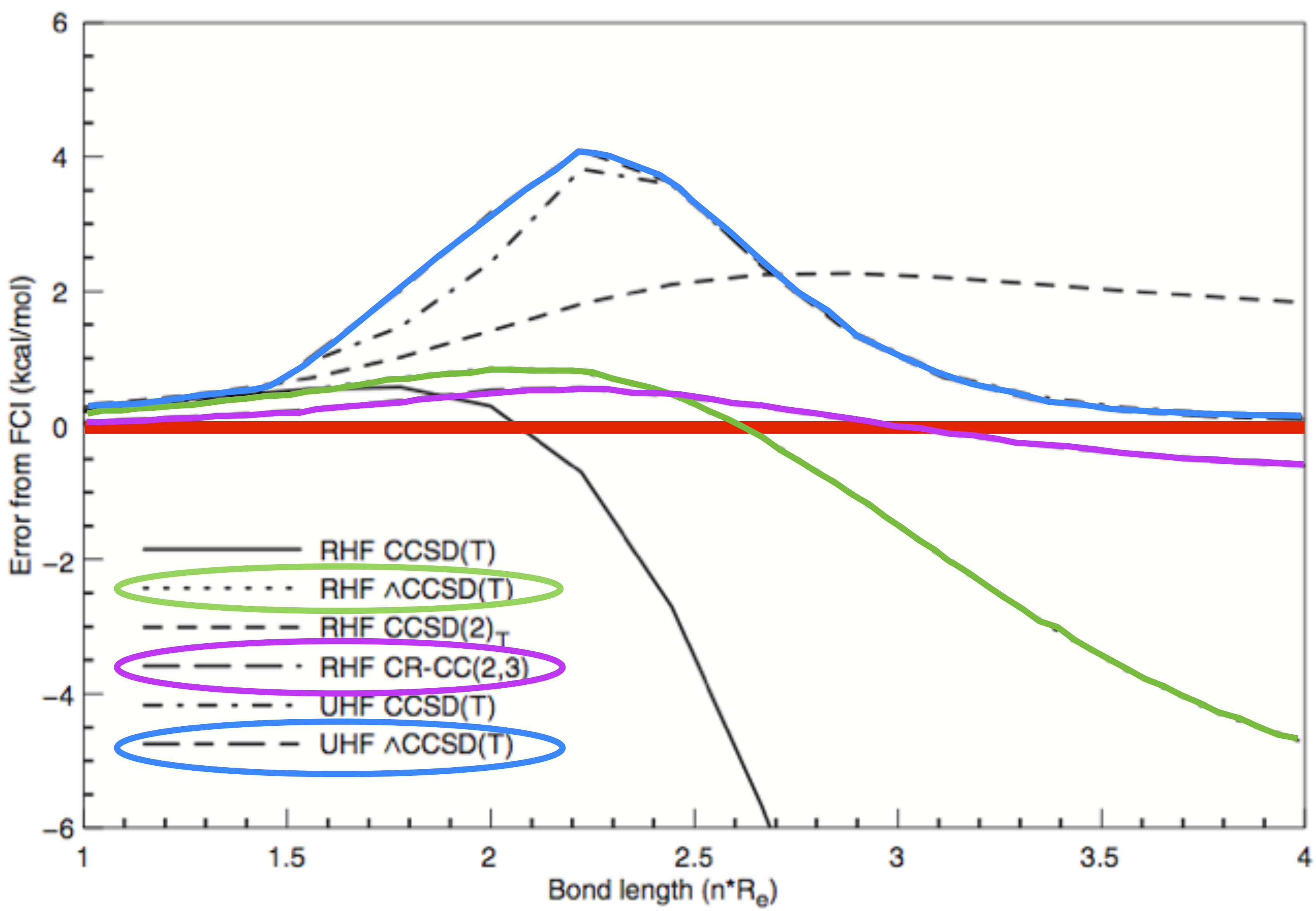

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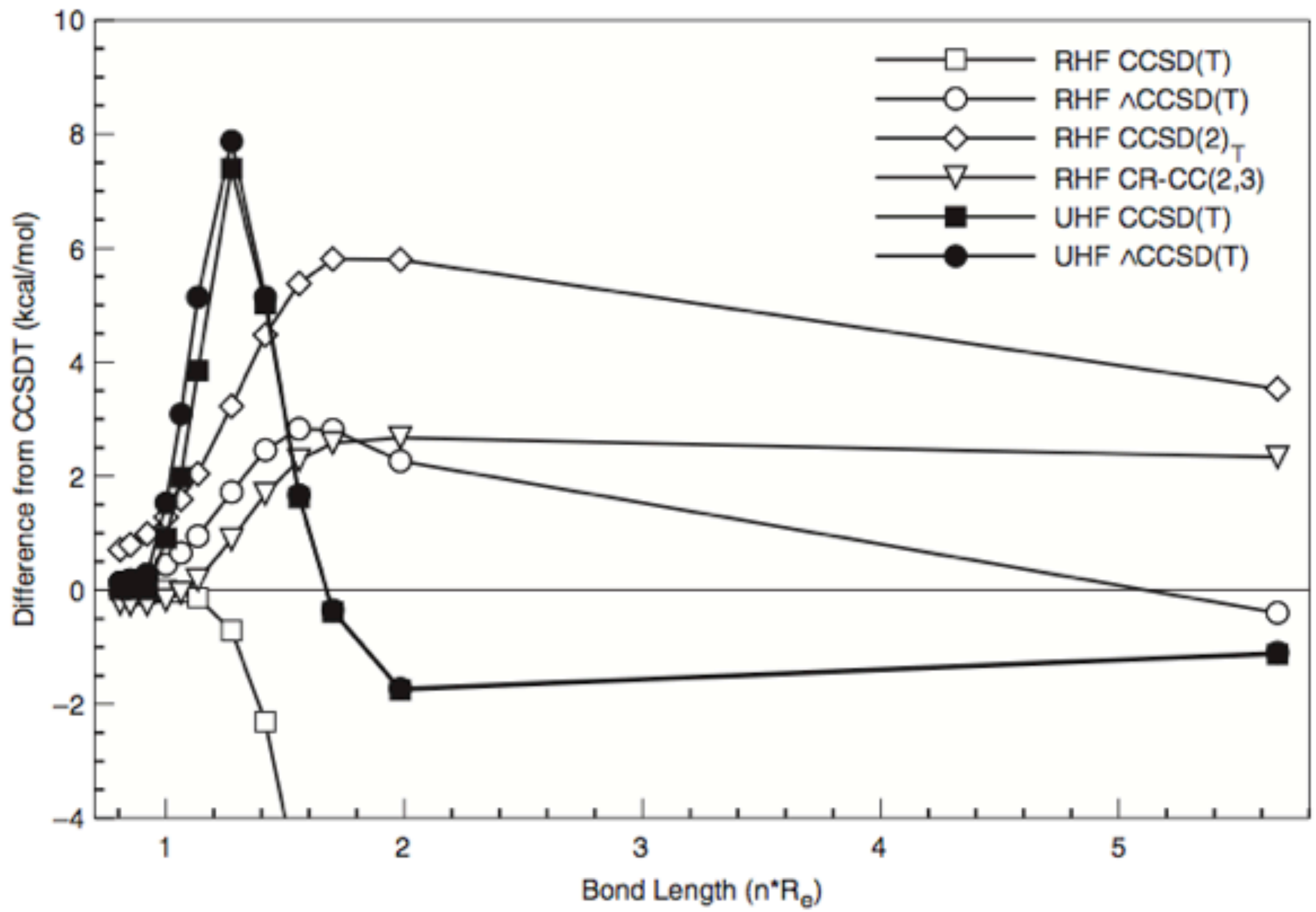

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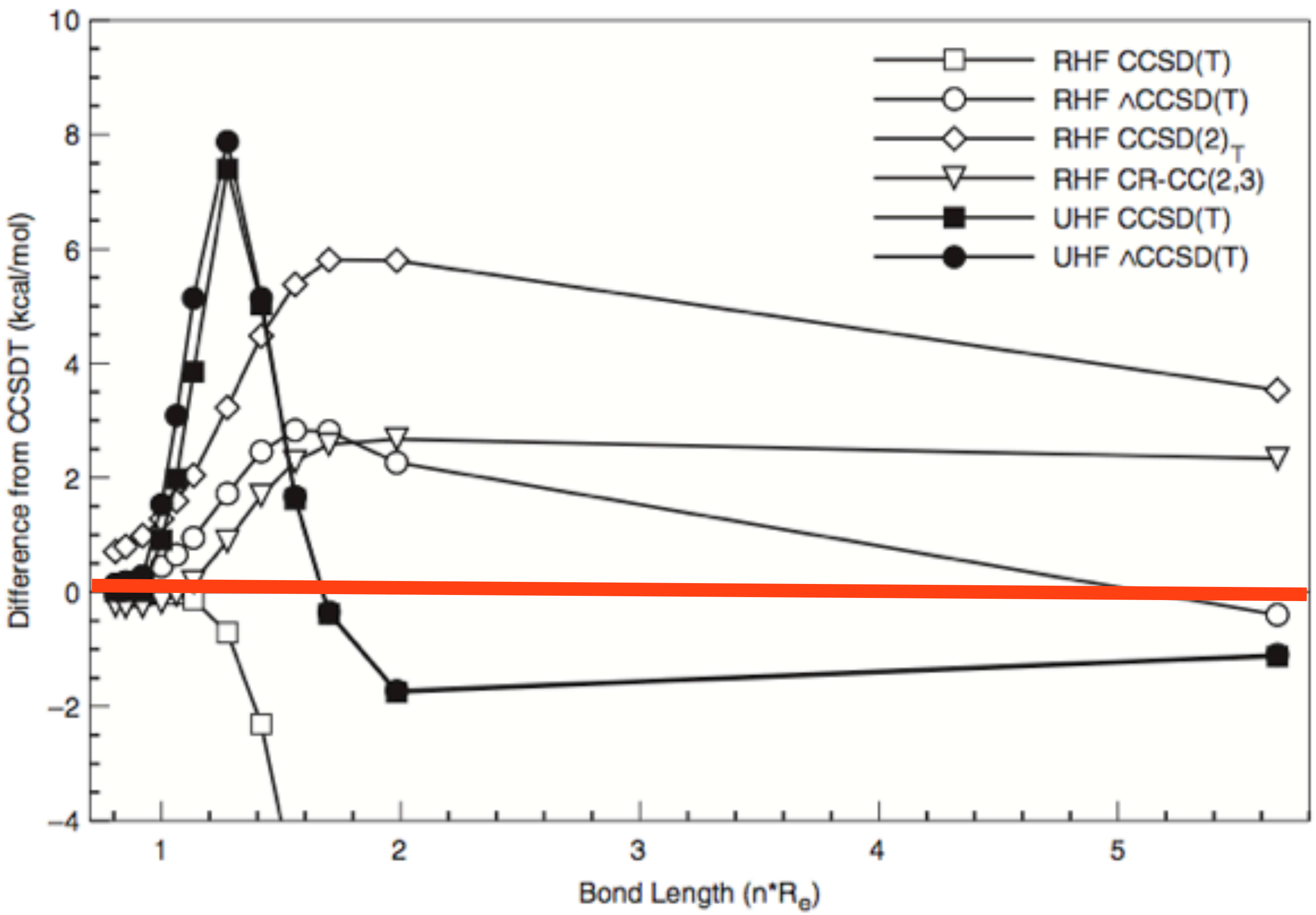

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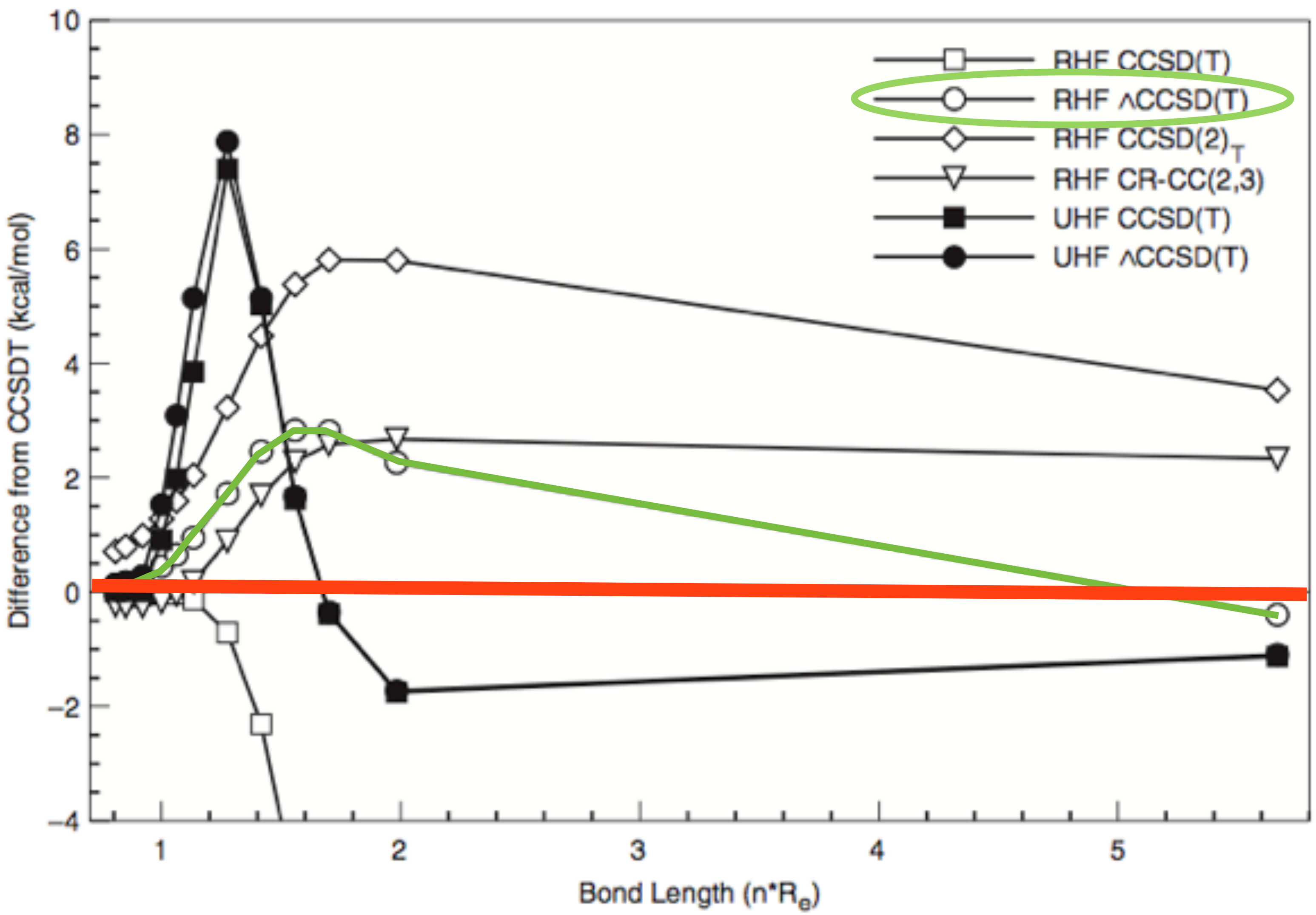

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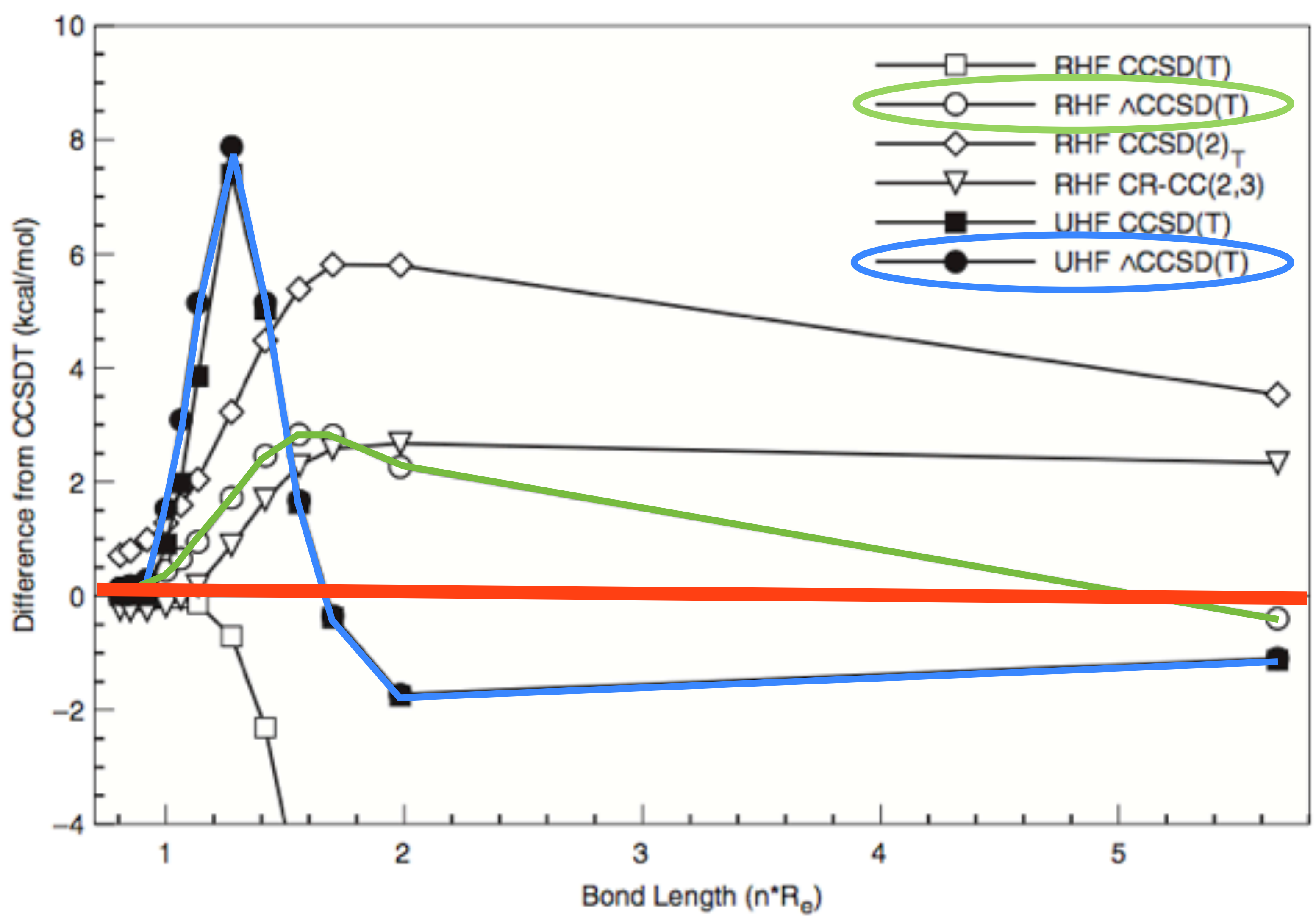

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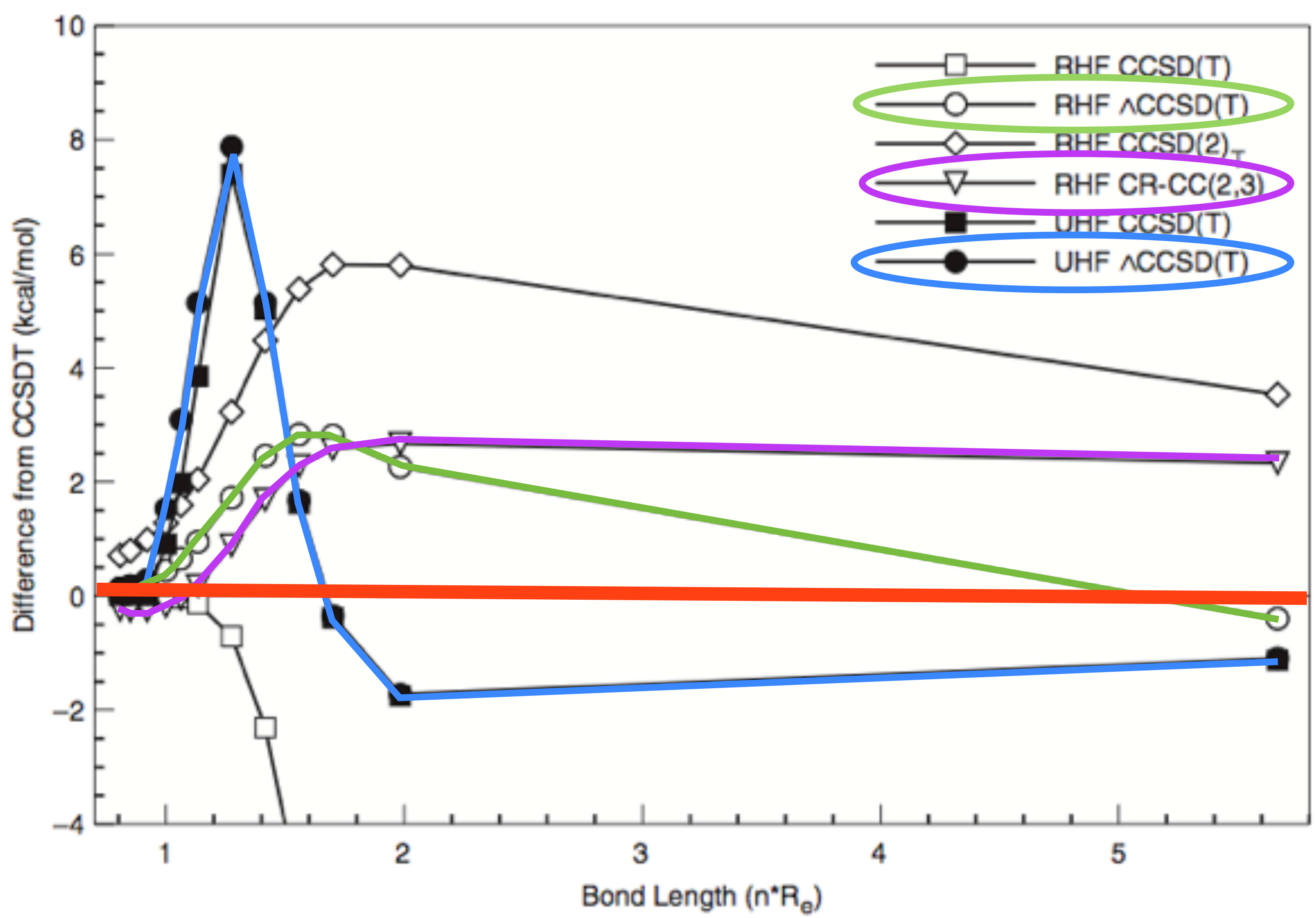

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Denominators in ΛCCSD(T), CR-CC(2,3)

$$\delta E^{(\mathrm{T})} = \frac{1}{(3!)^2} \sum_{\substack{abc \\ ijk}} \mathfrak{L}^{ijk}_{abc} \, \frac{1}{D^{abc}_{ijk}} \, \mathfrak{R}^{abc}_{ijk}$$

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  - **Two**- and **three-body** matrix elements of $\hat{\mathcal{H}} = e^{-\hat{T}} \hat{H}_N e^{\hat{T}}$ in denominator **cannot be treated exactly** in spherical formulation

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  - **Two**- and **three-body** matrix elements of $\hat{\mathcal{H}} = e^{-\hat{T}} \hat{H}_N e^{\hat{T}}$ in denominator **cannot be treated exactly** in spherical formulation
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Denominators in ΛCCSD(T), CR-CC(2,3)

$$\delta E^{(\mathrm{T})} = \frac{1}{(3!)^2} \sum_{\substack{abc\\ijk}} \mathfrak{L}^{ijk}_{abc} \frac{1}{D^{abc}_{ijk}} \mathfrak{R}^{abc}_{ijk}$$

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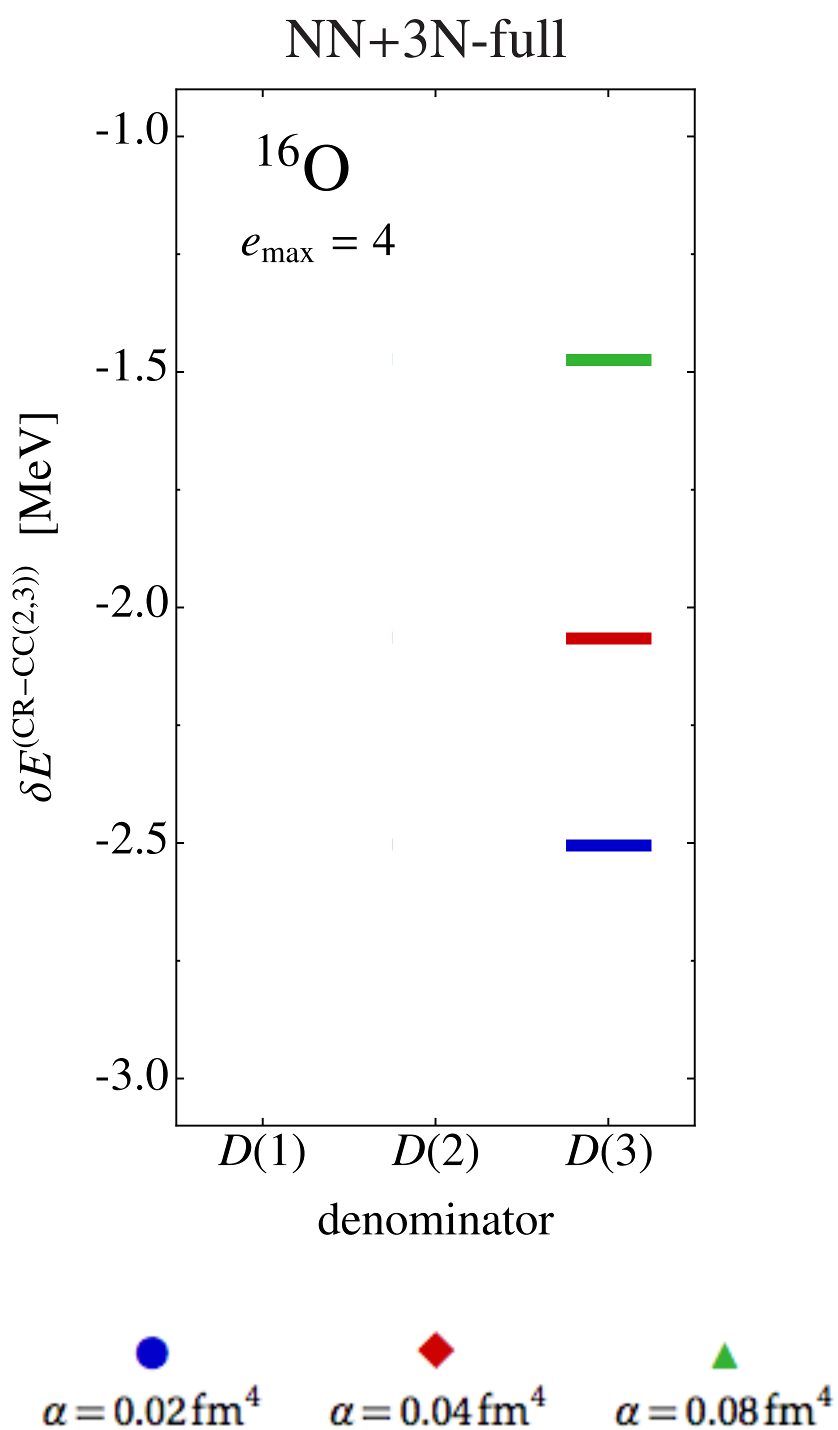
$$\Rightarrow D^{abc}_{ijk} \approx \overline{D}^{abc}_{ijk} = \mathcal{H}^i_i + \cdots + \overline{\mathcal{H}}^{ij}_{ij} + \cdots + \overline{\mathcal{H}}^{ijk}_{ijk} + \ldots$$

$$\overline{\mathcal{H}}^{p\ldots q}_{p\ldots q} = \frac{1}{(2j_p+1)\ldots(2j_q+1)} \sum_{m_p\ldots m_q} \mathcal{H}^{p\ldots q}_{p\ldots q}$$

Approximate CR–CC(2,3) Denominators

Option 1: Discard

- **D(k)**: up to **k-body** terms in denominator



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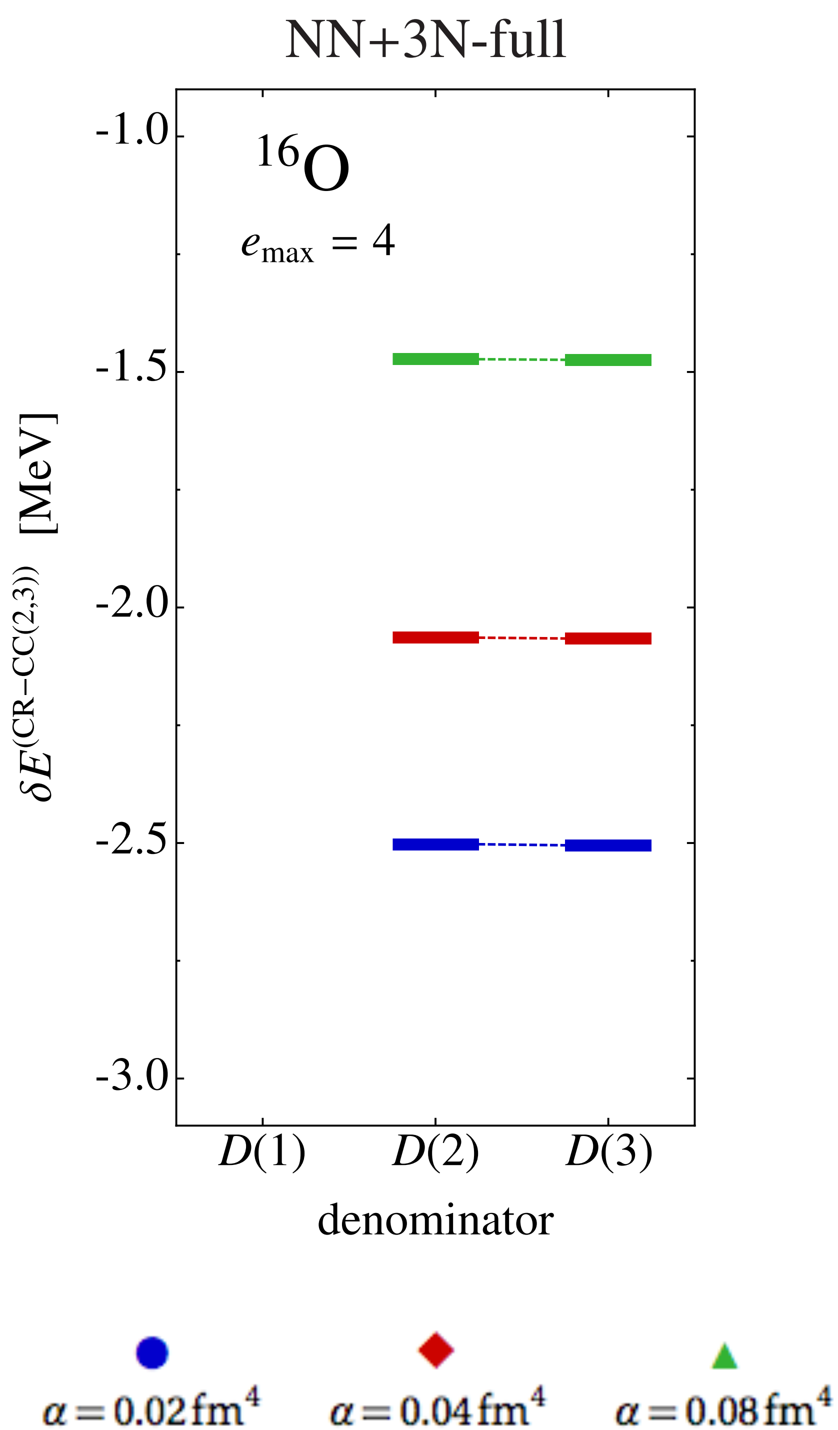

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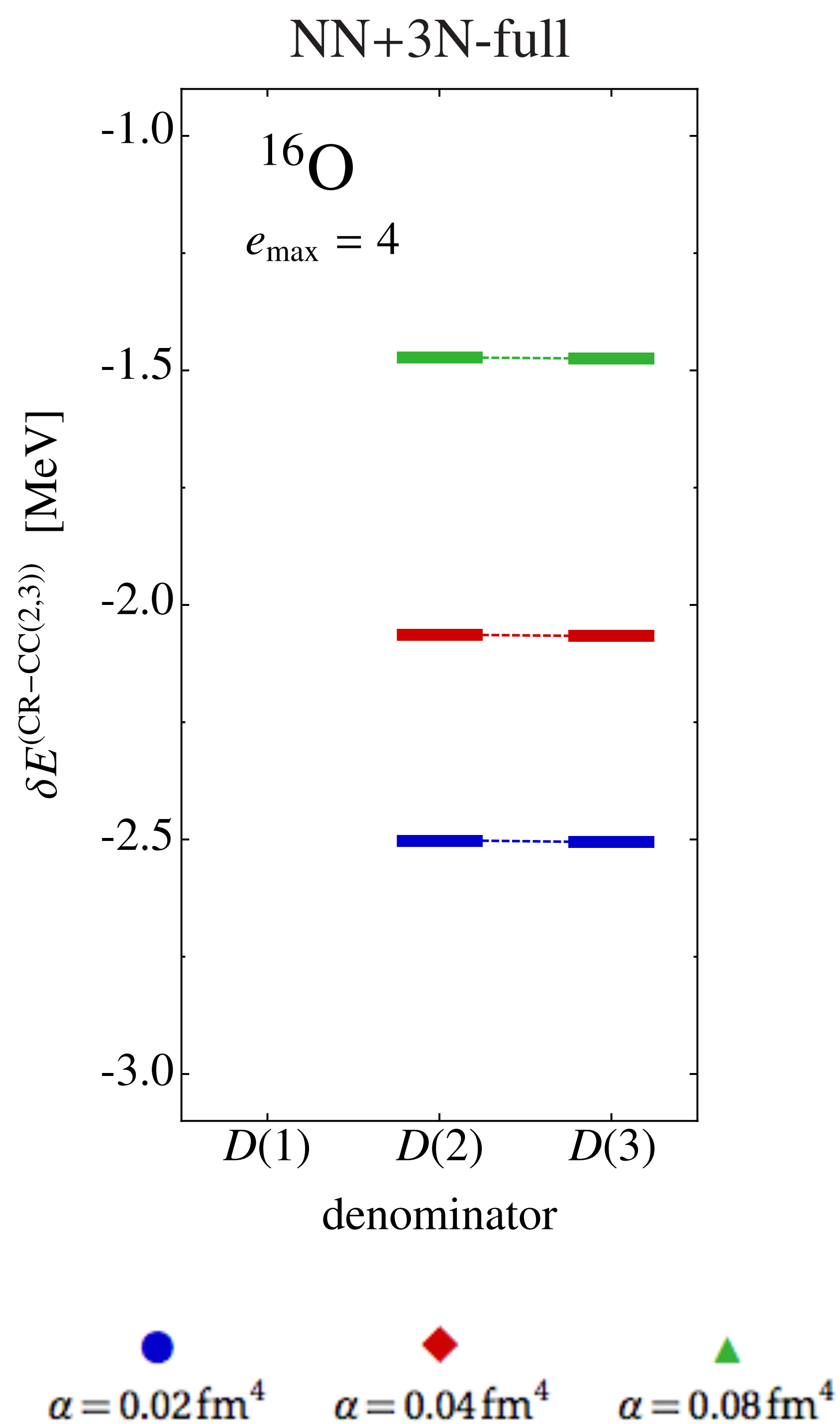

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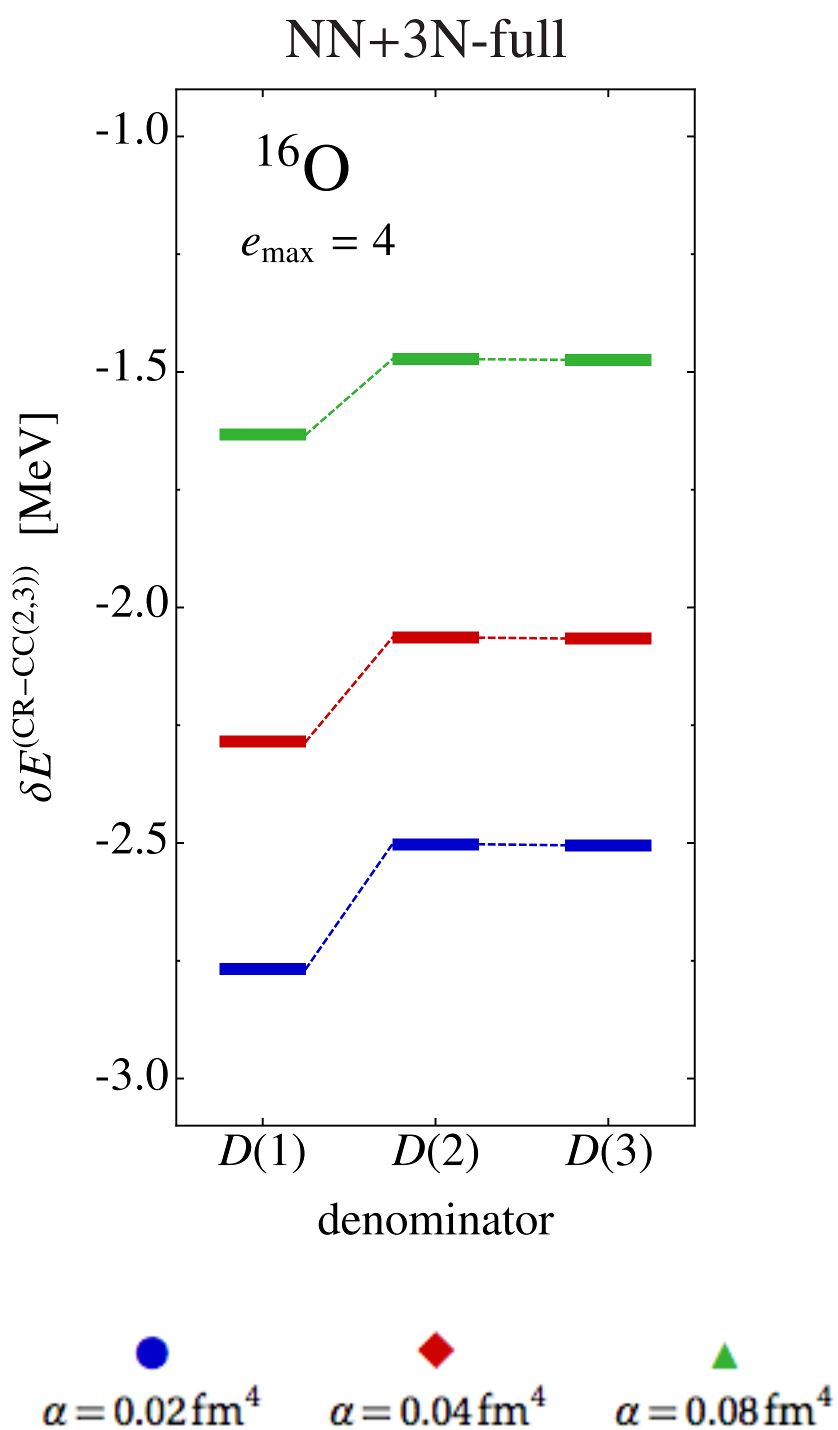

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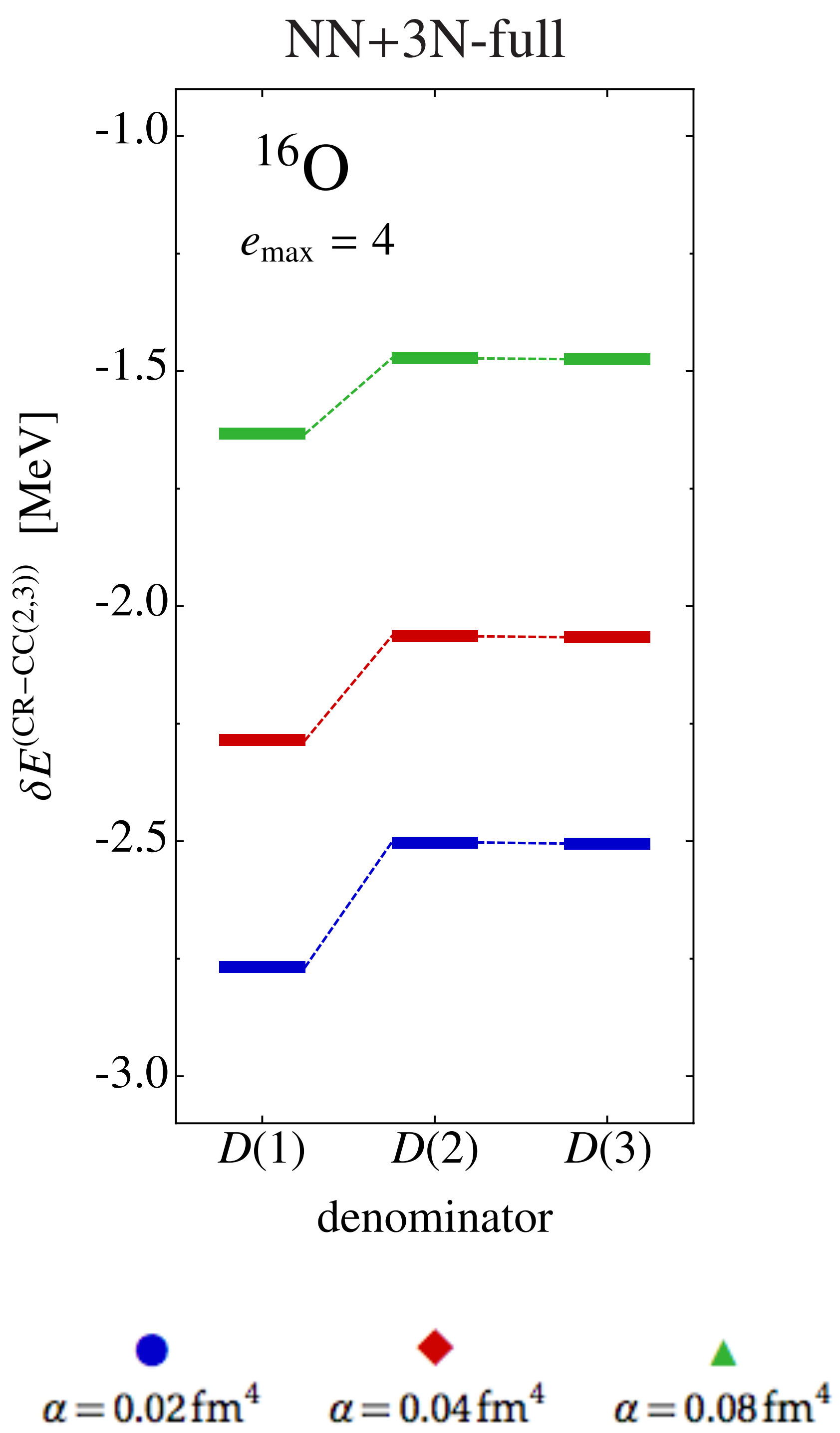

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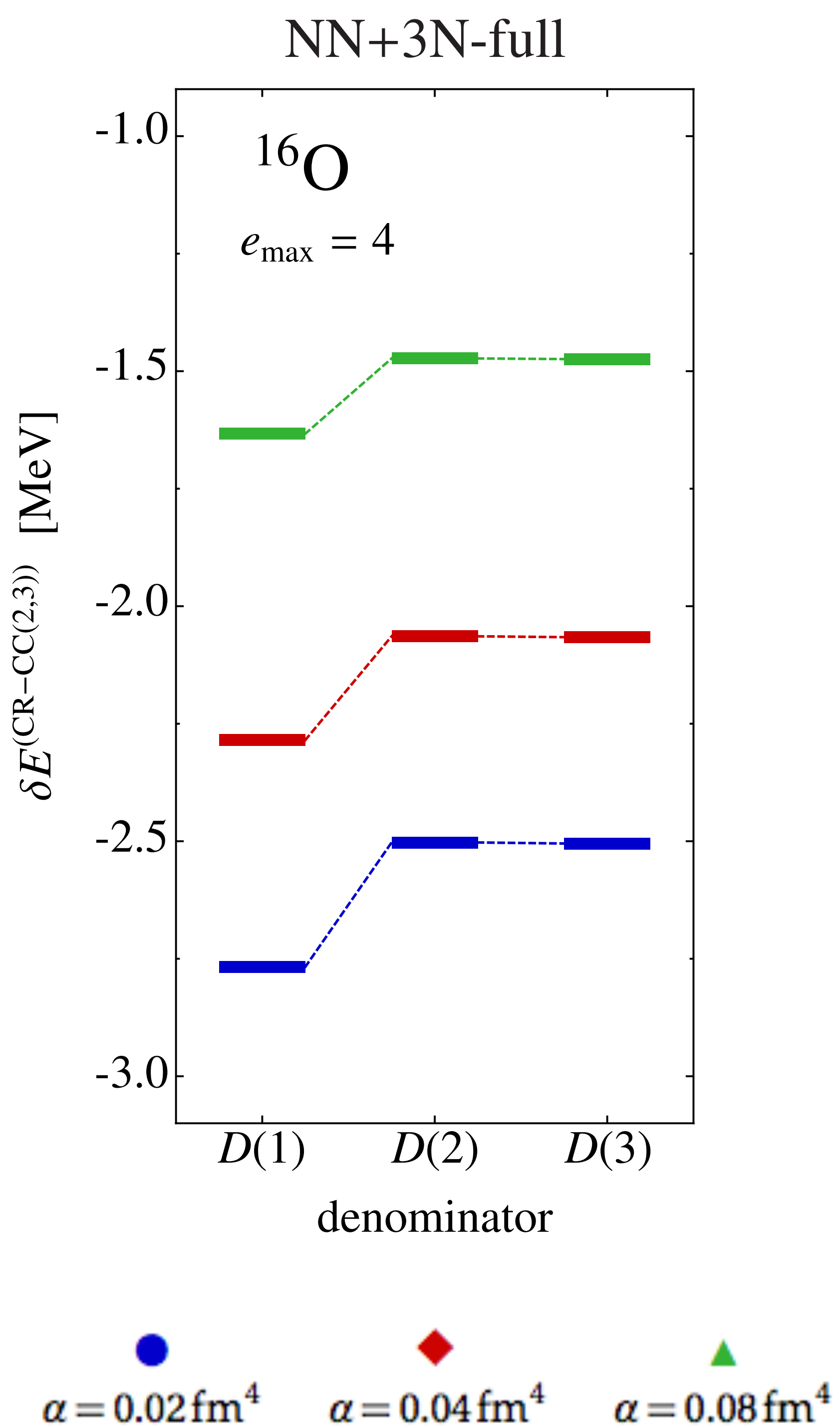

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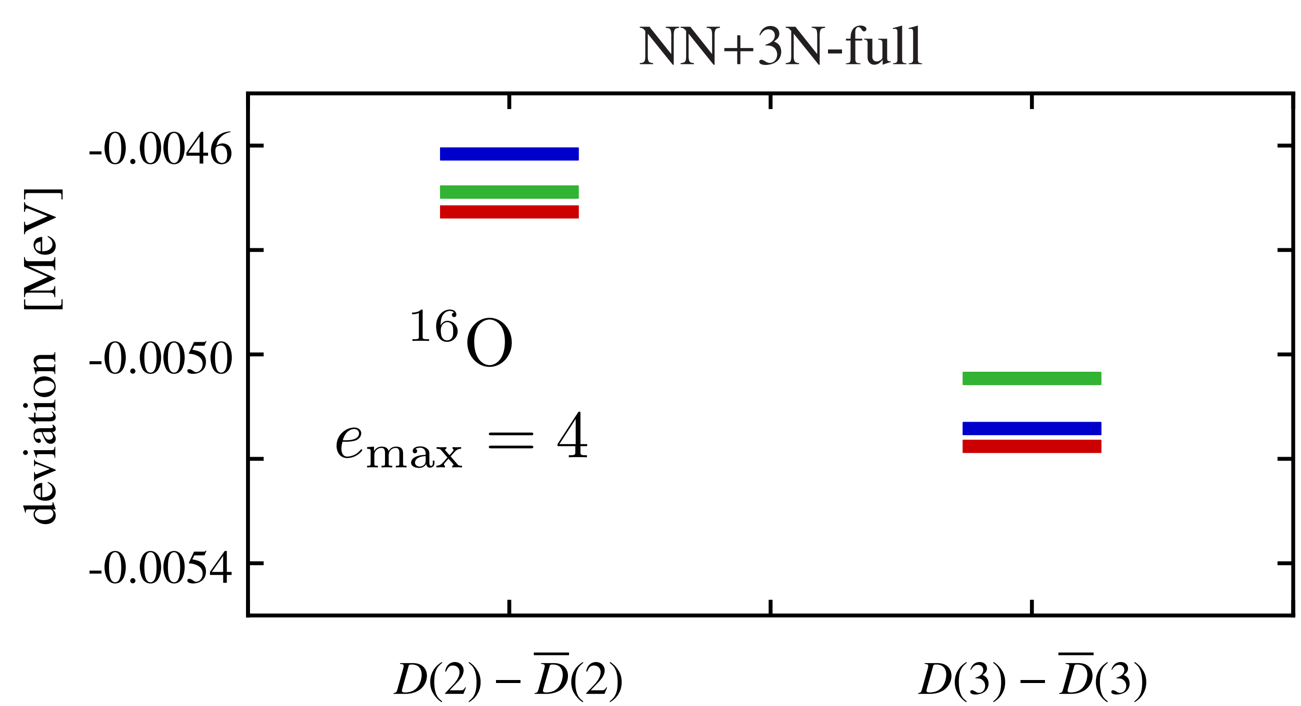
Option 2: Average



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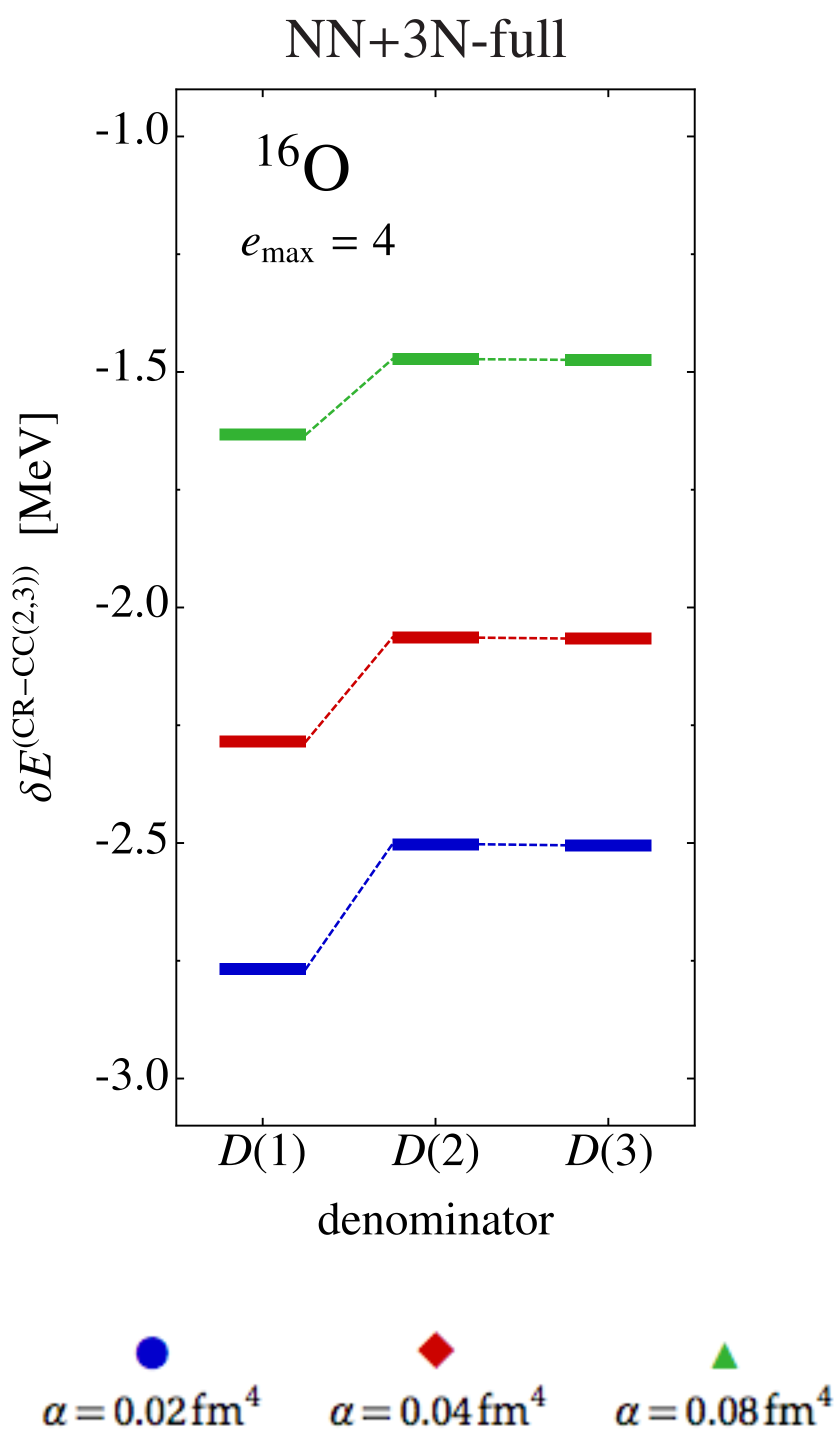

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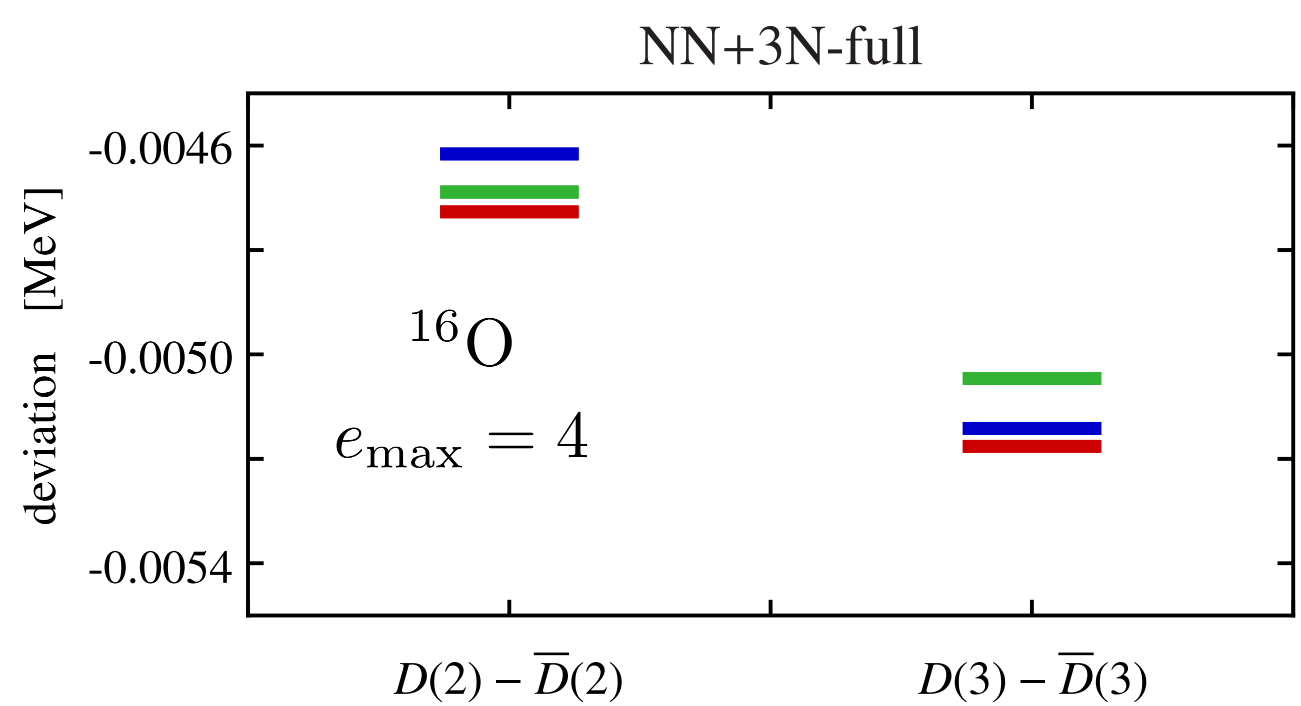
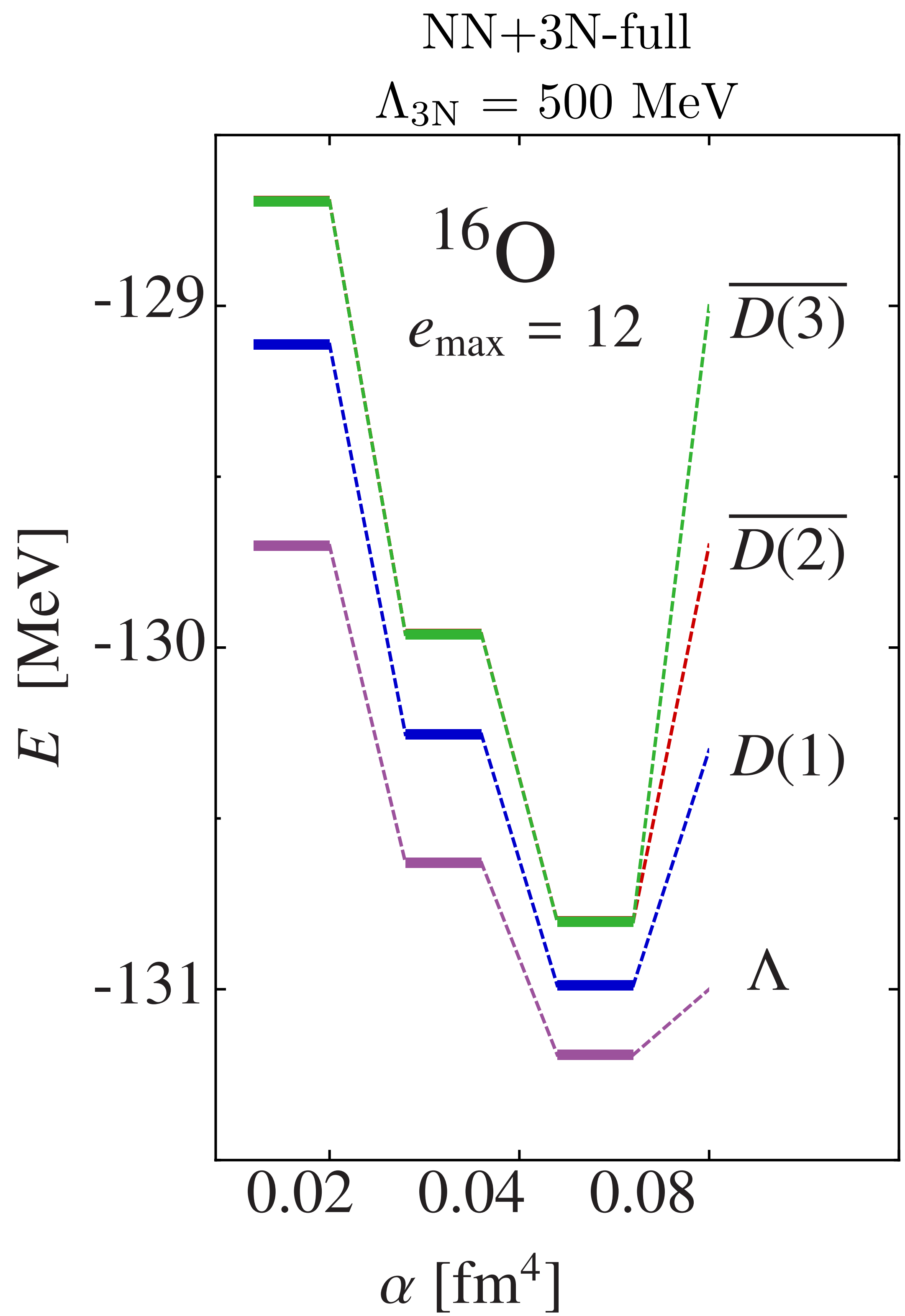


- Error from **averaging** ≈ **5 keV**

CR-CC(2,3) vs. ΛCCSD(T) and IT-NCSM



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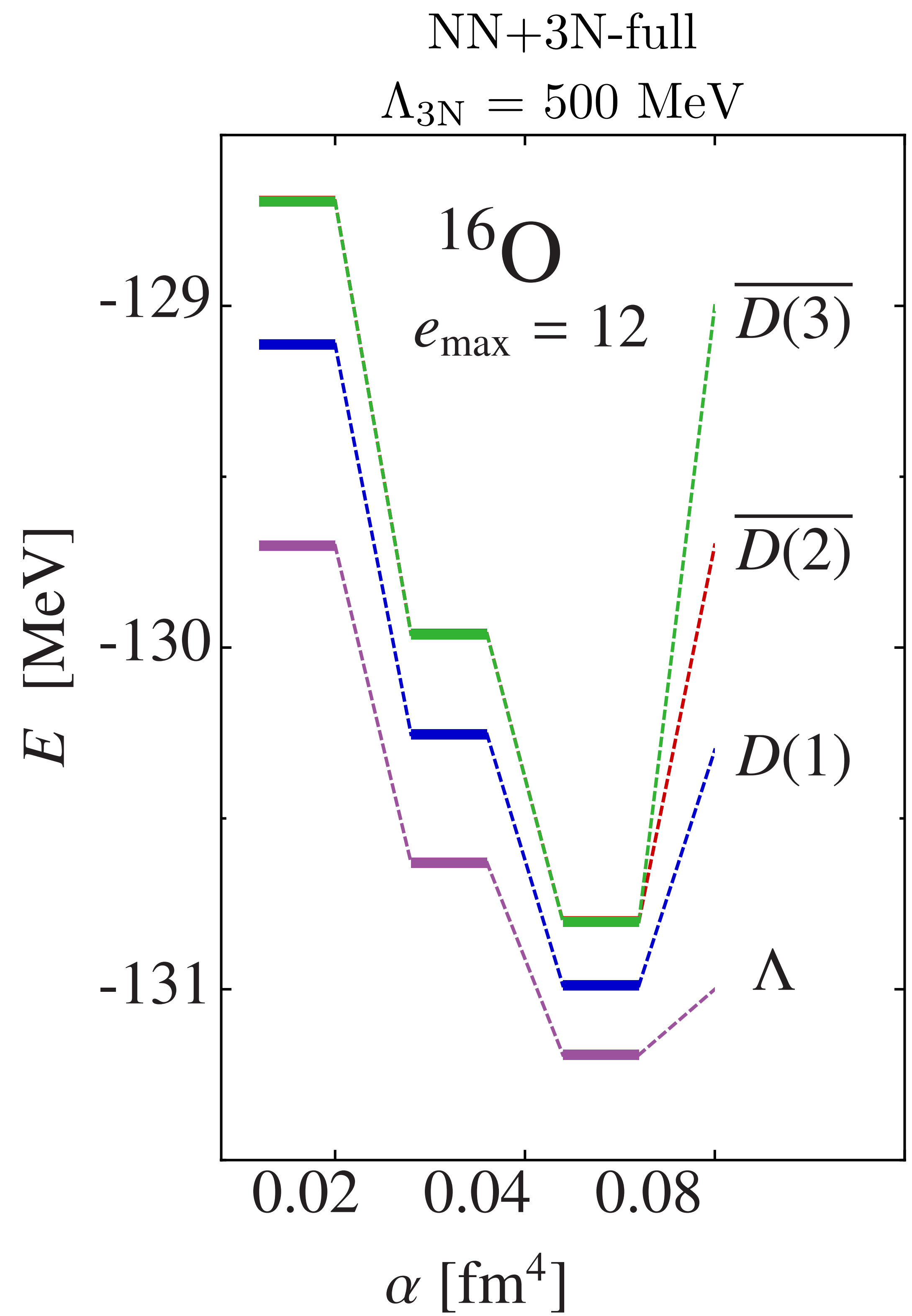
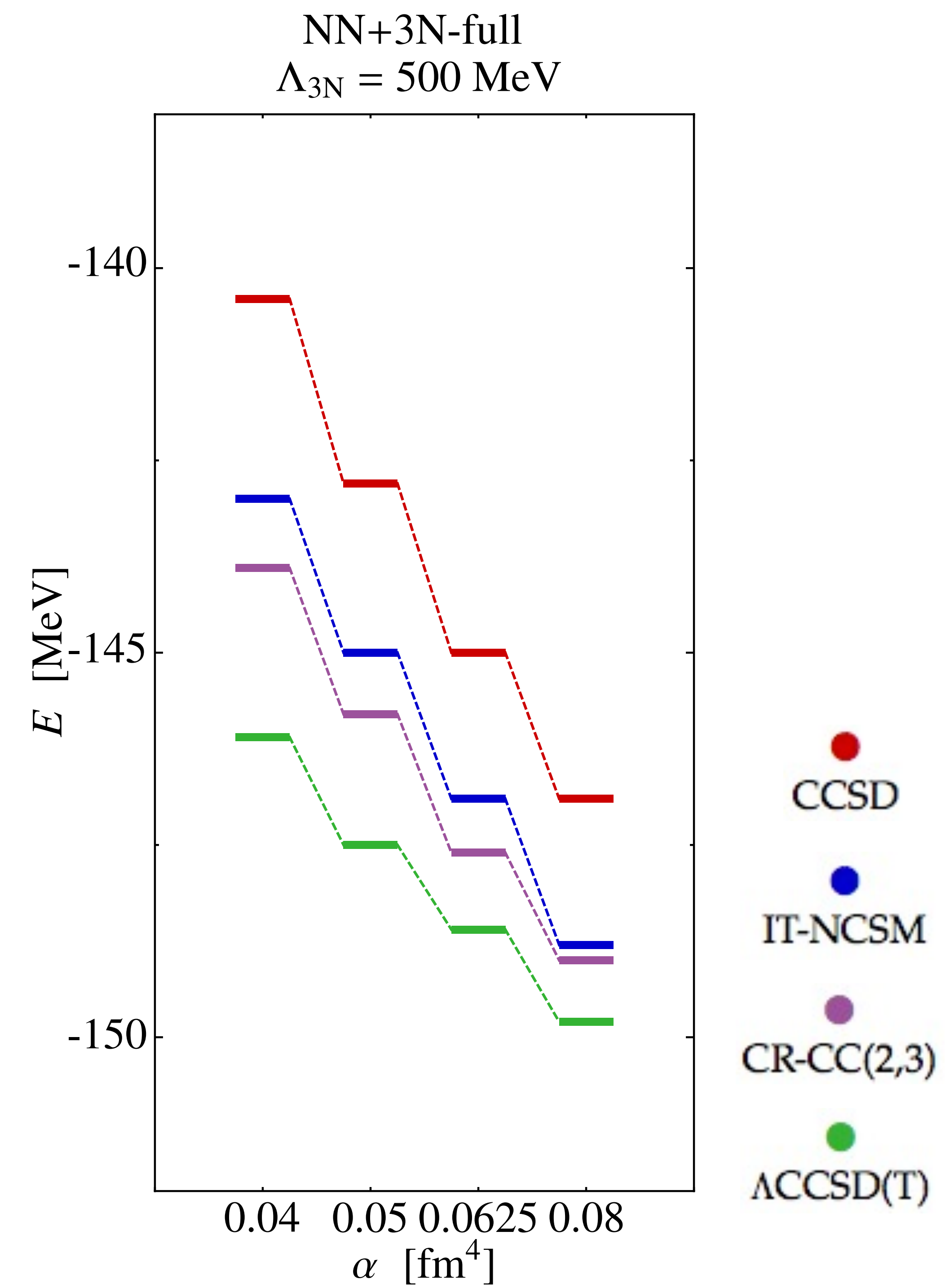
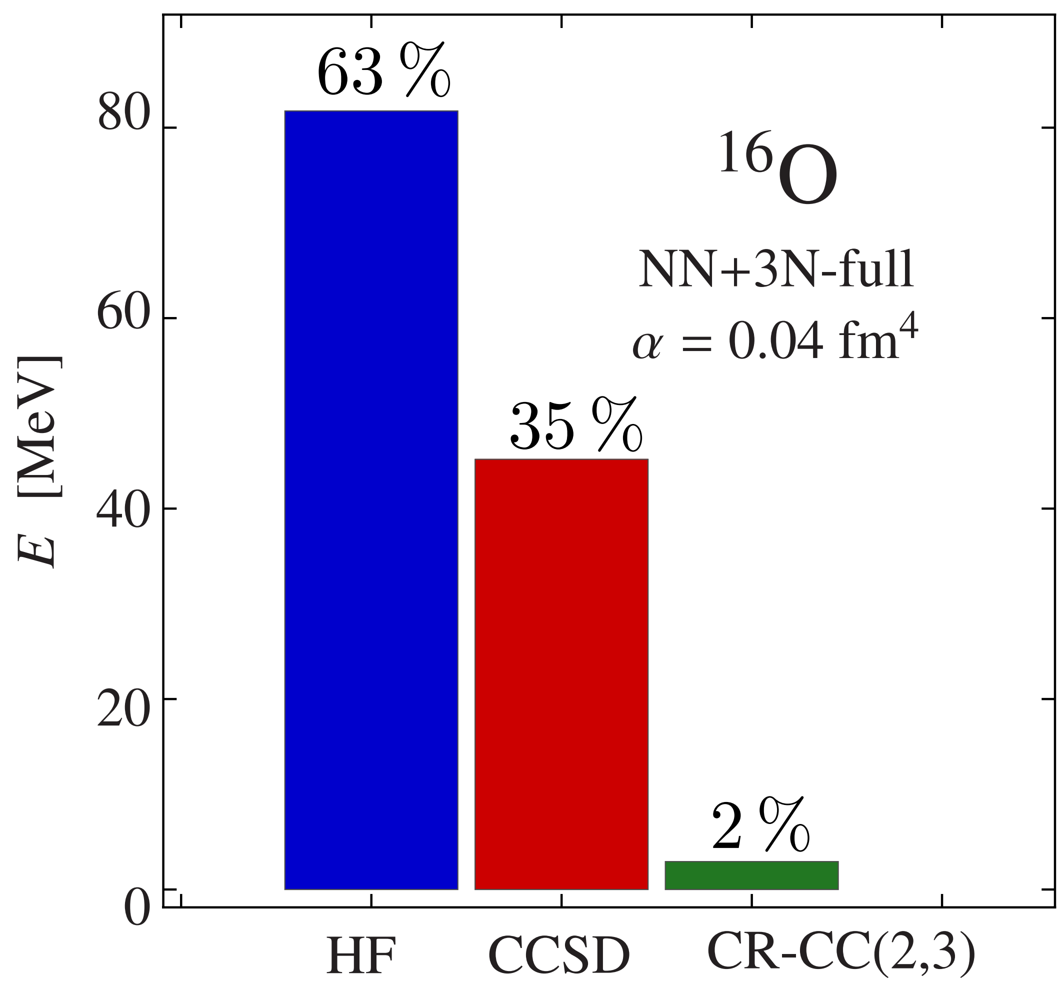




Cluster Convergence

- Use triples correction to **estimate errors** due to cluster truncation



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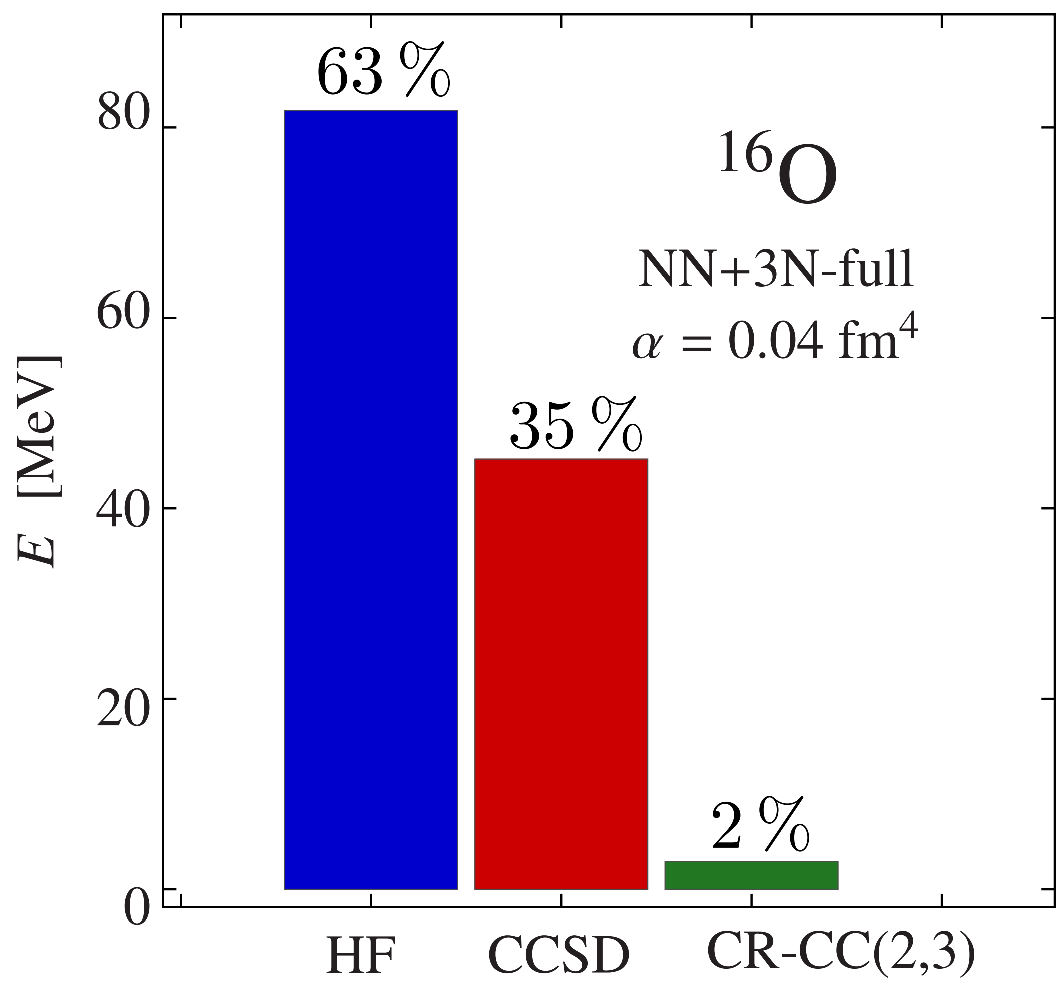

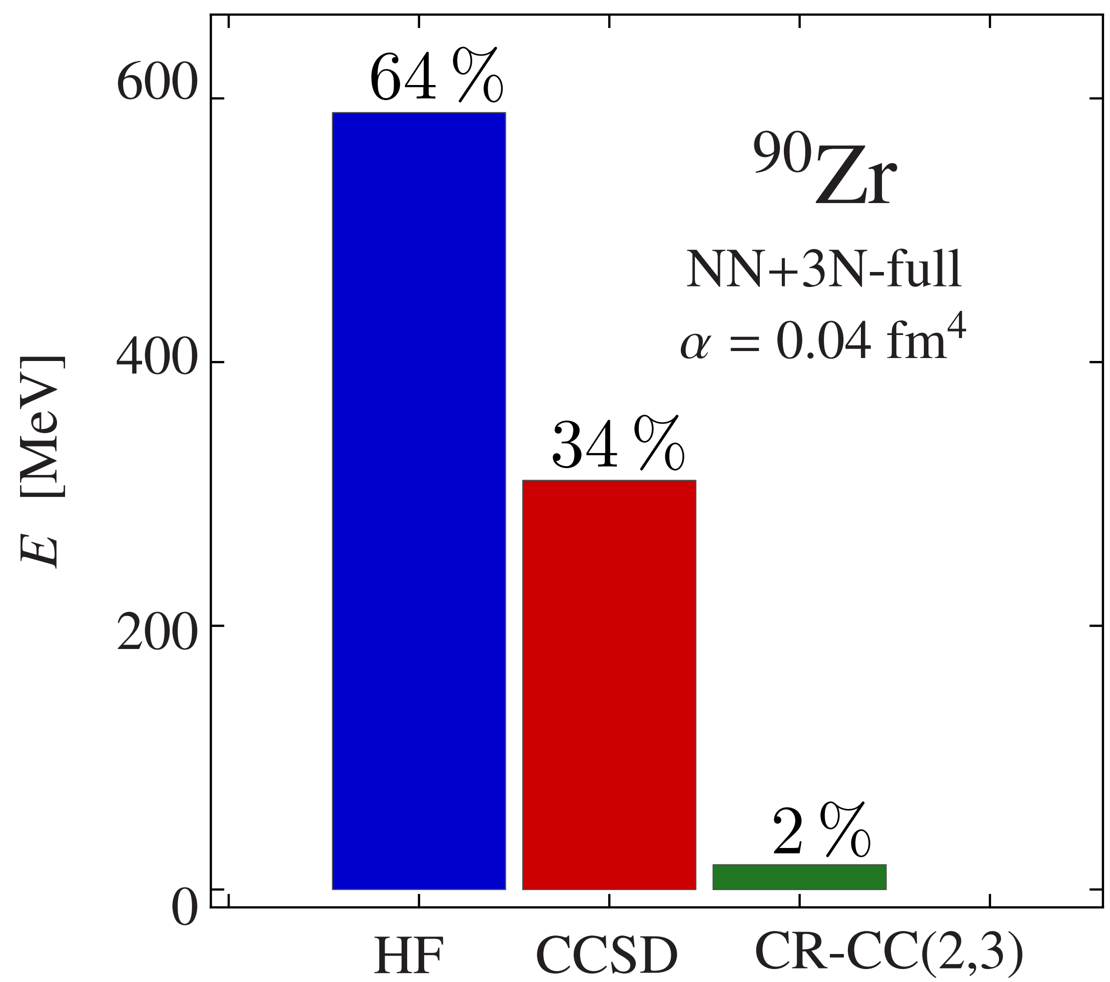

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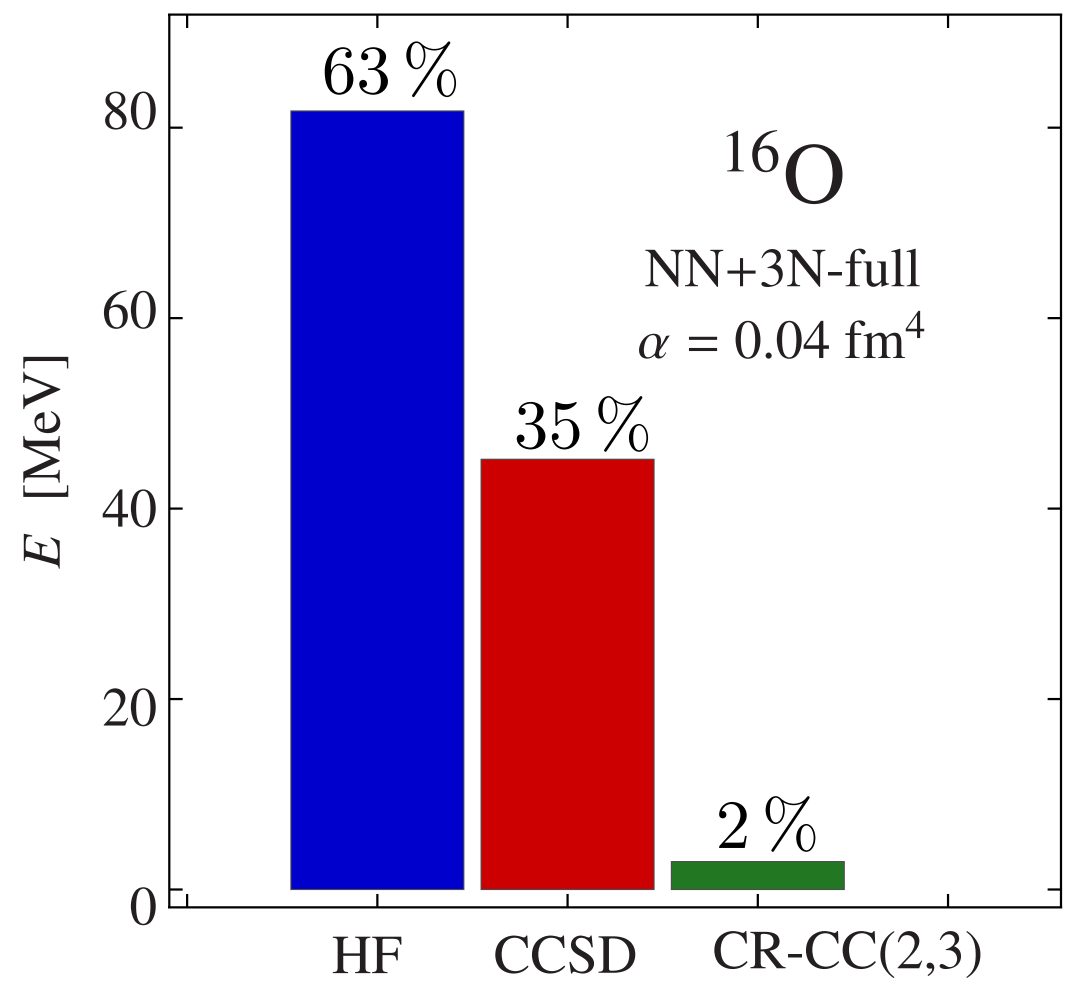
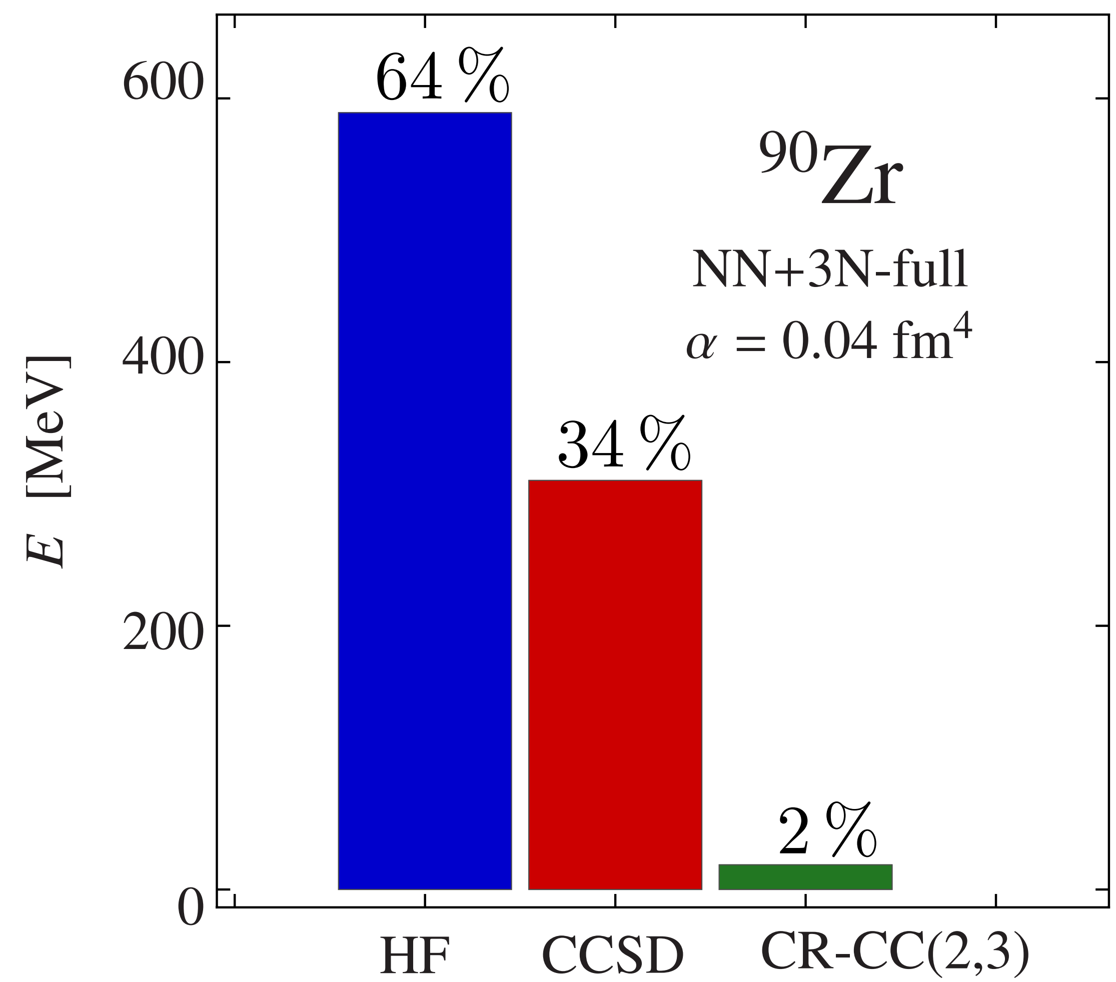


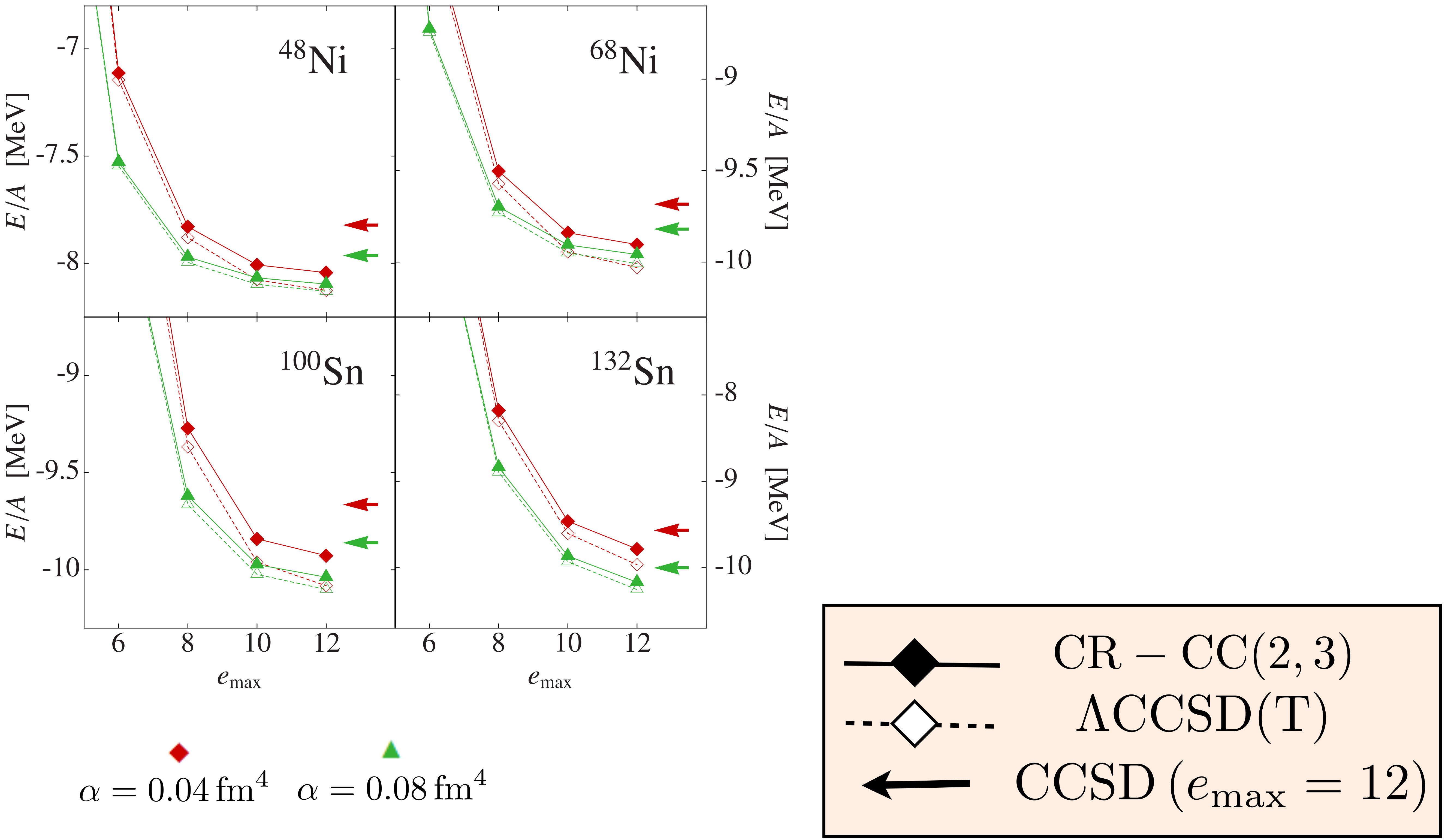


- typically **< 3 %** contributions from triples correction for all nuclear masses

Heavy Nuclei

S. Binder, J. Langhammer, A. Calci, R. Roth, arXiv:1312.5685

Coupled-Cluster for Heavy Nuclei



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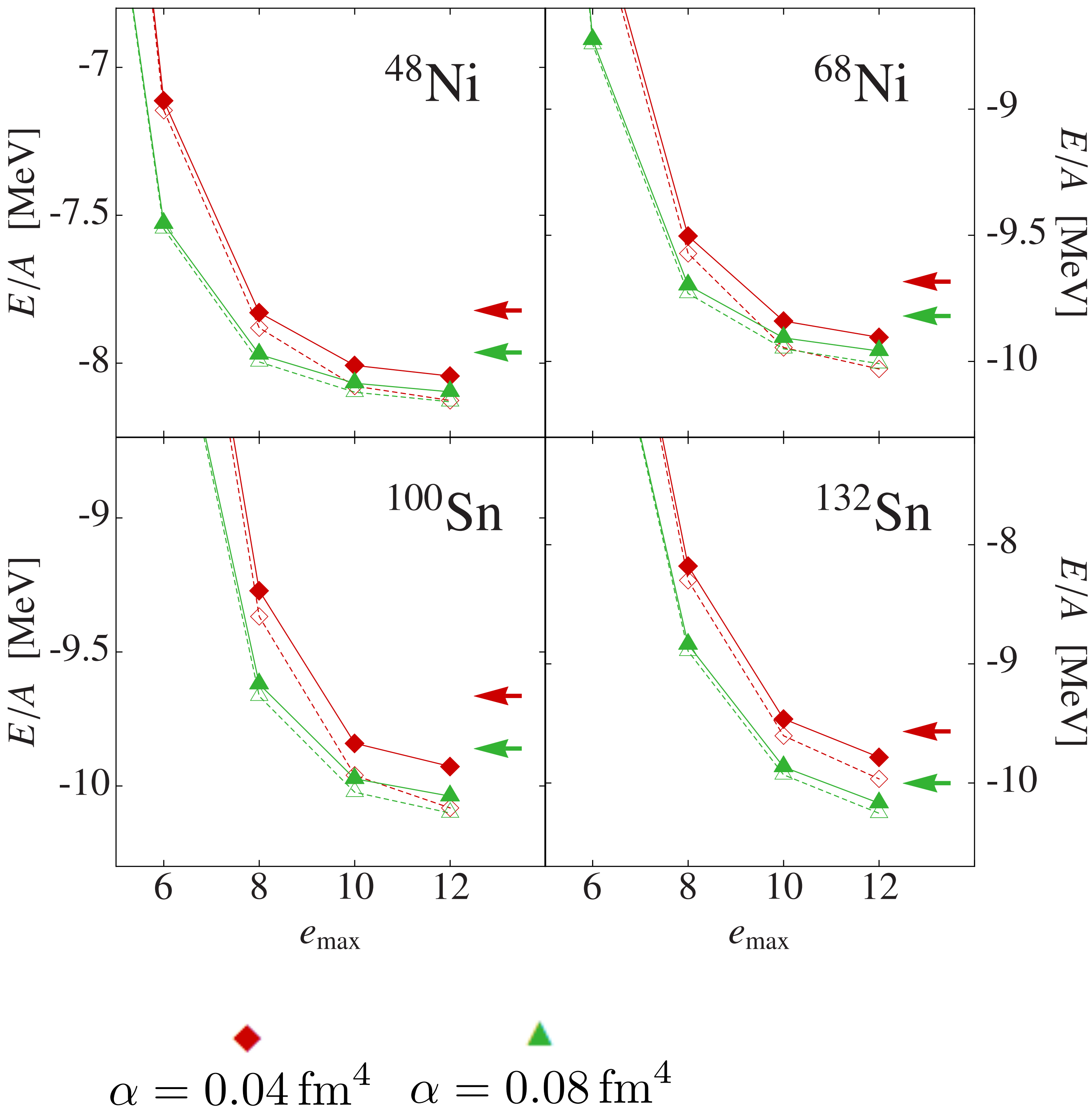

- **soft interactions**: reasonably converged triples calculations possible for heavy nuclei

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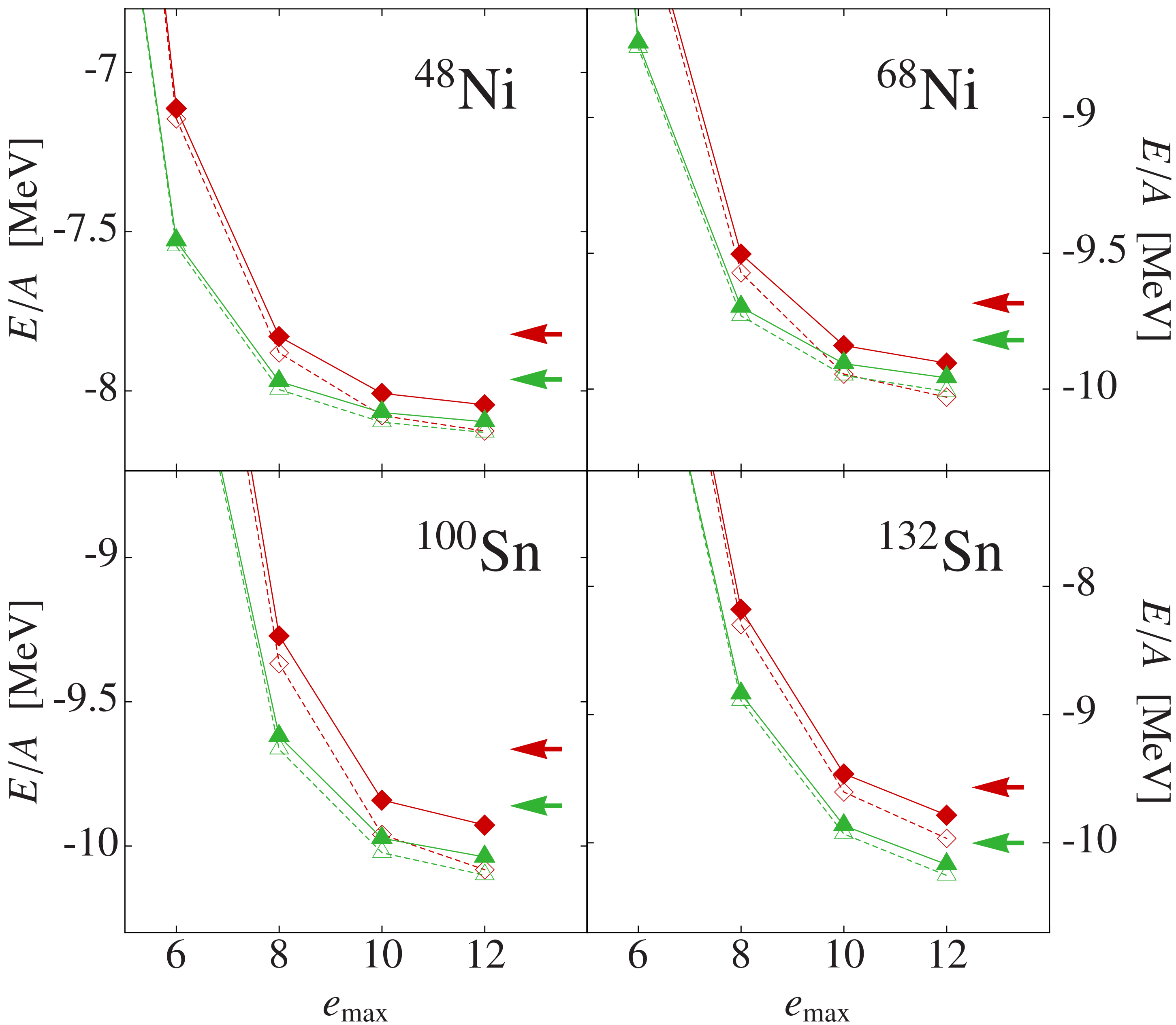
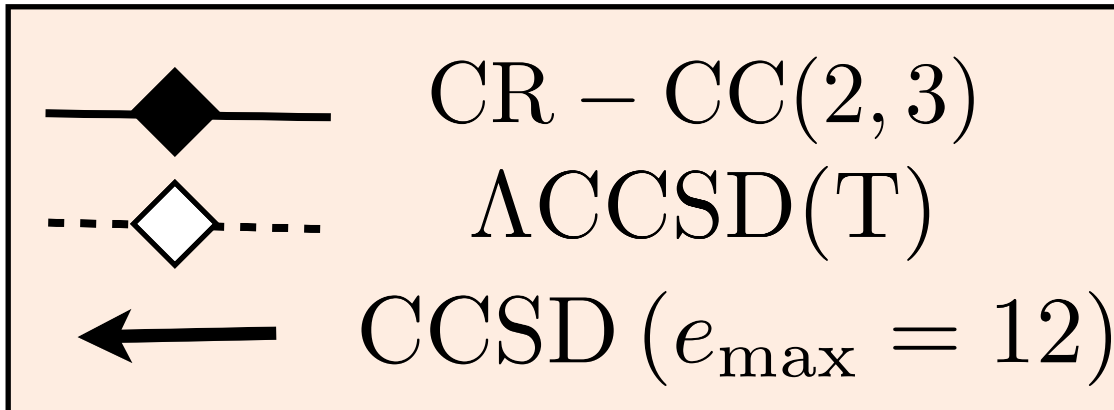


$\alpha = 0.04\,\mathrm{fm}^4$ $\alpha = 0.08\,\mathrm{fm}^4$

- **soft interactions**: reasonably converged triples calculations possible for heavy nuclei
- calculations are rather **inexpensive**



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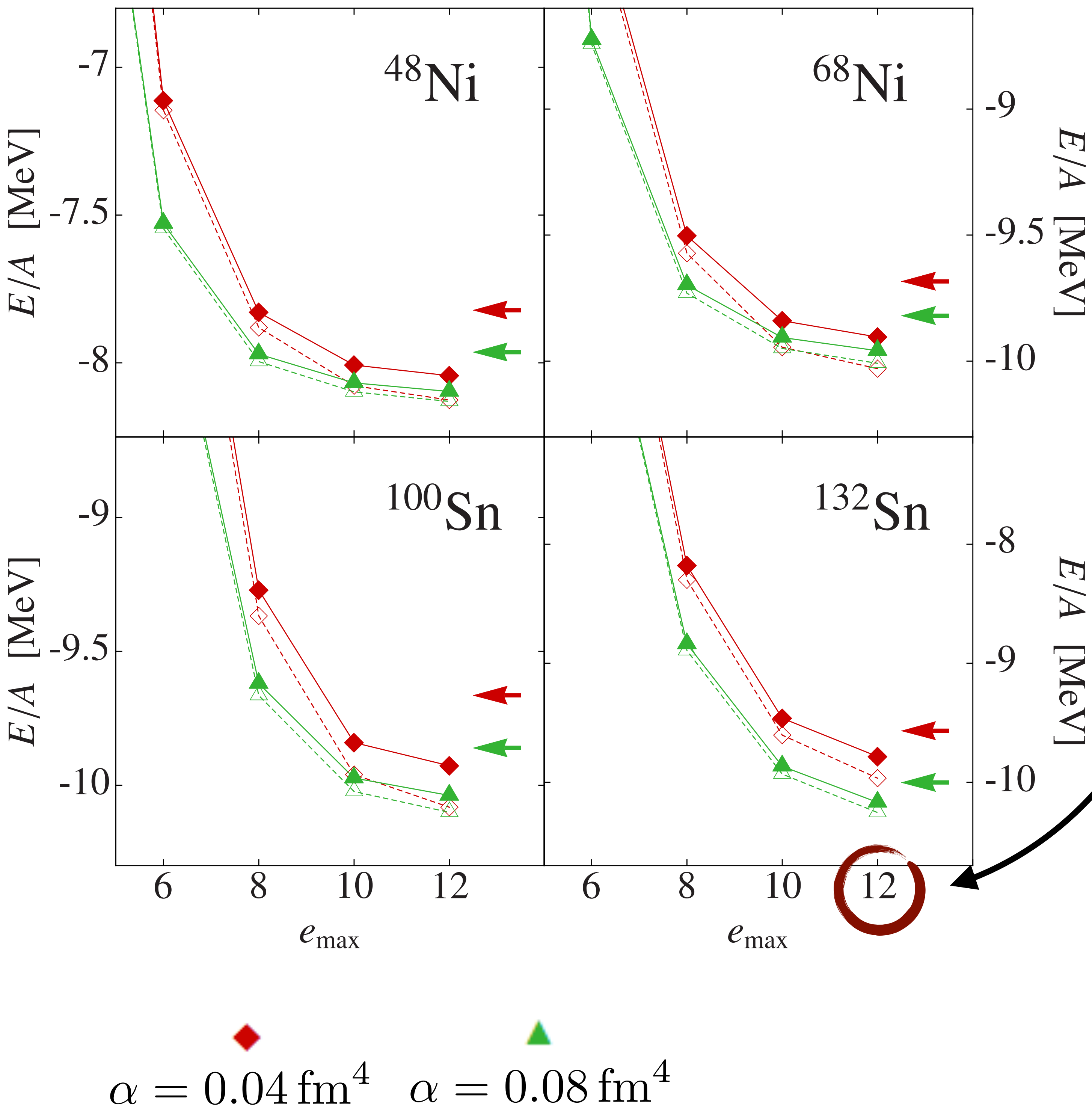

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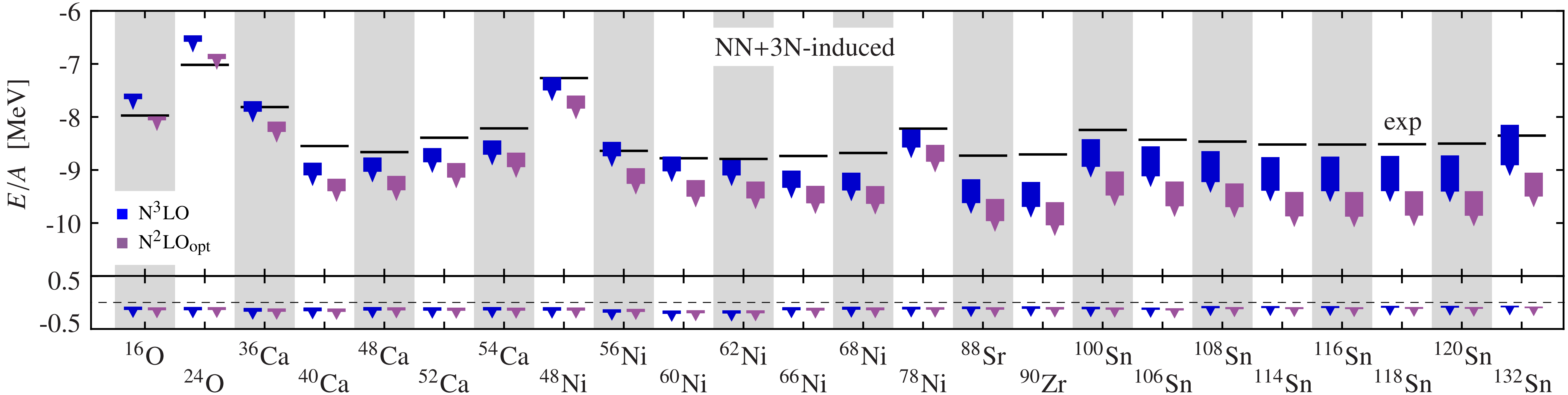
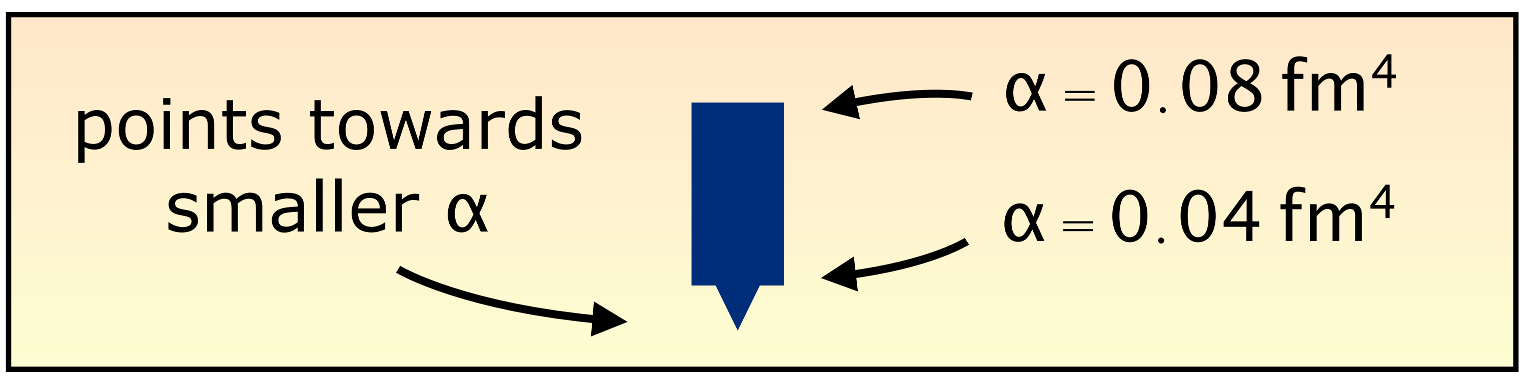
- CR-CC(2,3) : **7.200** CPU h for ^{132}Sn, e_{max}=12

Heavy Nuclei from Chiral Interactions





CR-CC(2,3)

HF basis

$\hbar\Omega = 24$ MeV

$E_{3\max} = 18$

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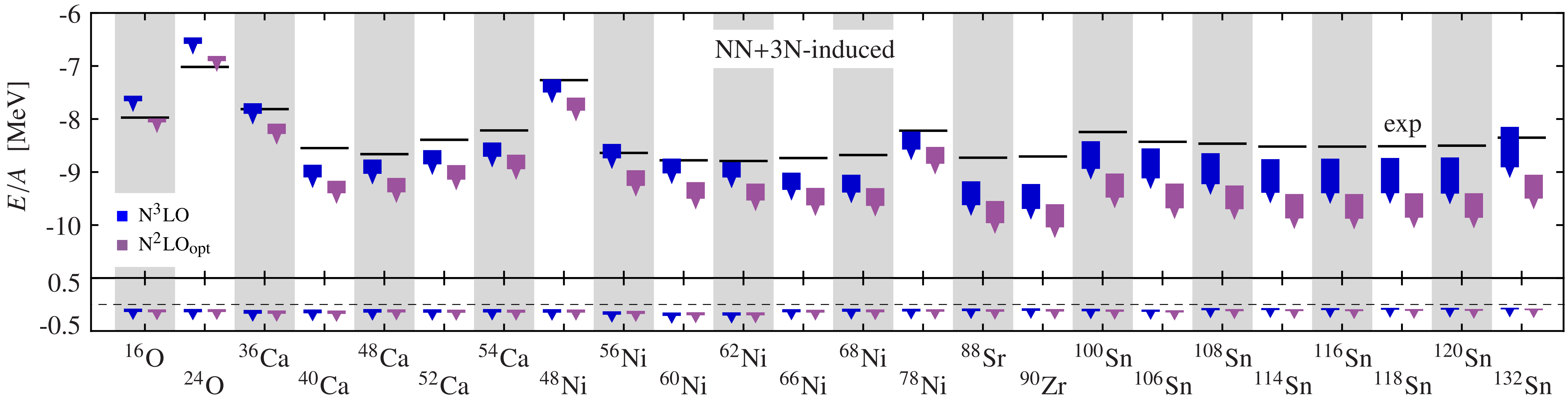

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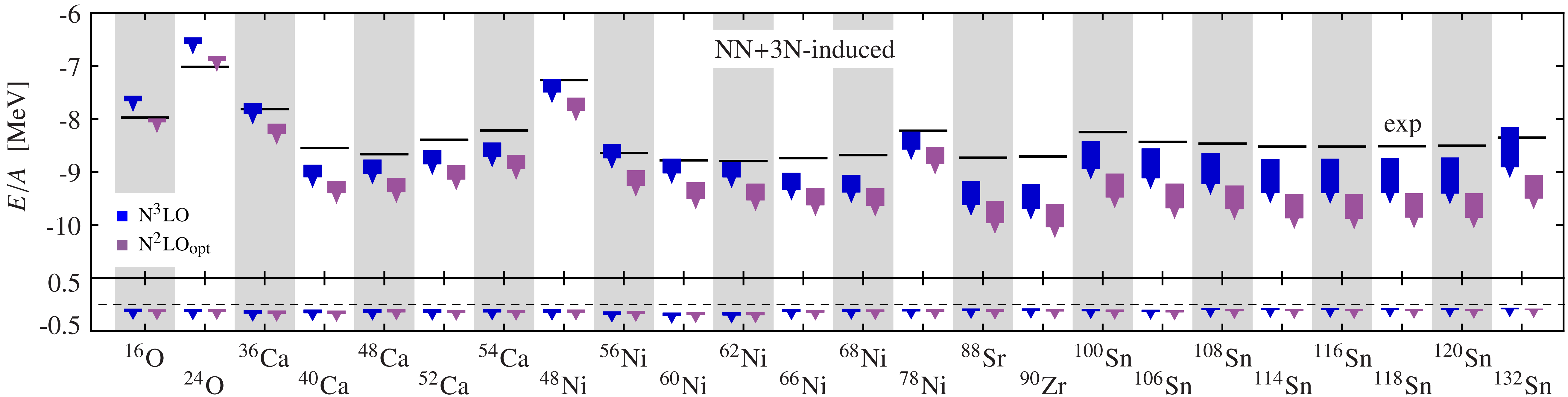

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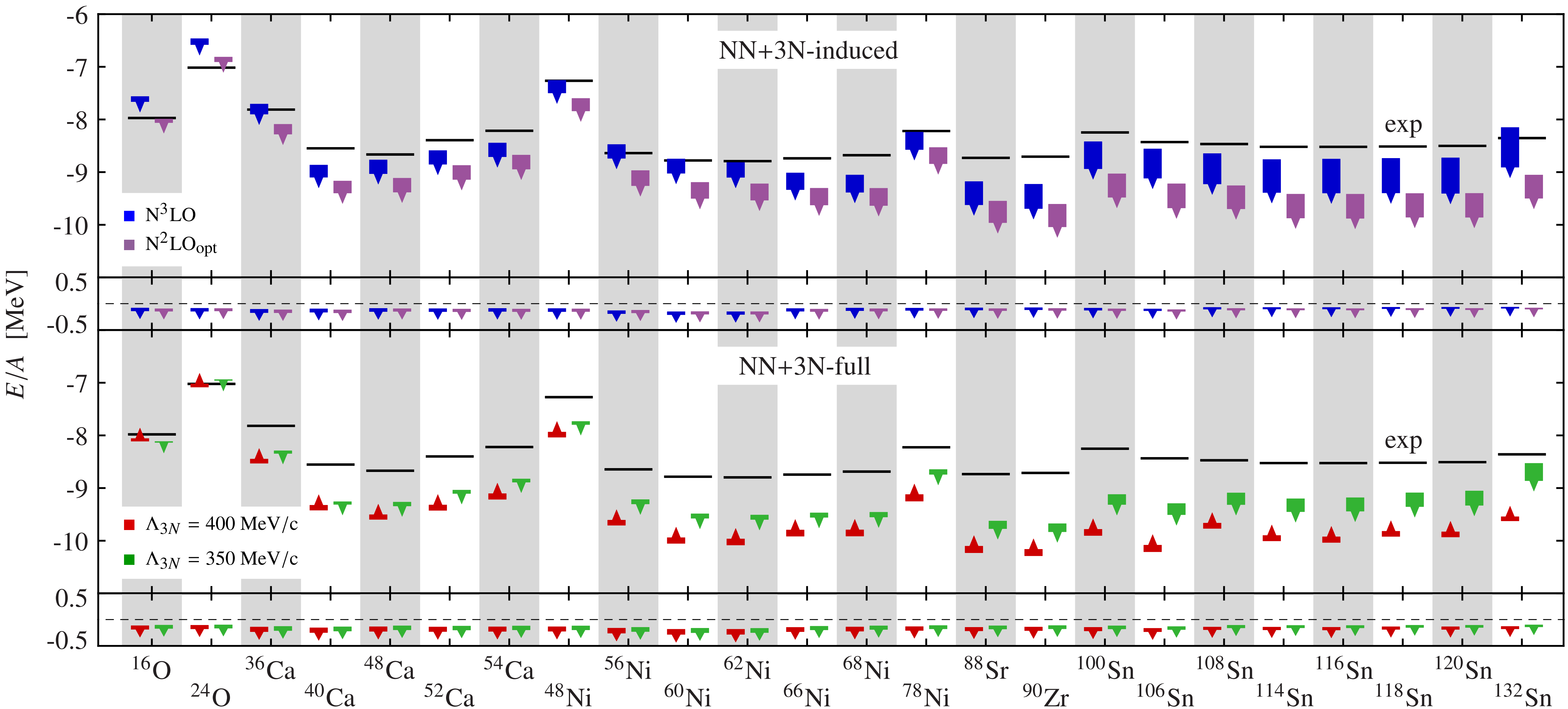

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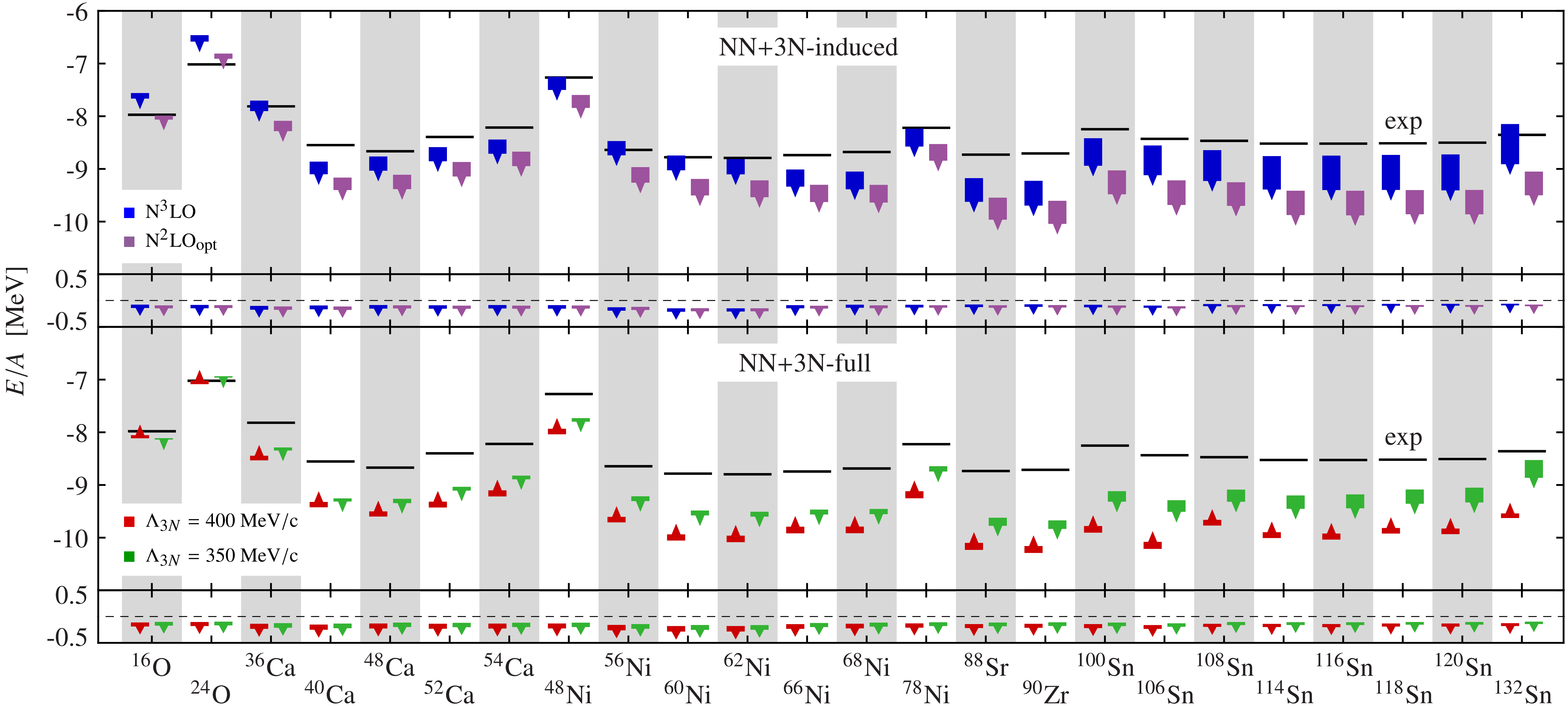

- NN+3N-induced: **strong** SRG-induced **4N**, ... interactions
- NN+3N-full: **cancellation** of SRG-induced **4N**, ... interactions

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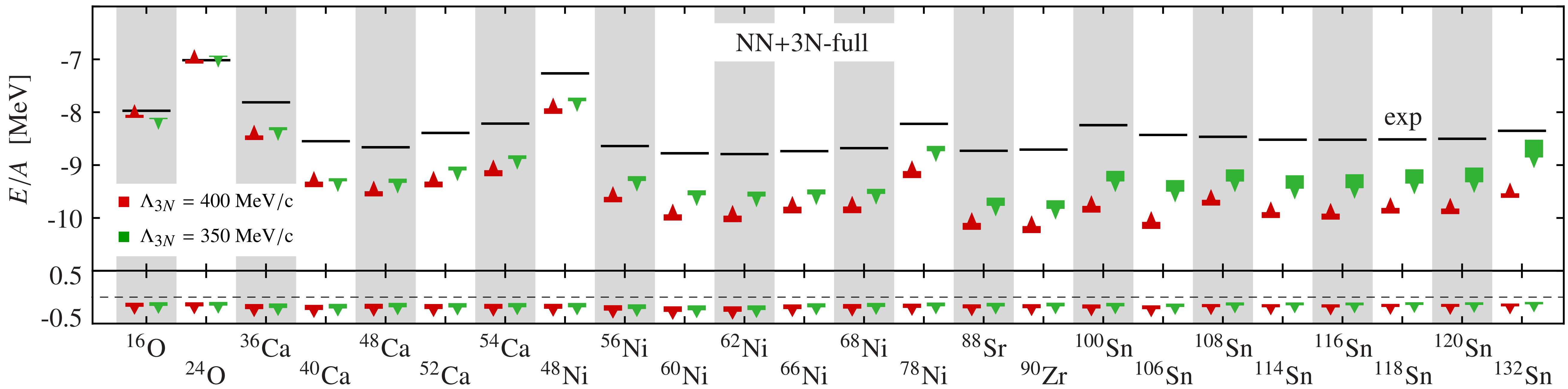

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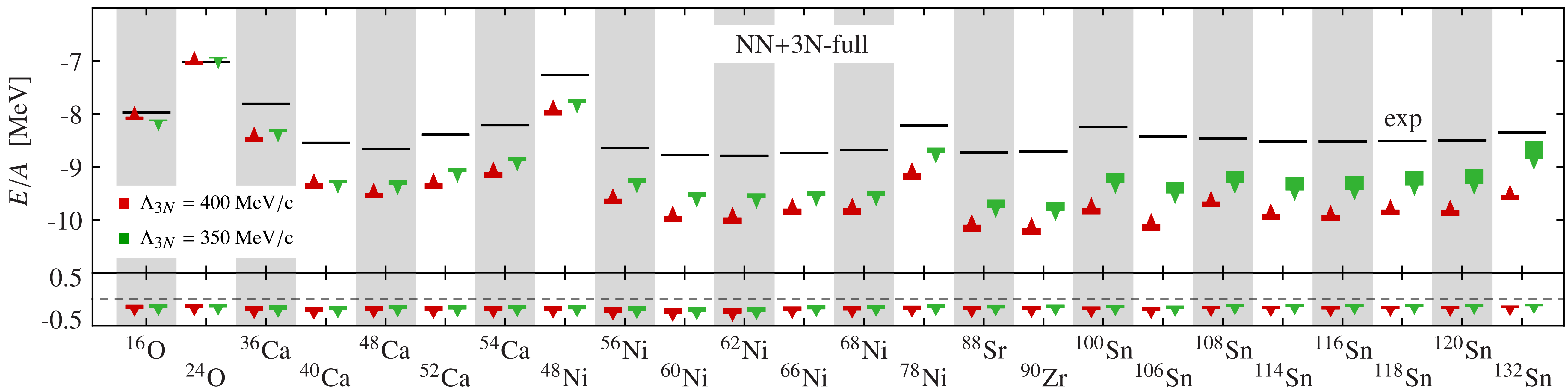

- Hamiltonians fixed in **A≤4** systems

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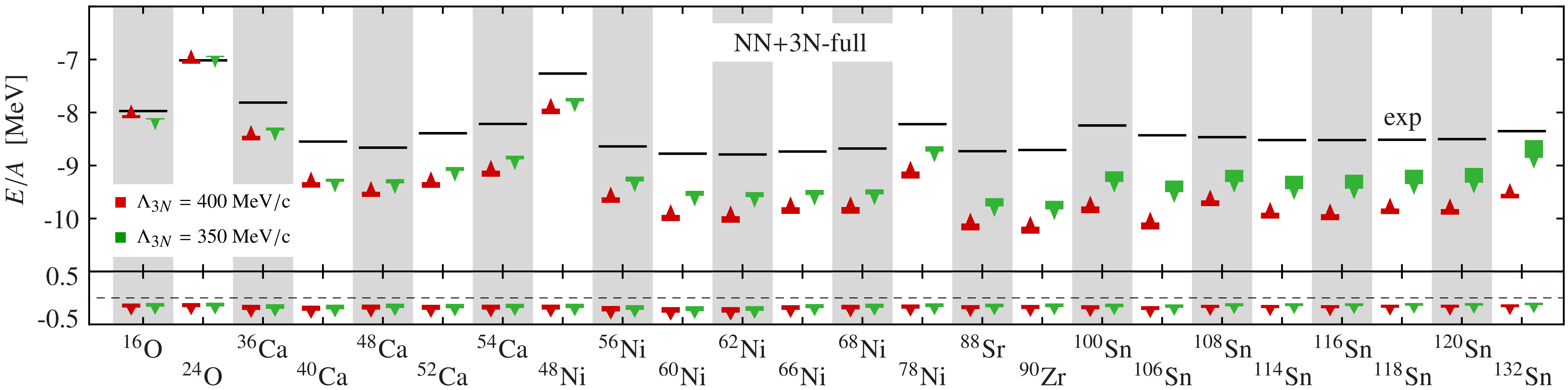

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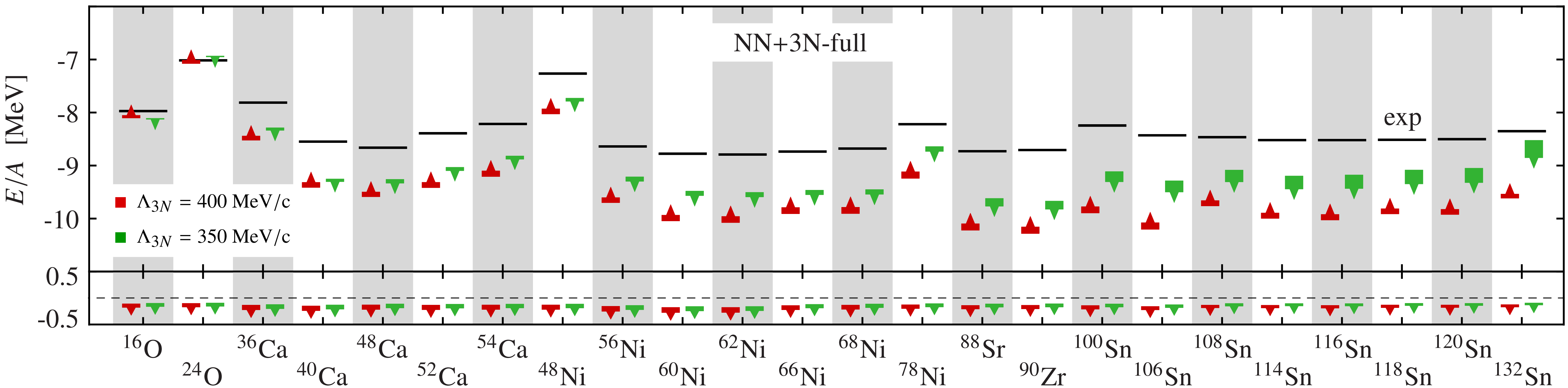

- Hamiltonians fixed in **A≤4** systems

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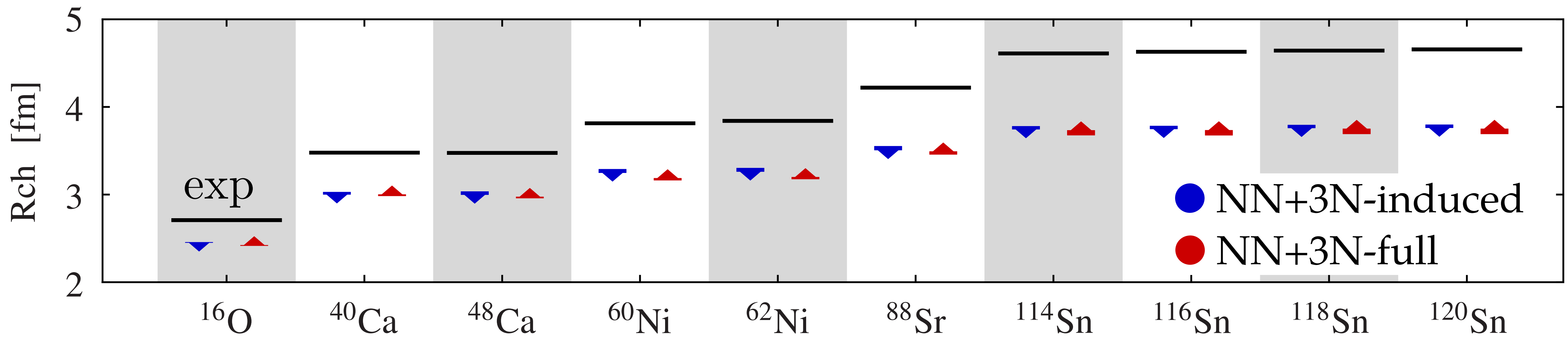
- systematic overbinding ⇒ still **deficiencies**
  - **consistent 3N** interaction at N^{3}LO, and **4N** interaction
  - SRG-induced **4N, ...** interactions

Radii



Hartree-Fock

$\hbar\Omega = 24$ MeV

$E_{3\text{max}} = 18$

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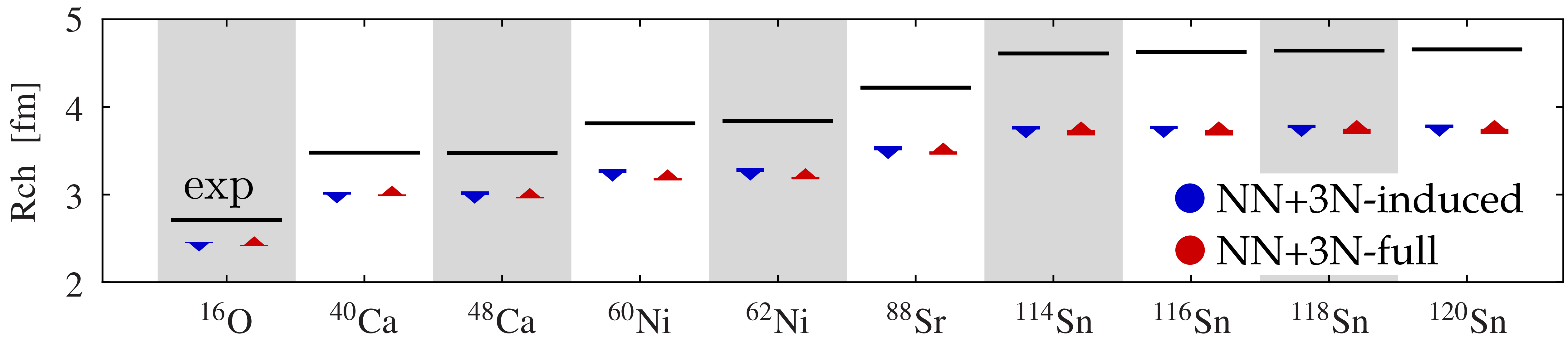

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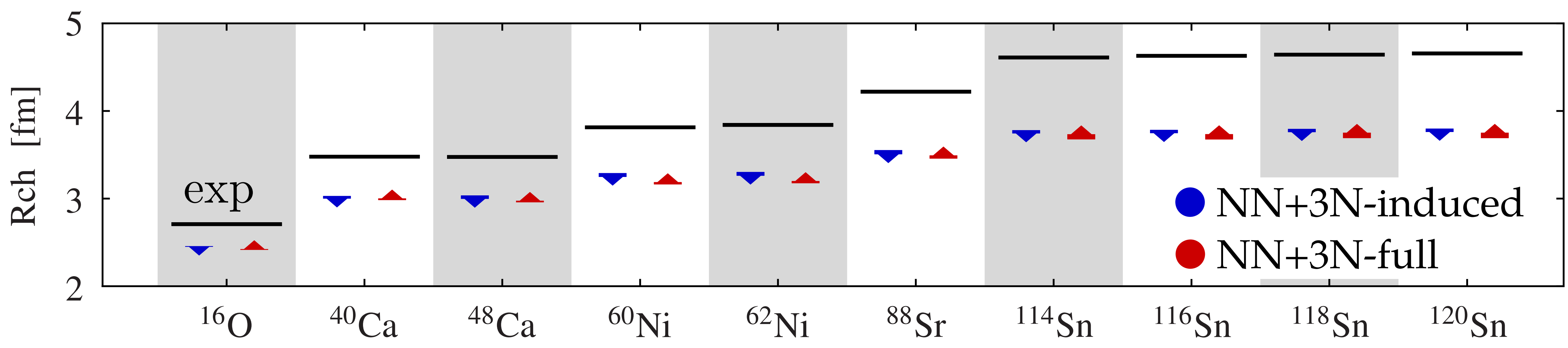

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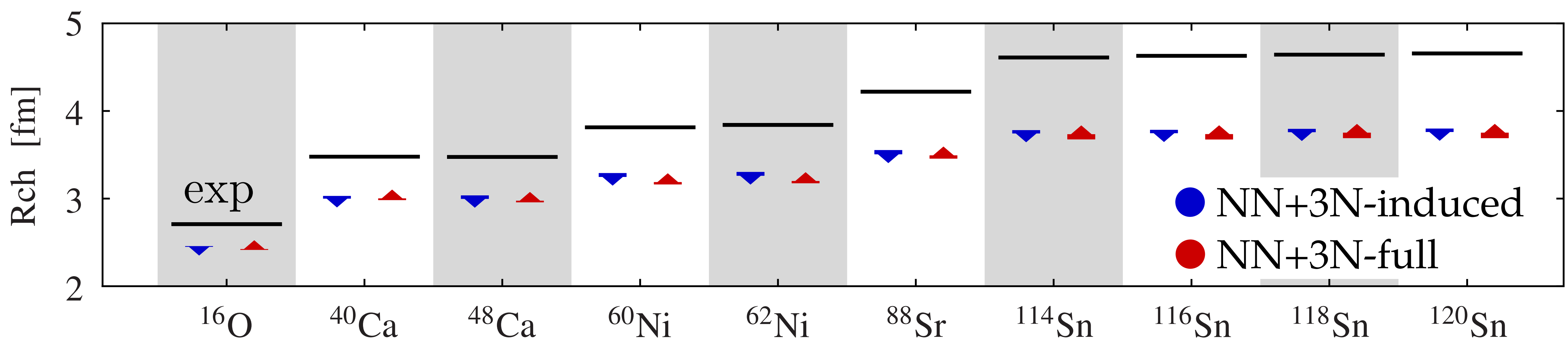

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$\Rightarrow$ **challenge** for chiral Hamiltonians, already for **lighter nuclei**

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  - **Observables** other than energy, e.g., **Radii**

Epilogue

- **thanks to my group & collaborators**
  - A. Calci, E. Gebrerufael, J. Langhammer, S. Fischer, R. Roth, S. Schulz, H. Krutsch, 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
    The Ohio State University, USA
  - K. Hebeler
    TU Darmstadt

Computing Time

JÜLICH FORSCHUNGSZENTRUM — NERSC — CSC Center for Scientific Computing Frankfurt

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HELMHOLTZ GEMEINSCHAFT

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  TU Darmstadt

Thanks for your attention!

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