Heavy Nuclei

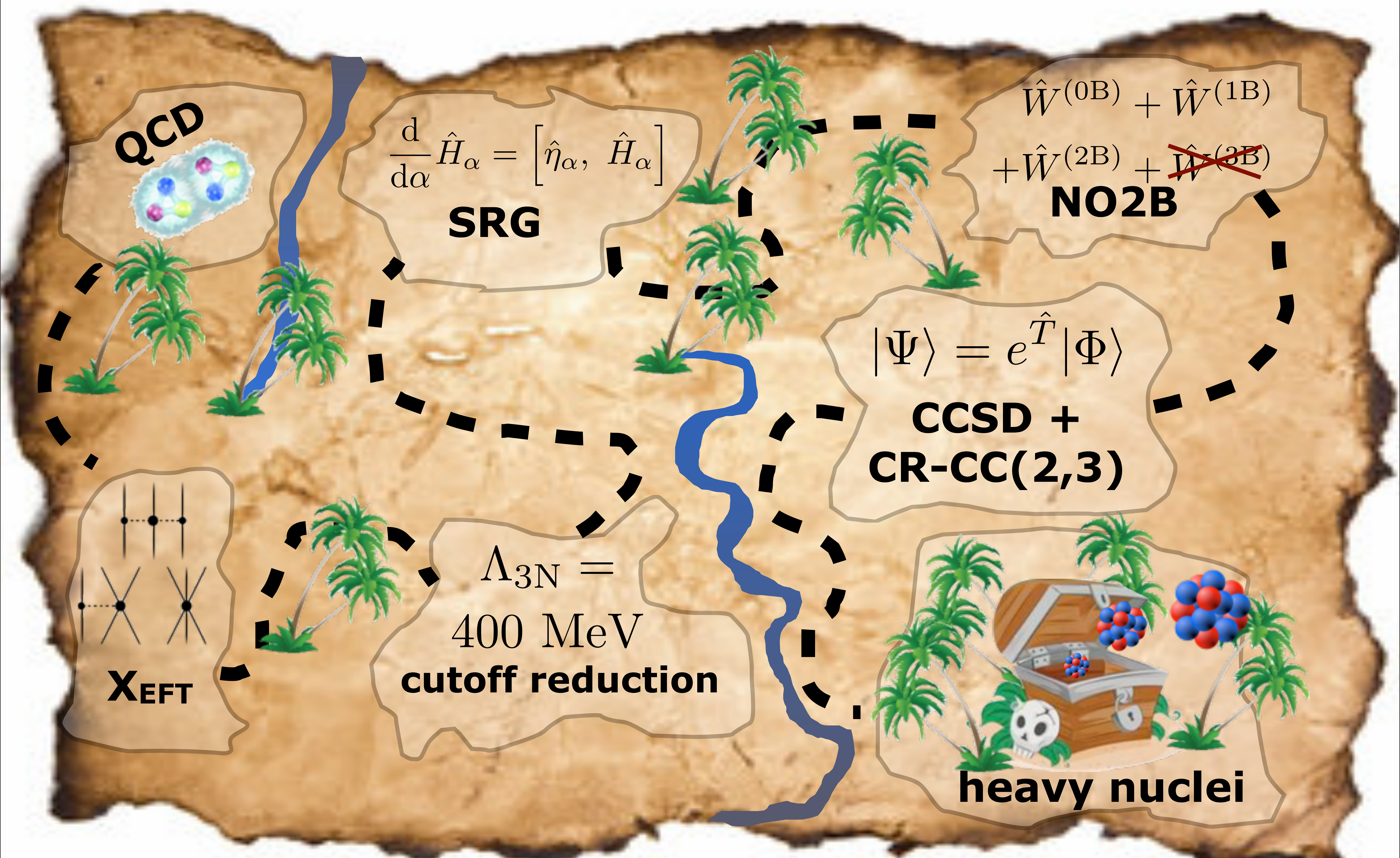
Ab Initio

Sven Binder

INSTITUT FÜR KERNPHYSIK

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Path to Heavy Nuclei



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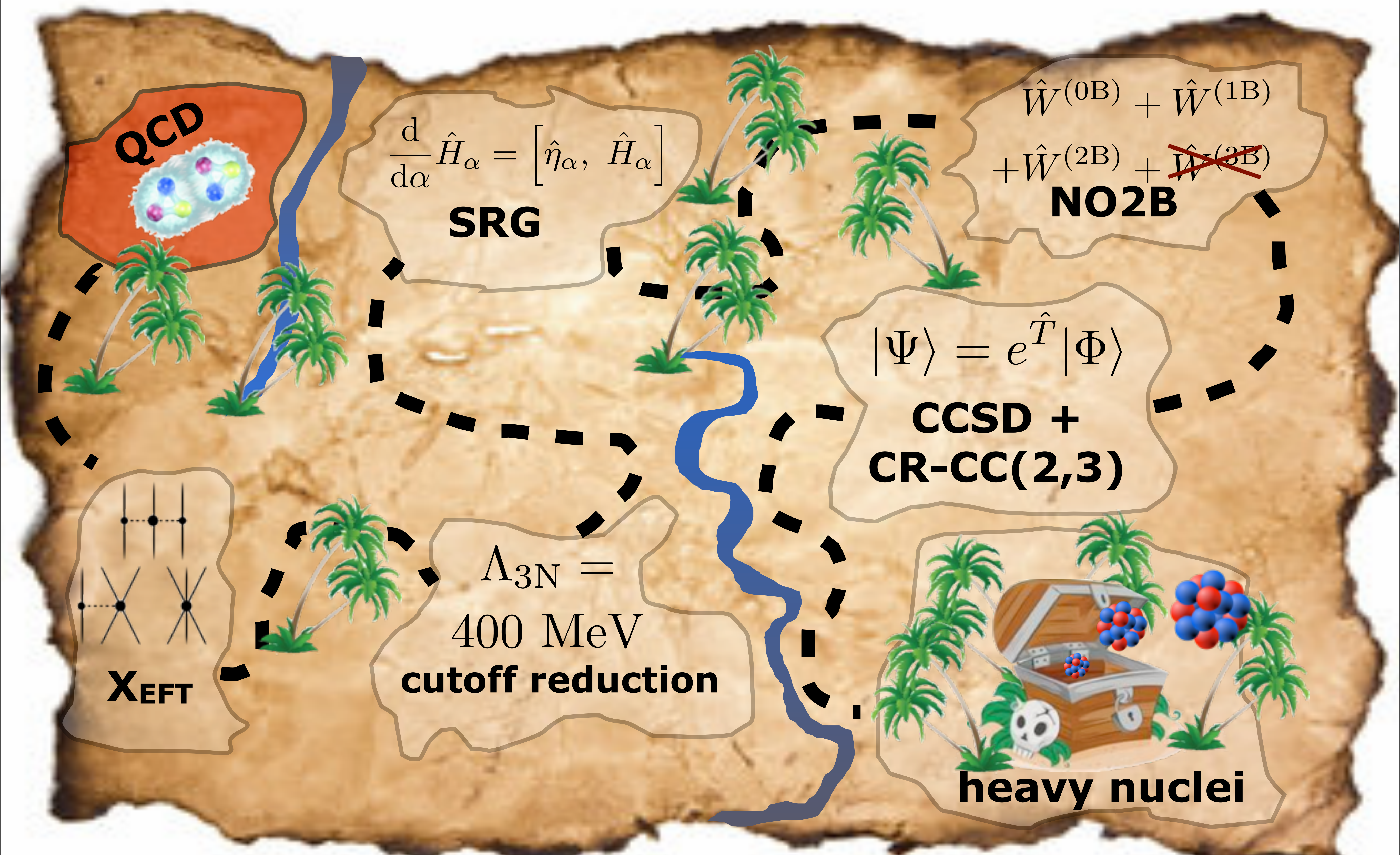

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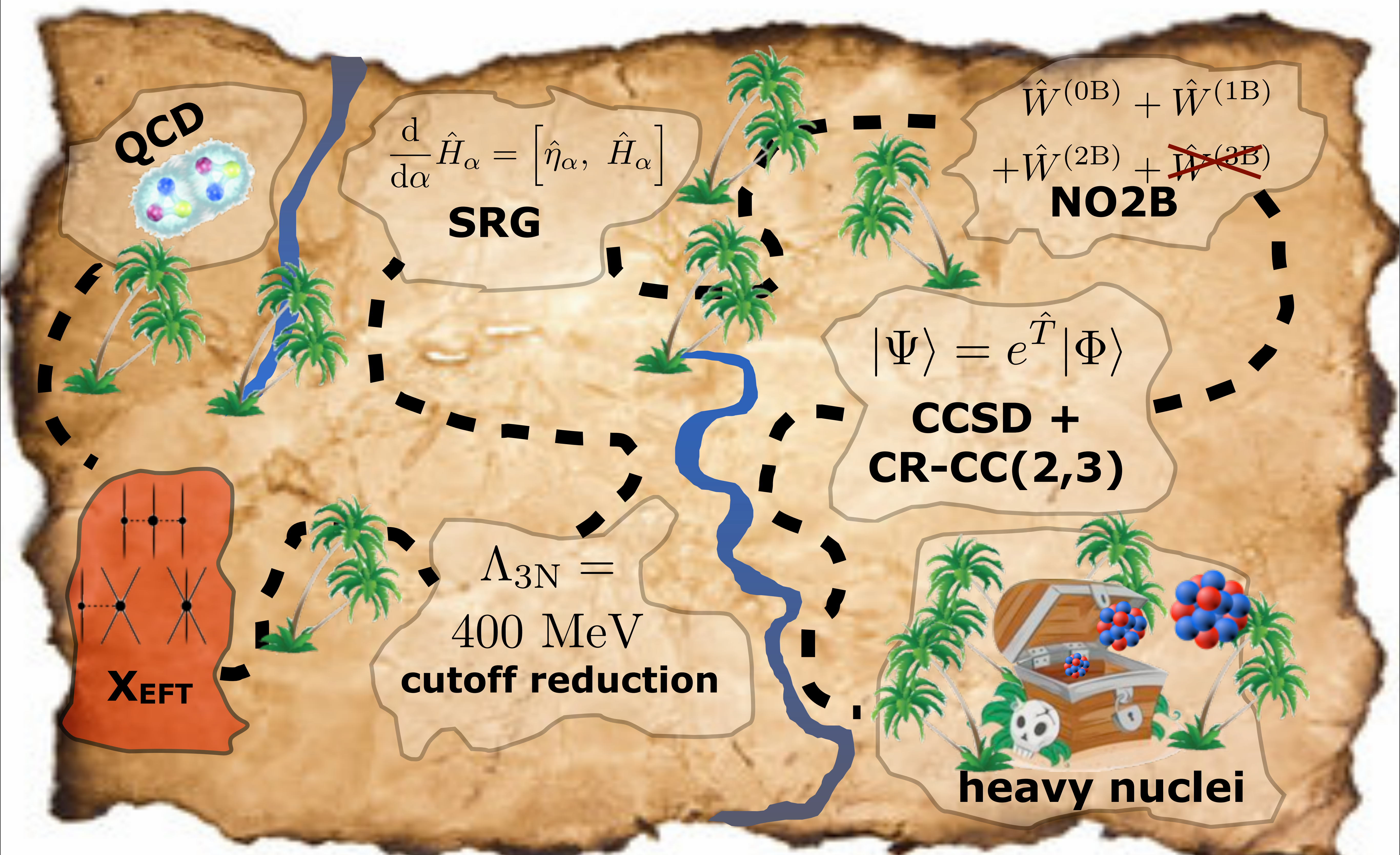

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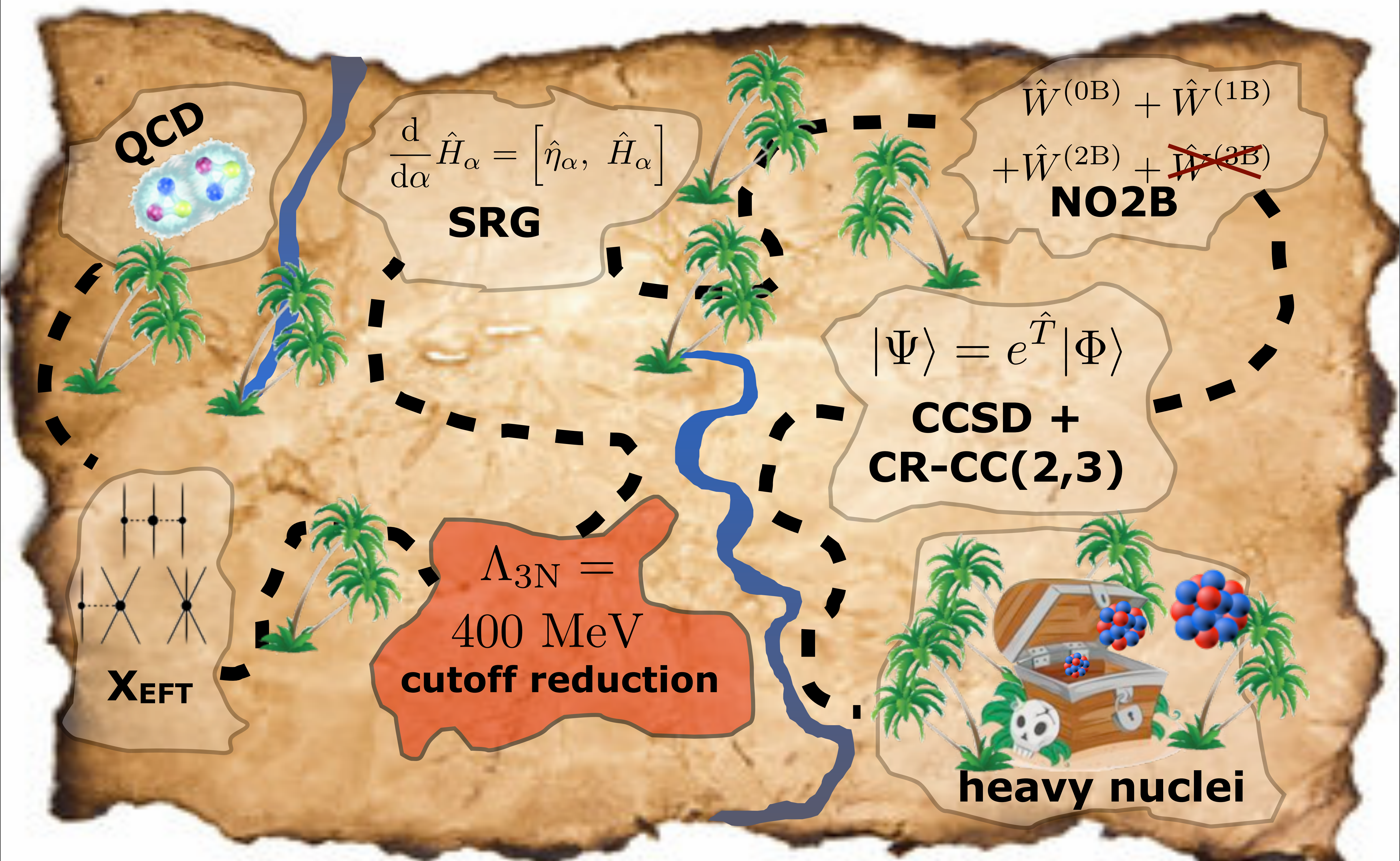

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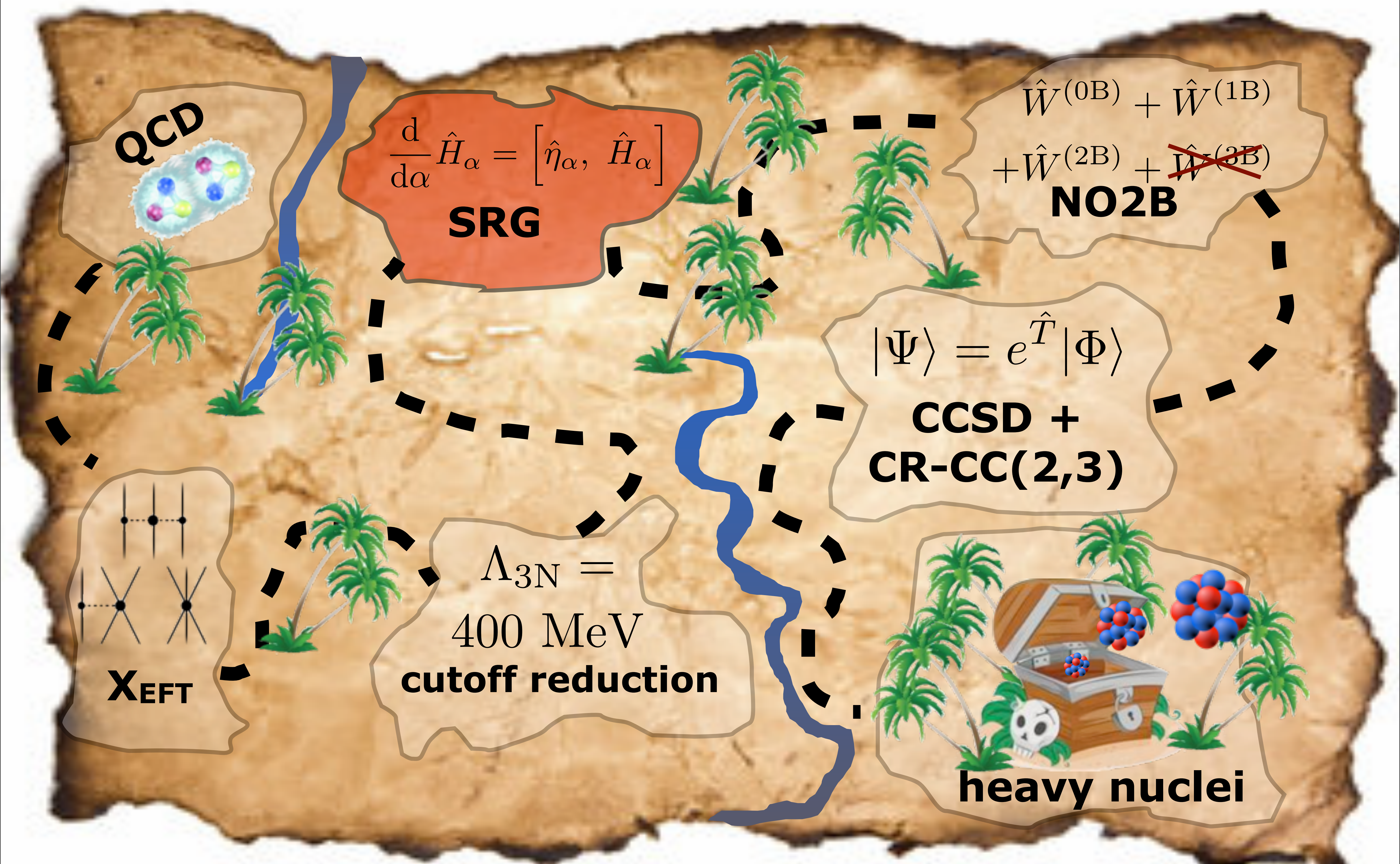

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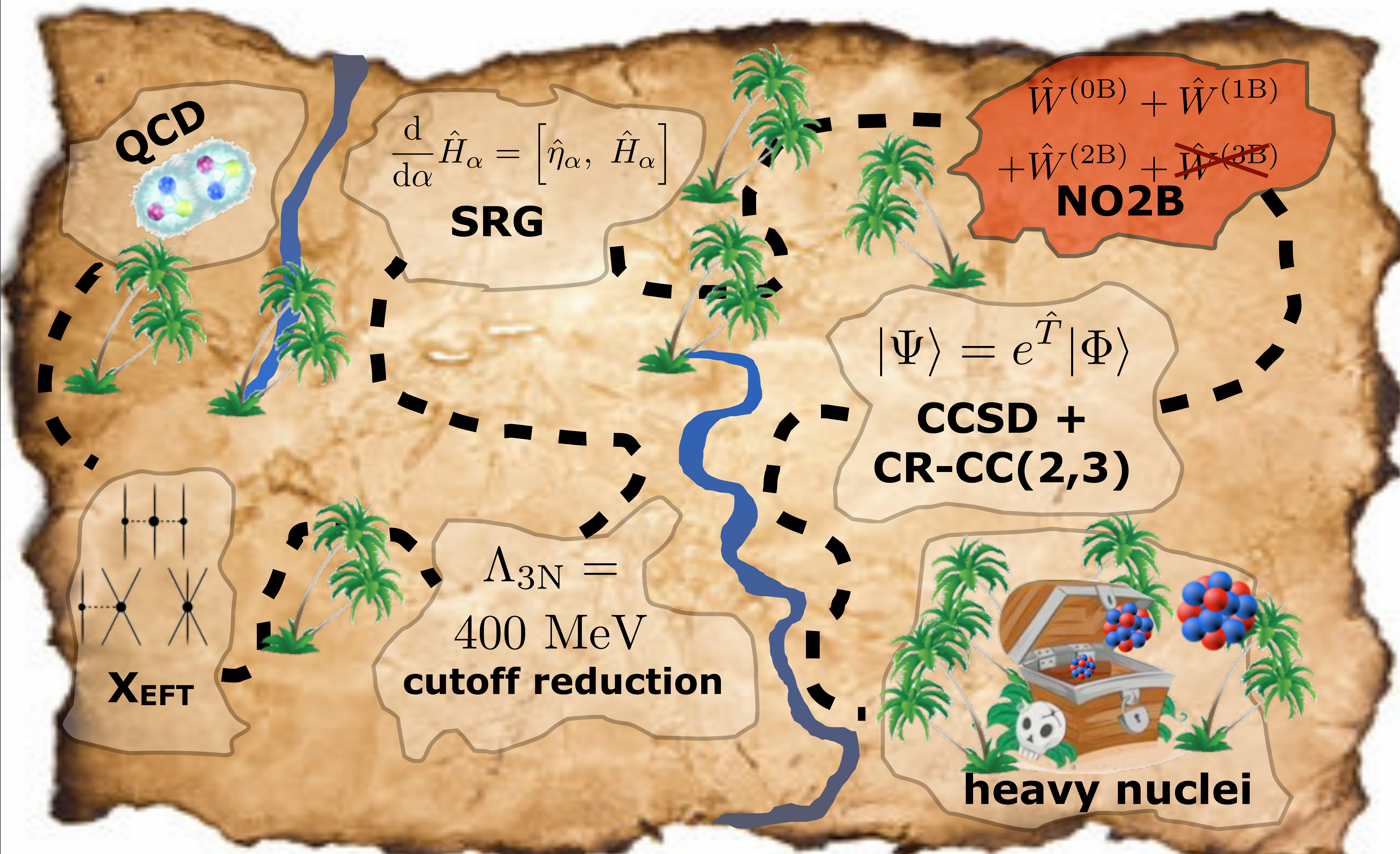

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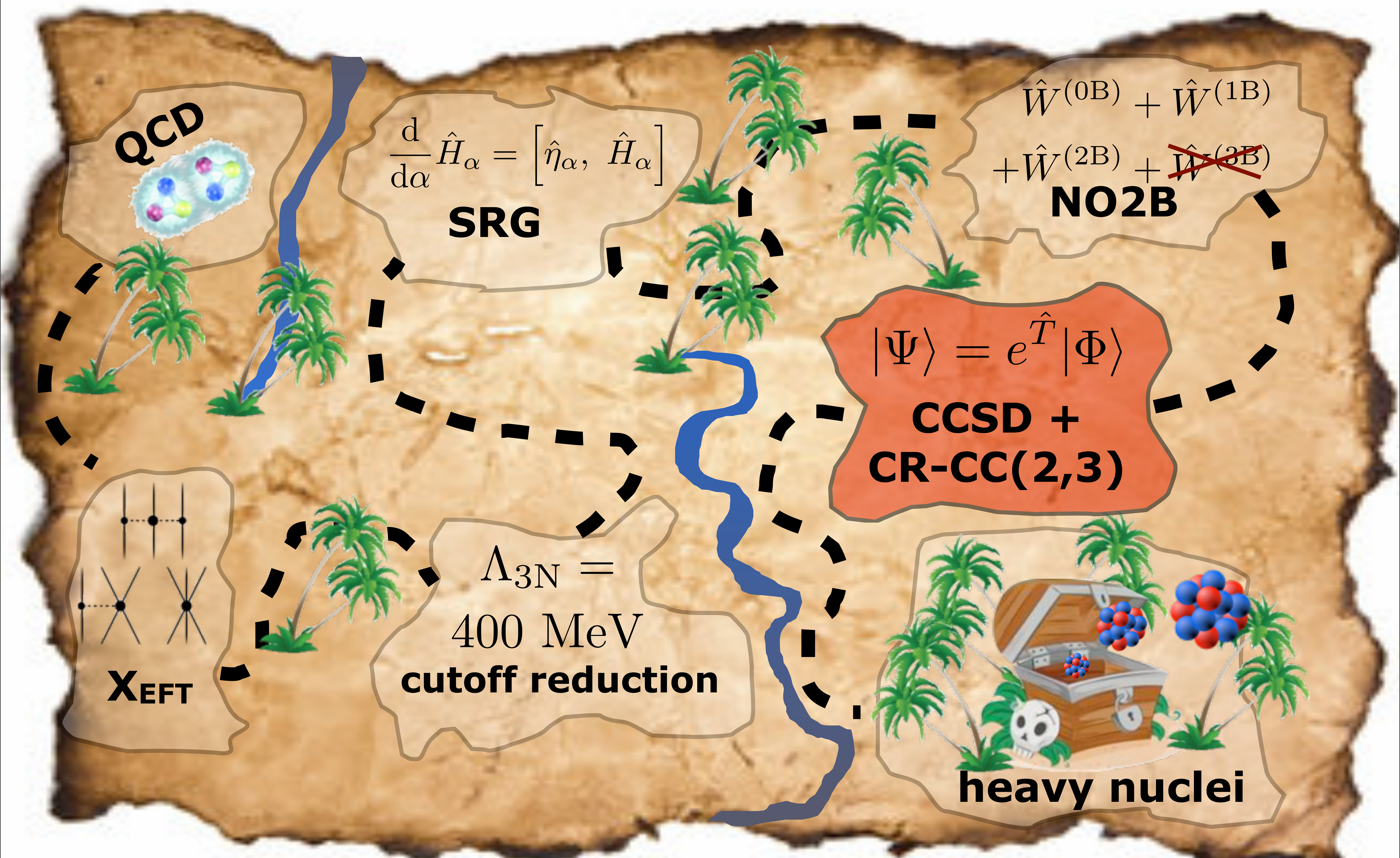

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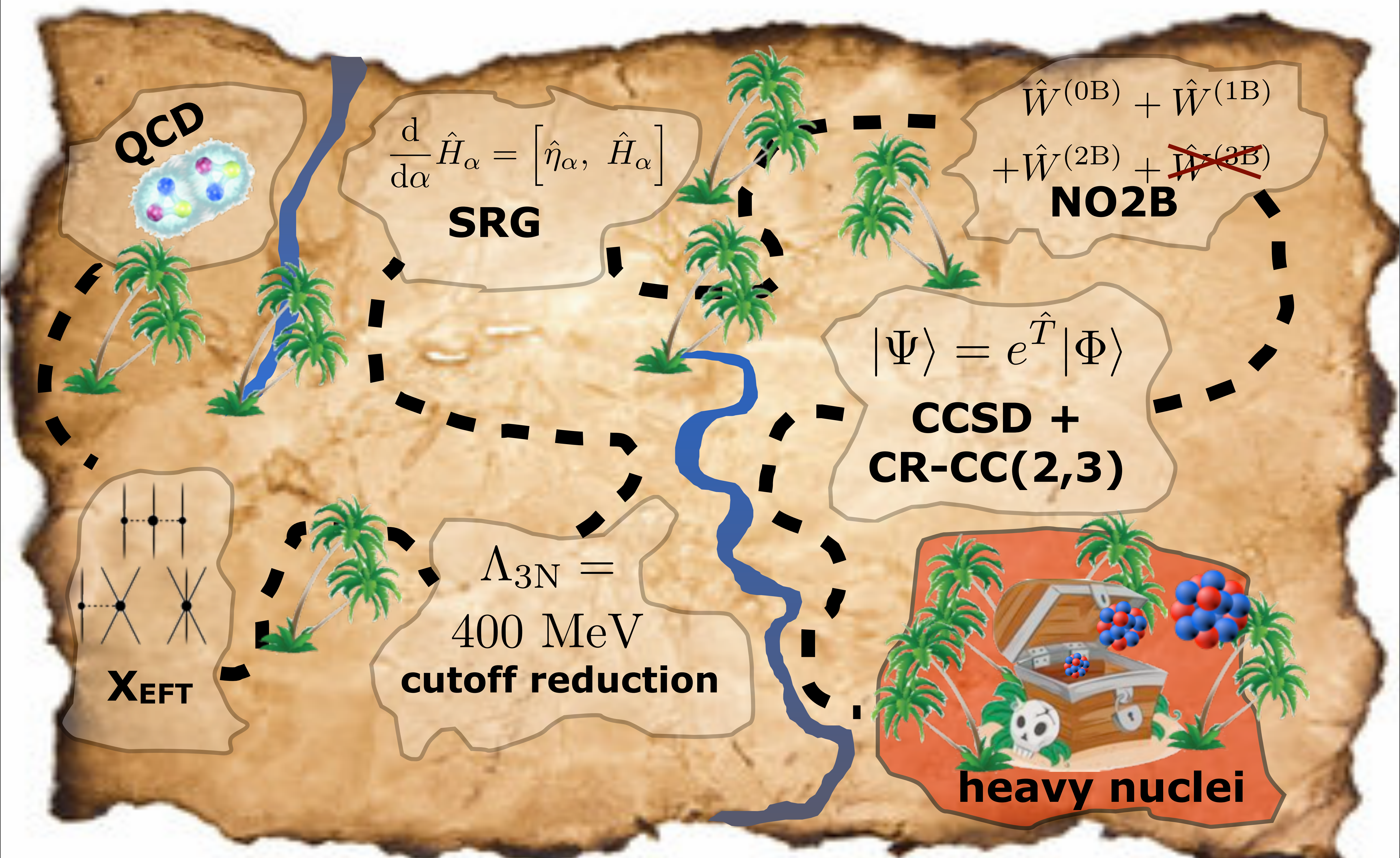


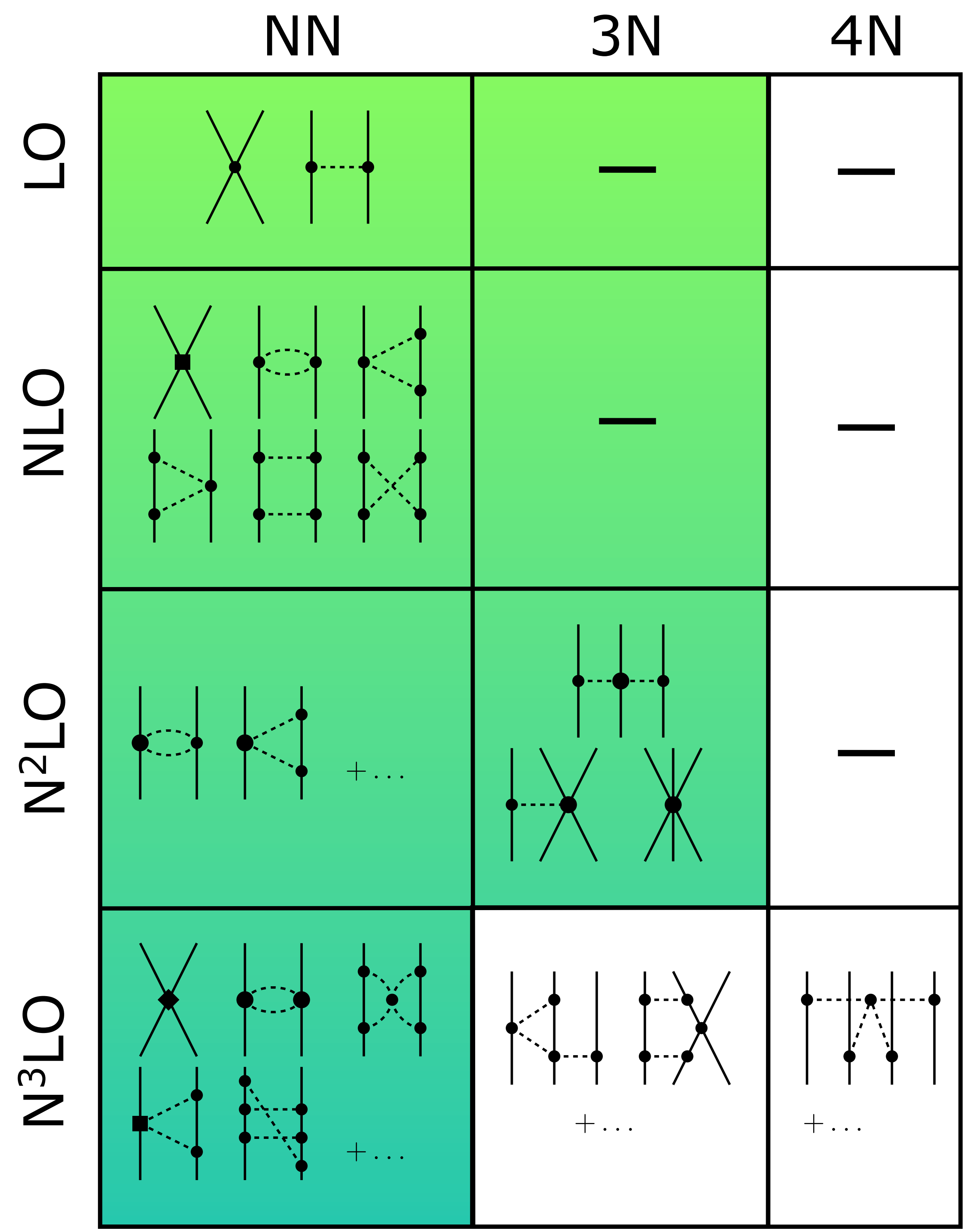
Nuclear Interactions from Chiral EFT

NN interaction

- **N^3LO**: Entem and Machleidt, Λ_{NN} = 500 MeV
- **N^2LO optimized**: Ekström *et al.*, Λ_{NN} = 500 MeV

3N interaction

- **N^2LO**: Navrátil
  - Λ_{3N} = 500 MeV, ^3H fit
  - Λ_{3N} = 350 MeV, ^3H & ^4He fit
  - Λ_{3N} = 400 MeV, ^3H & ^4He fit



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

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

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- **similarity-transformed** Schrödinger equation

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

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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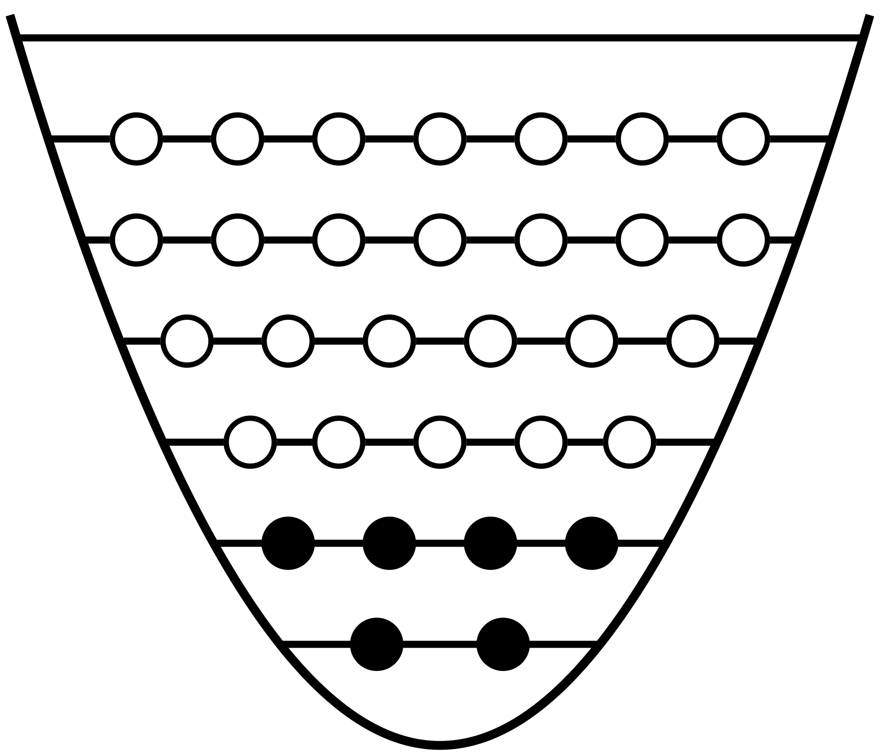

$|\Phi_0\rangle$

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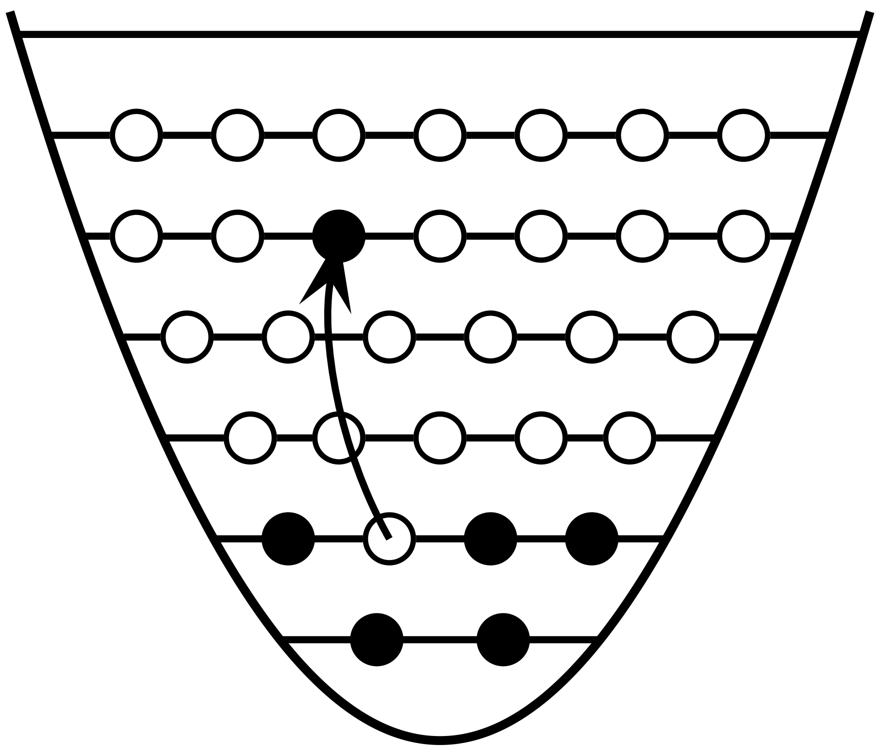

$$\hat{T}_1 \, |\Phi_0\rangle$$

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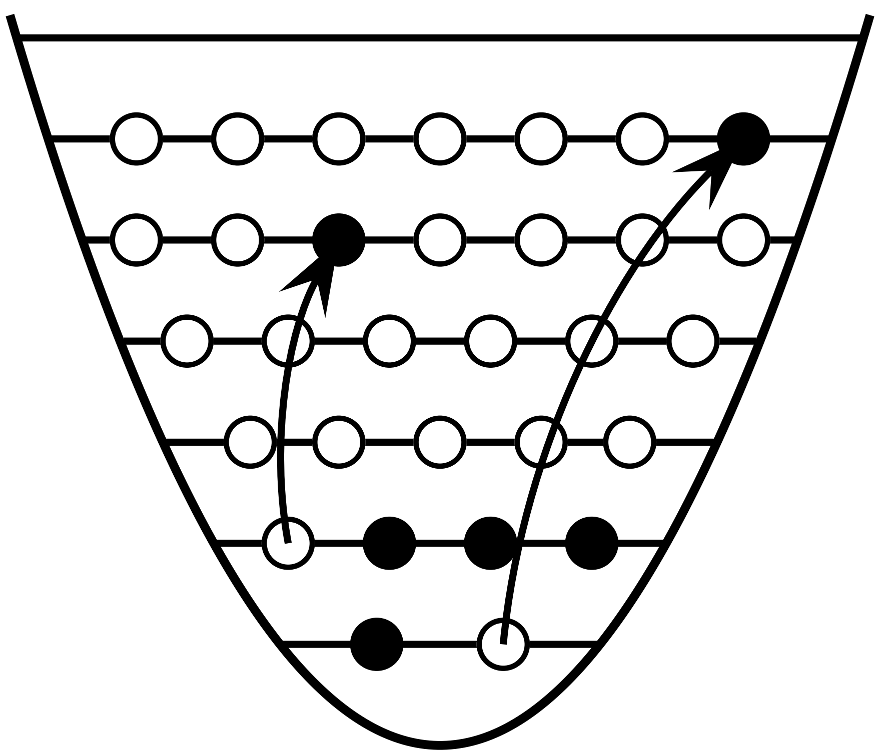

$$\hat{T}_2 \, |\Phi_0\rangle$$

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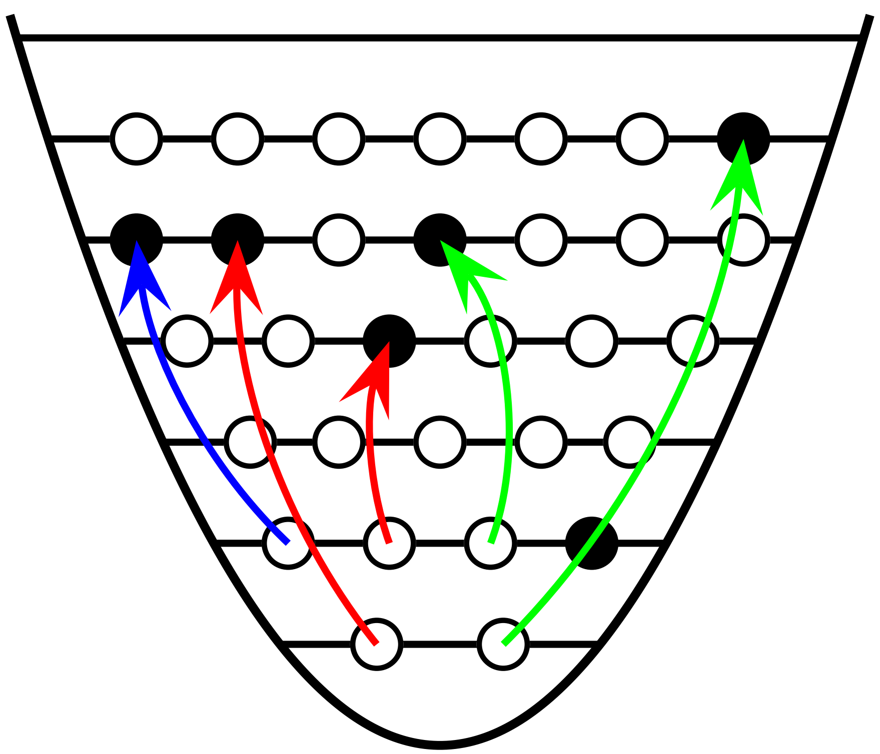

$\hat{T}_1 \, \hat{T}_2 \, \hat{T}_2 \, |\Phi_0\rangle$

- $e^{\hat{T}}$- Ansatz: **higher** excitations from **products** of lower excitation operators

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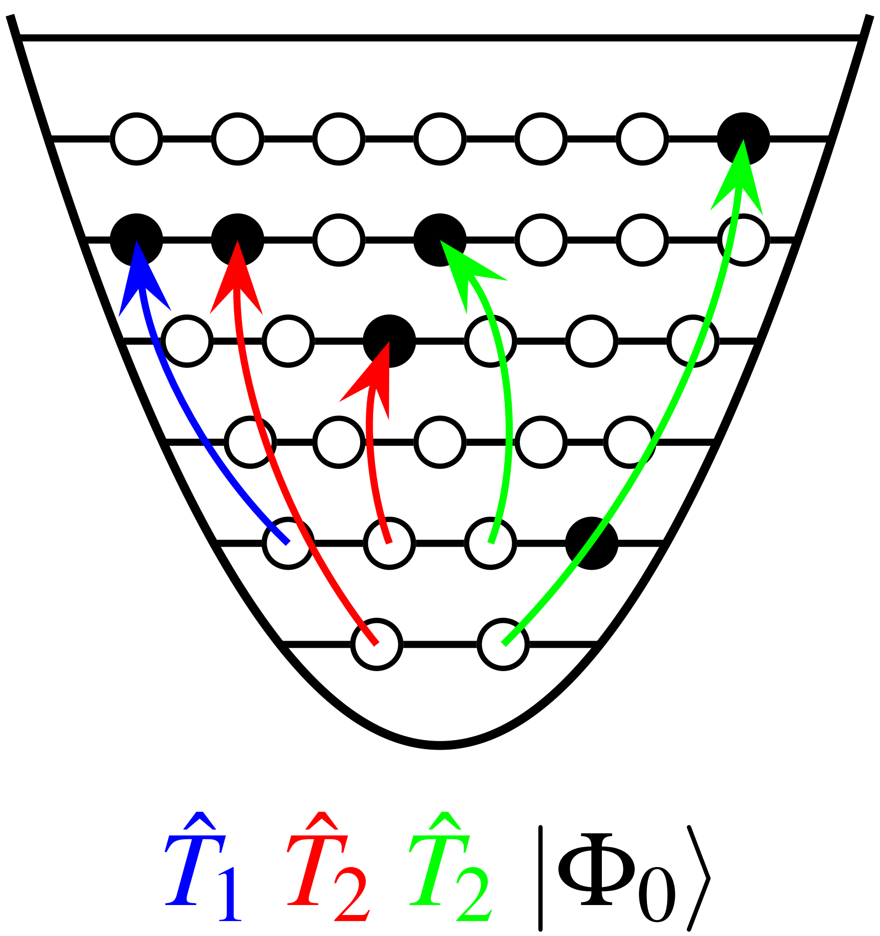

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- CCSD equations

$$\Delta E^{(\mathrm{CCSD})} = \langle \Phi_0 | \hat{\mathcal{H}} | \Phi_0 \rangle$$

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

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

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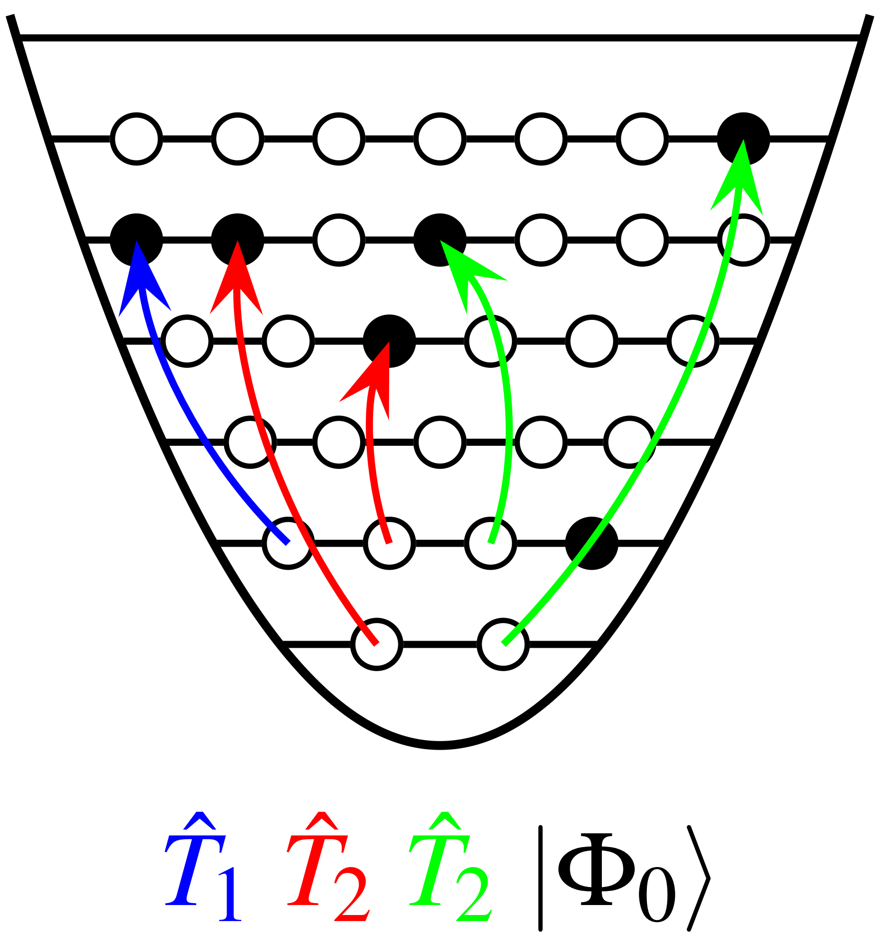

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- Coupled system of **nonlinear equations**

Coupled-Cluster Triples Corrections

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perturbation theory

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

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perturbation theory → $\Lambda\mathrm{CCSD(T)}$

method of moments → $\mathrm{CR-CC}(2,3)$

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$$
\begin{tikzcd}
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\Lambda\mathrm{CCSD(T)} & & \mathrm{CR-CC(2,3)}
\end{tikzcd}
$$

- Non-iterative **triples corrections**

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

Denominators in ΛCCSD(T), CR-CC(2,3)

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    - Option 2: **Average** them

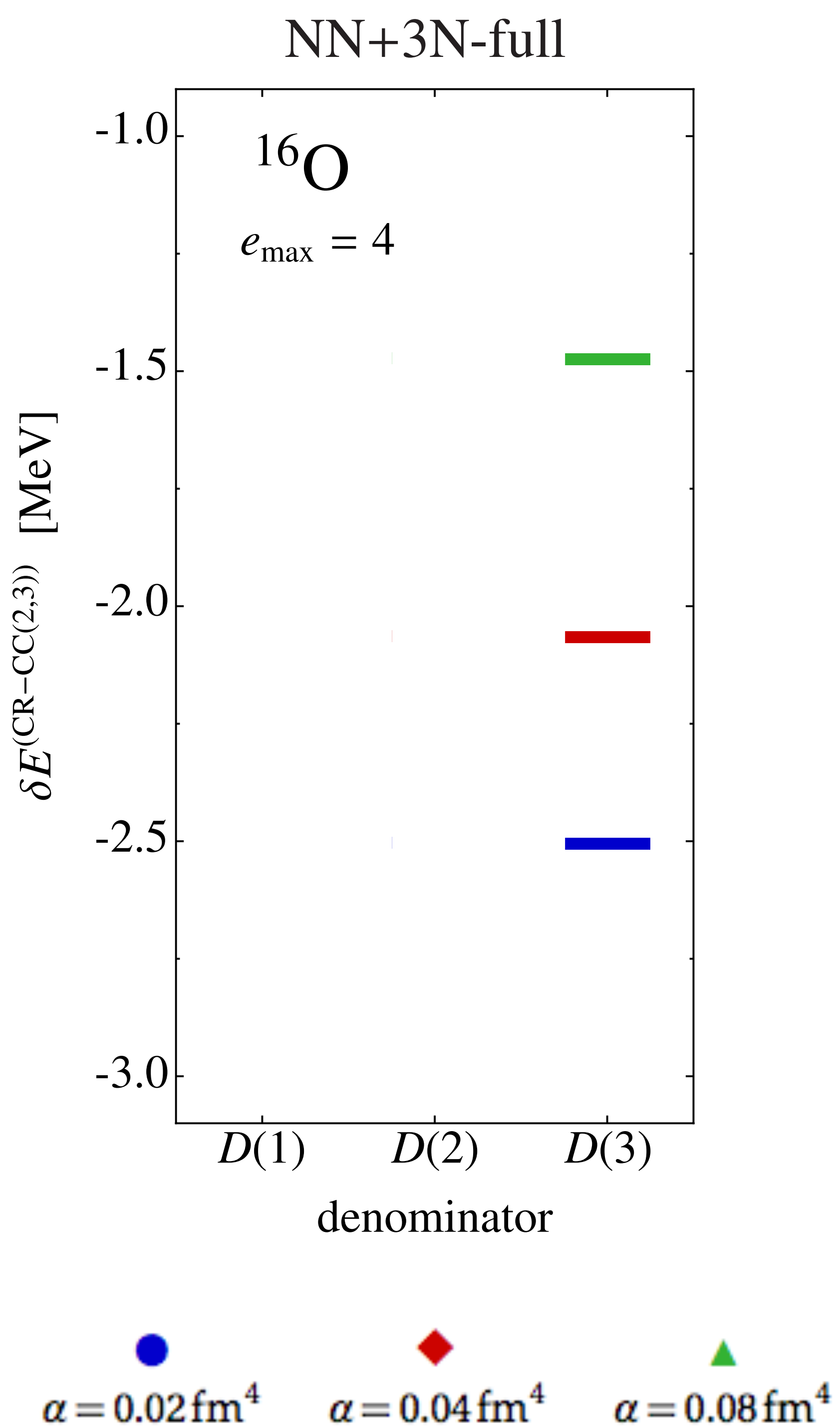
$$\Rightarrow D^{abc}_{ijk} \approx \overline{D}^{abc}_{ijk} = \mathcal{H}^i_i + \dots + \overline{\mathcal{H}}^{ij}_{ij} + \dots + \overline{\mathcal{H}}^{ijk}_{ijk} + \dots$$

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

Approximate CR-CC(2,3) Denominators

Option 1: Discard

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



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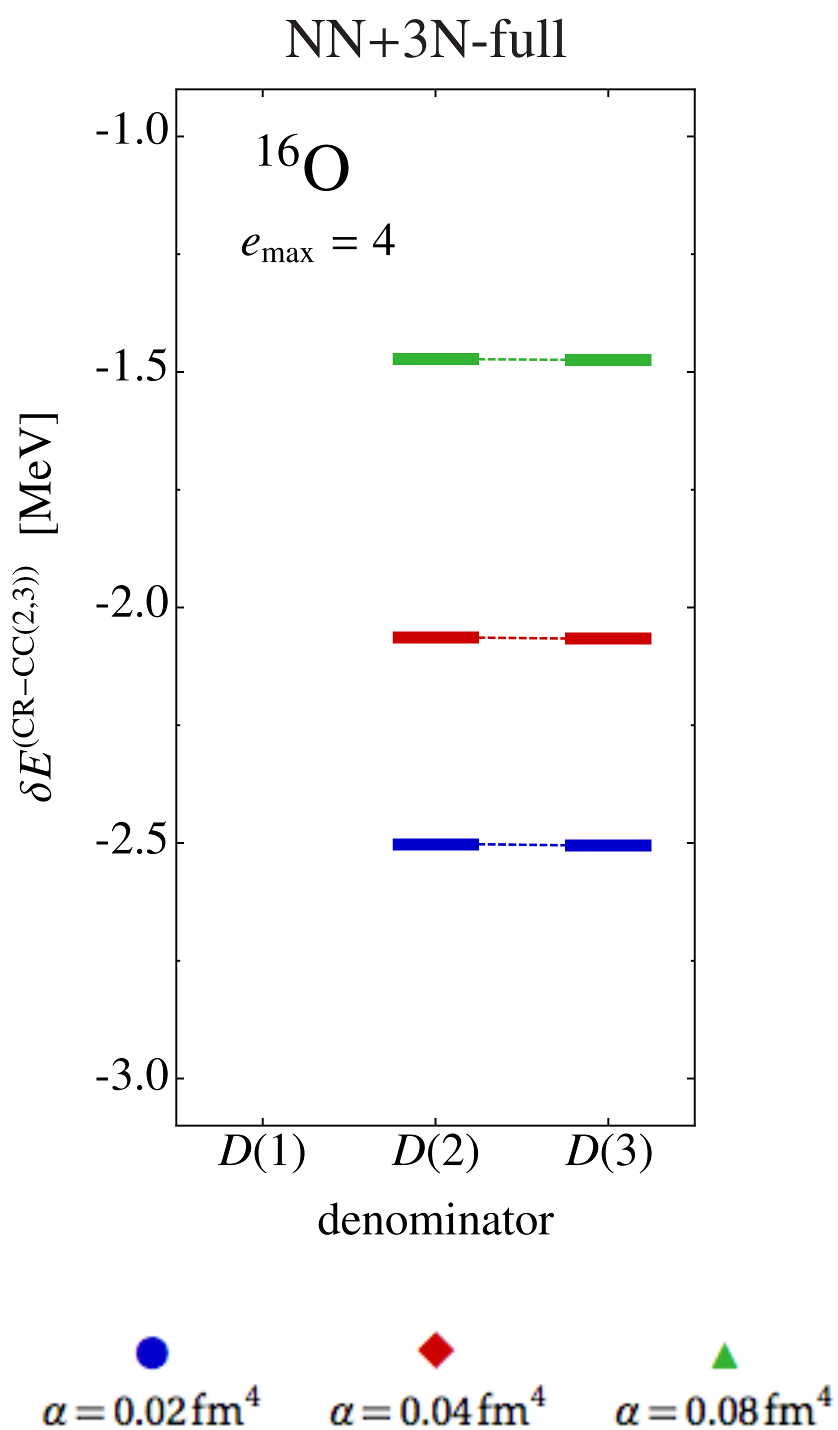

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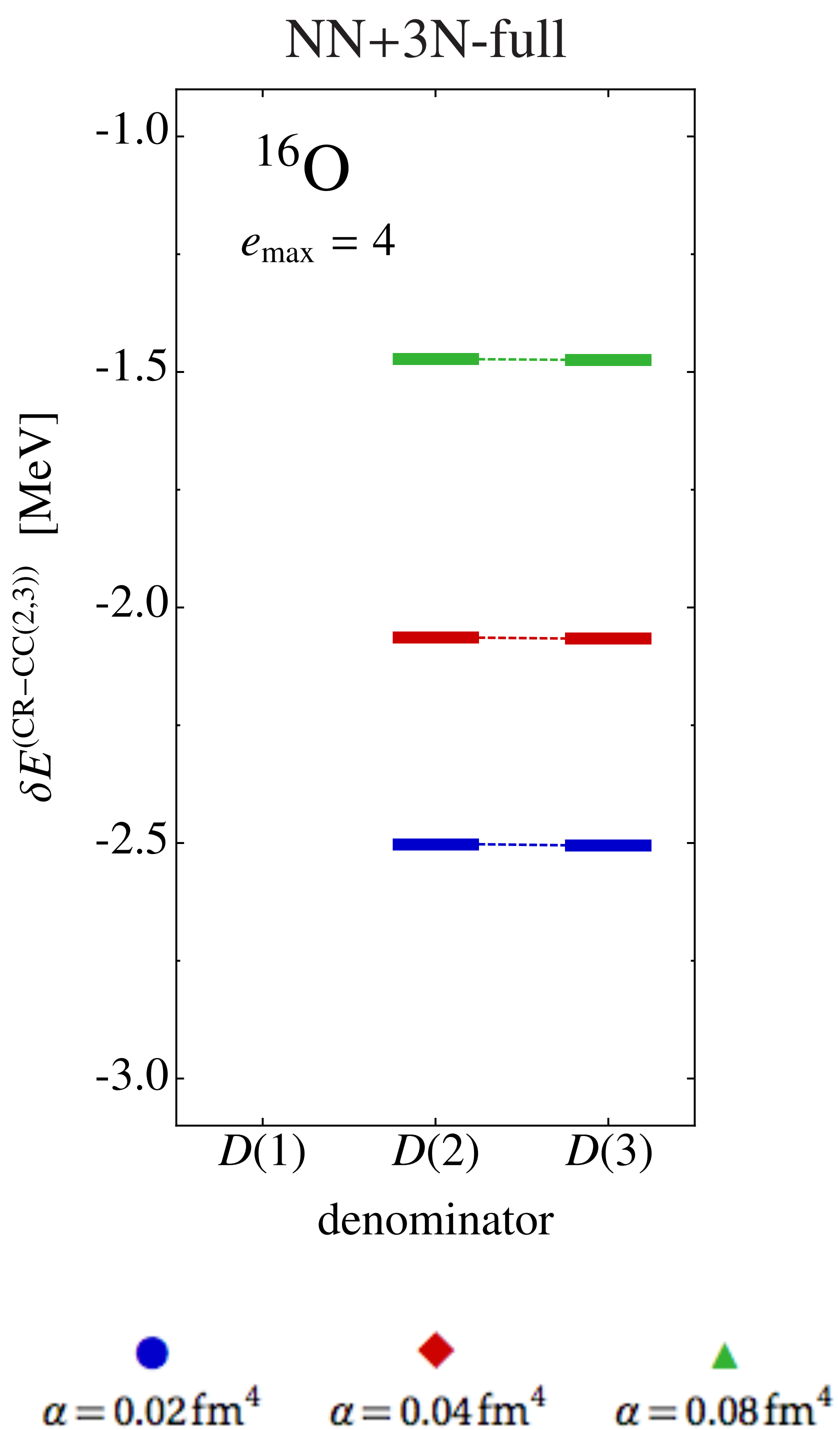

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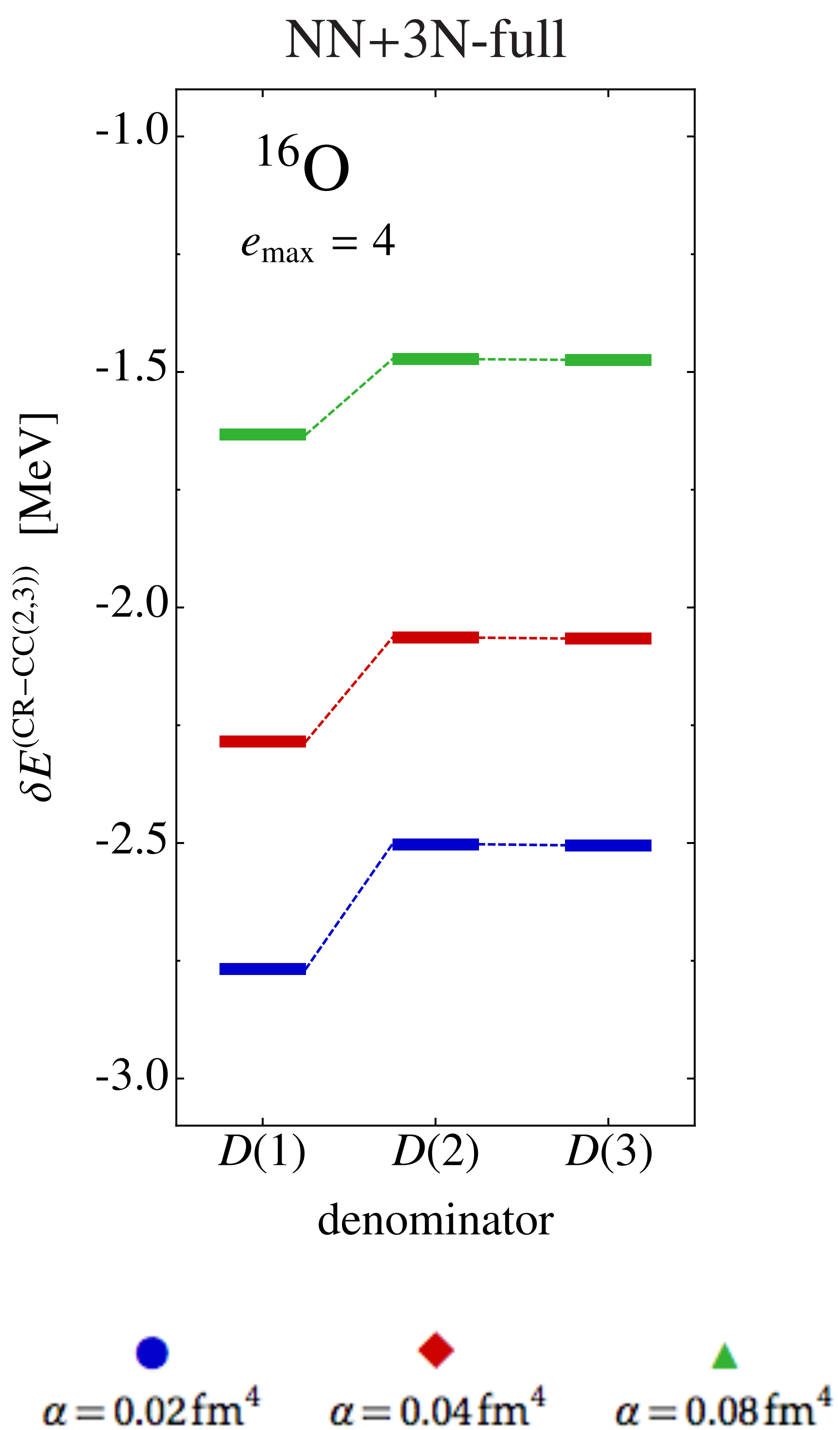

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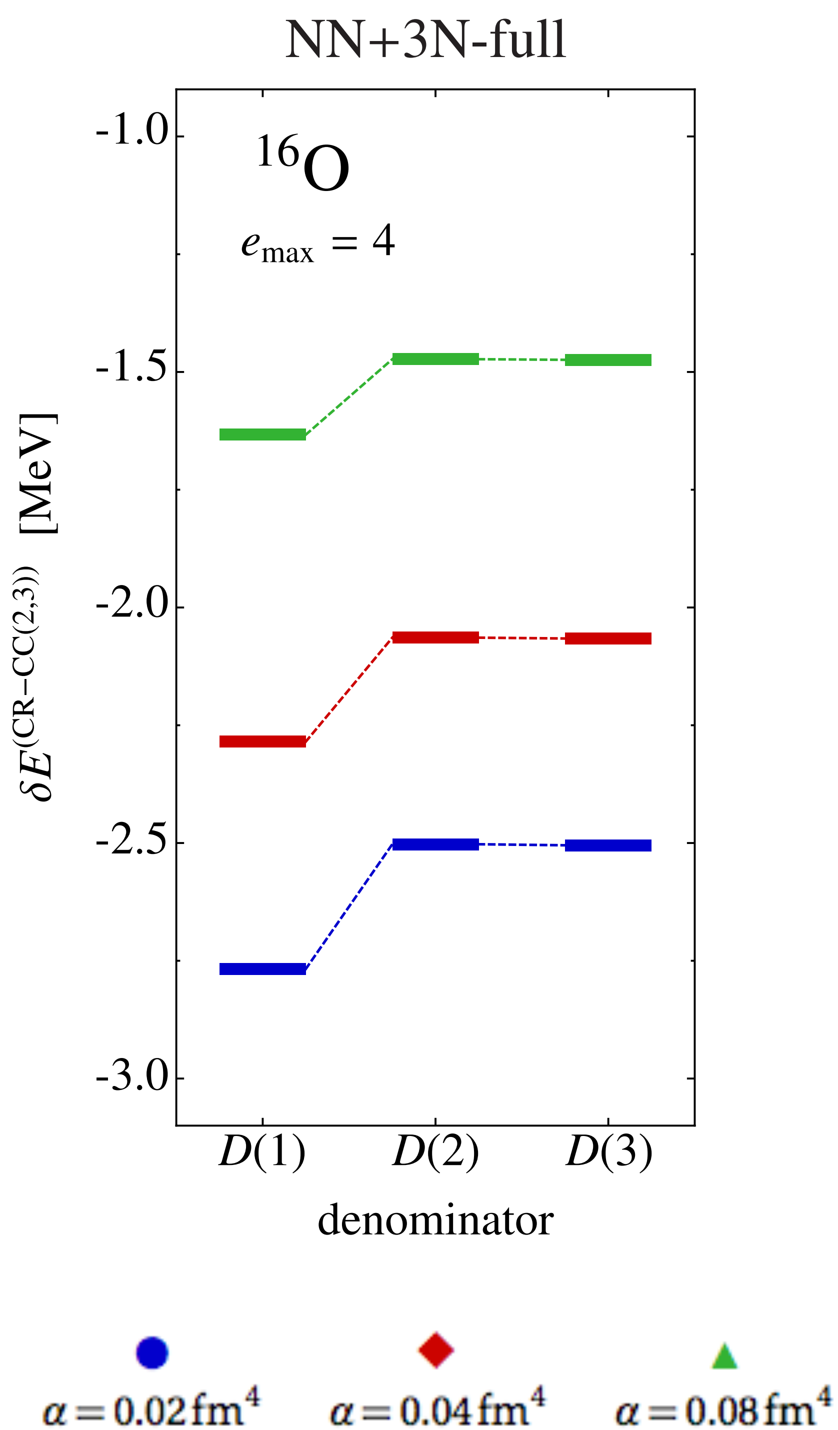

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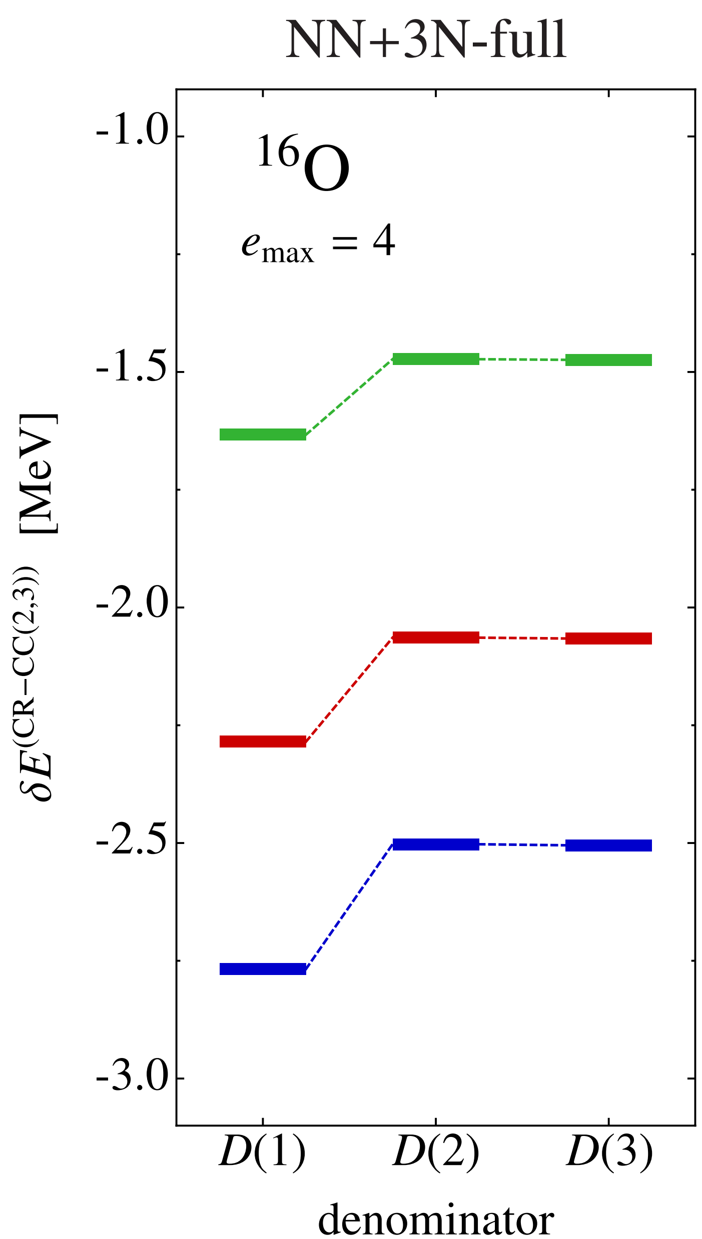

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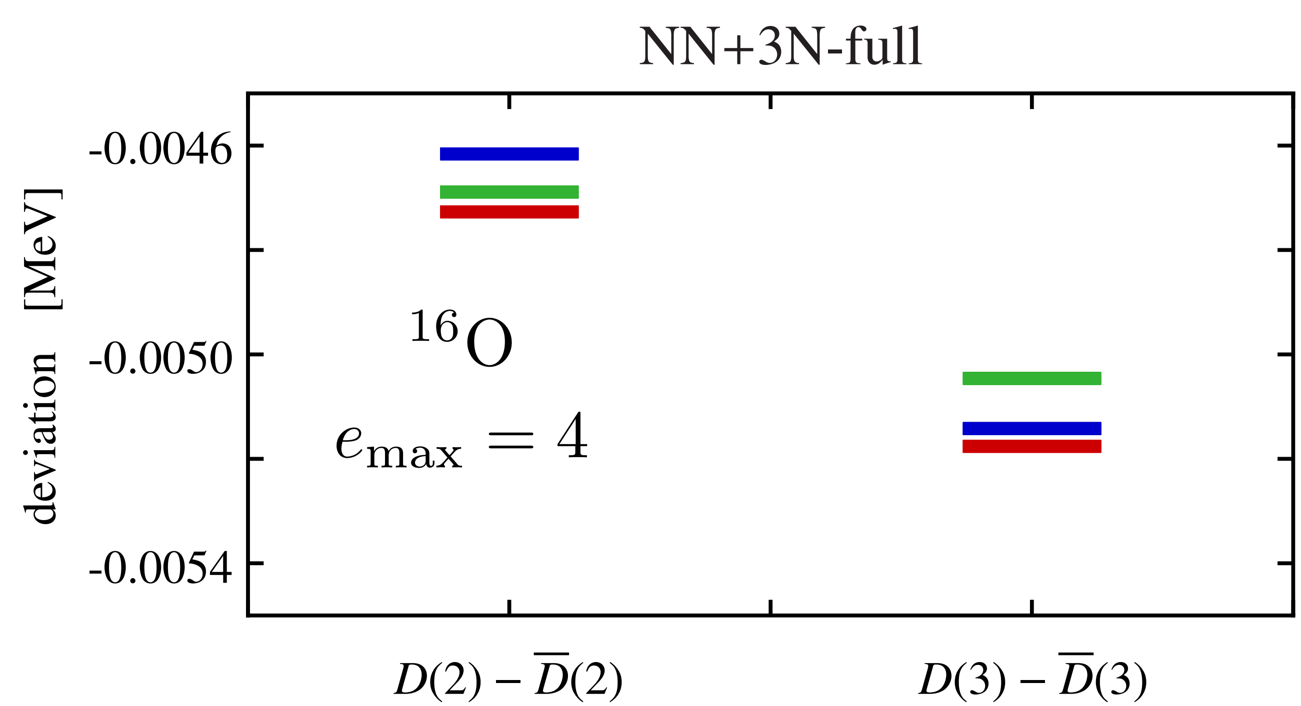
Option 2: Average



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

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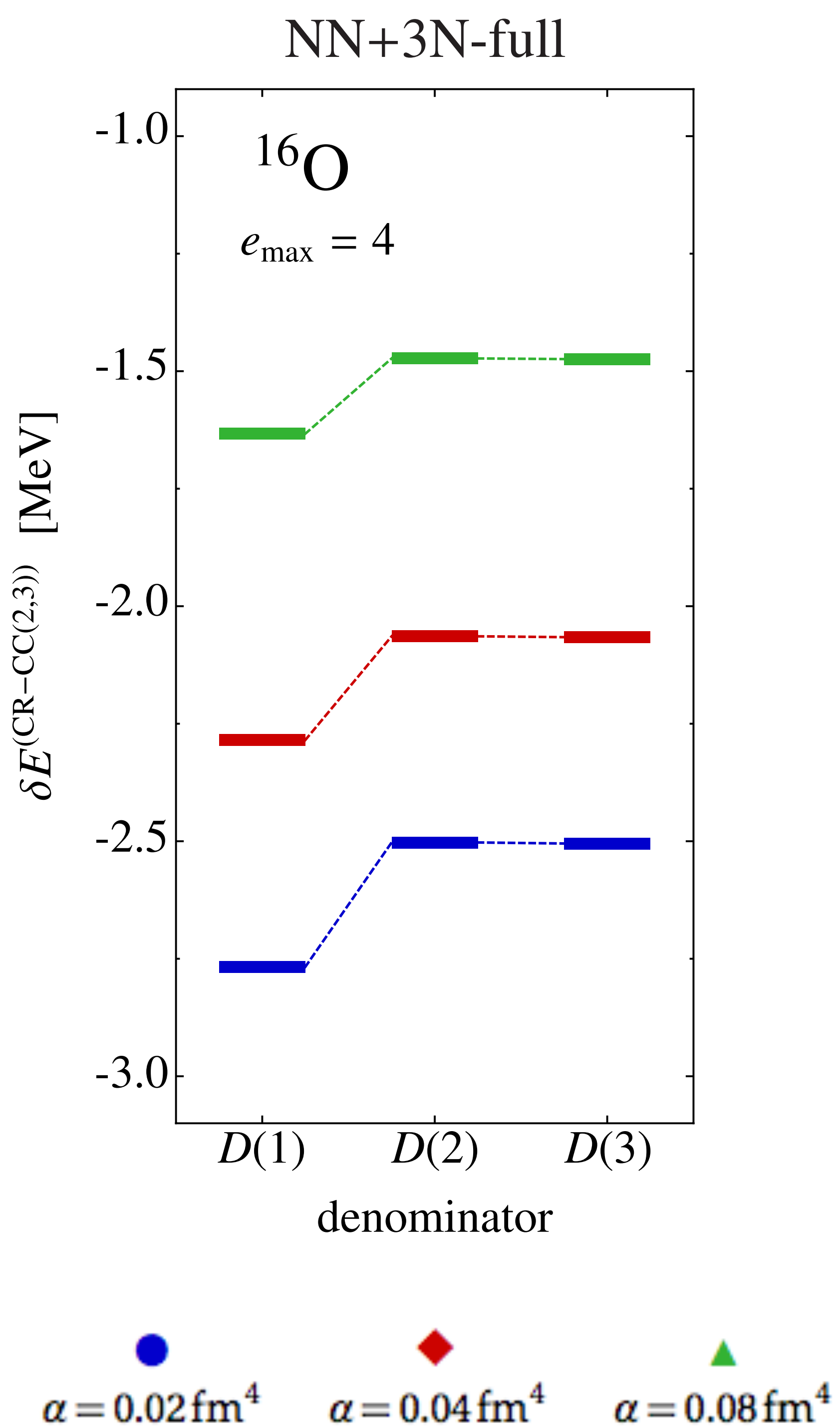

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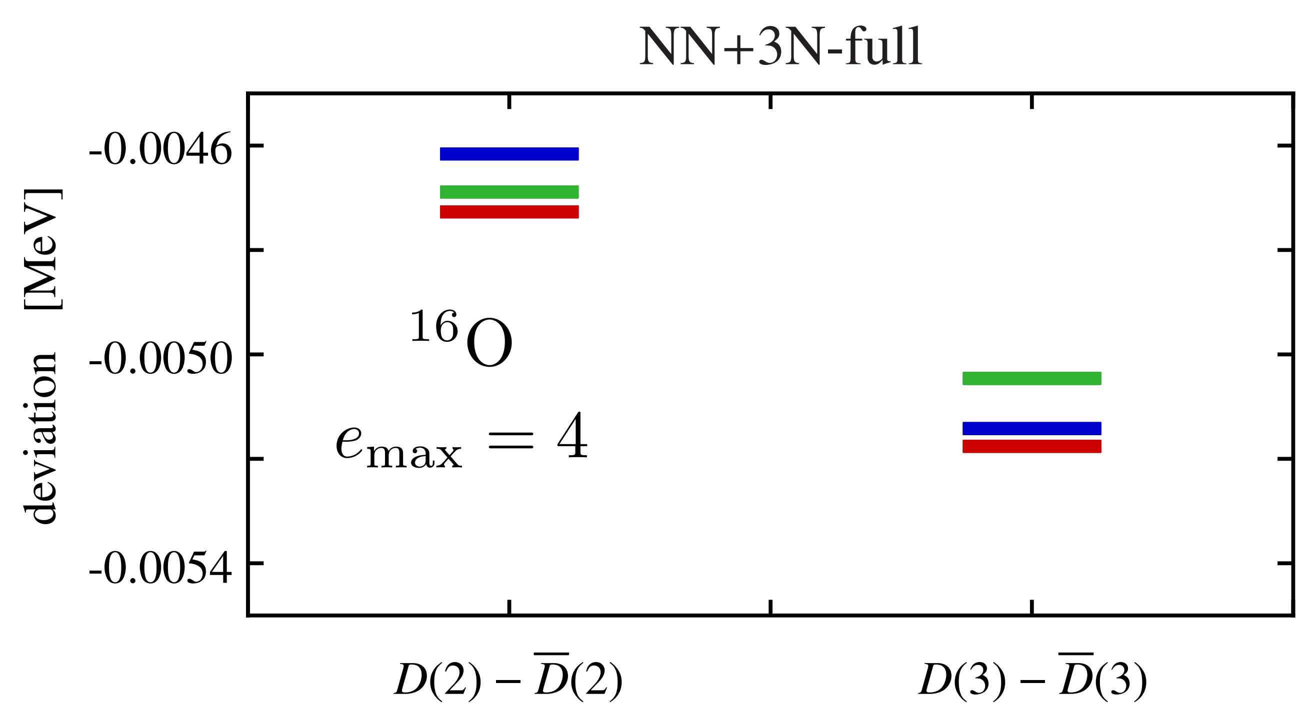
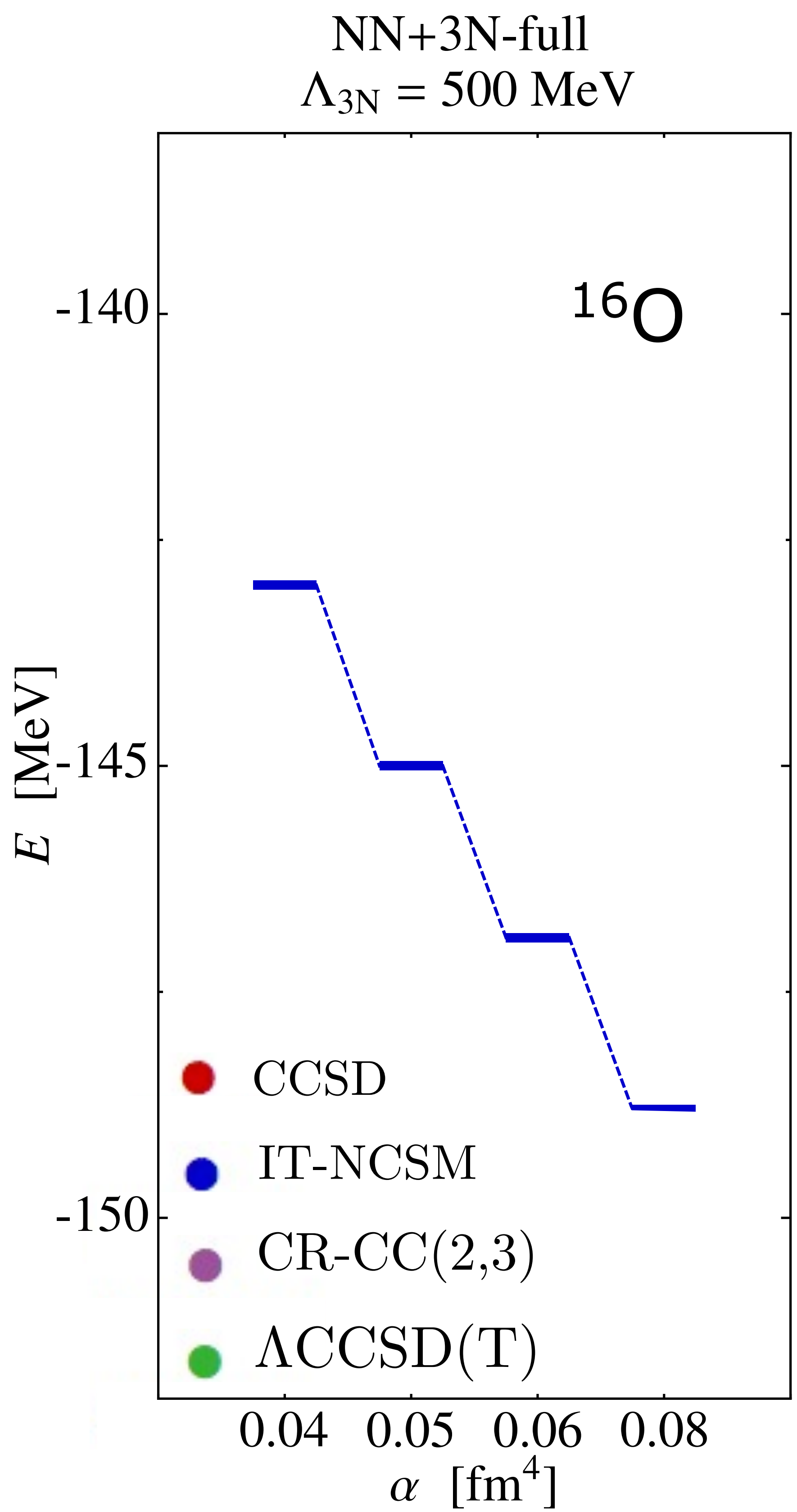


- Error from **averaging** ≈ **5 keV**

CR-CC(2,3) vs. ΛCCSD(T) and IT-NCSM



CR-CC(2,3)

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

$$\mathfrak{M}^{abc}_{ijk} = \langle \Phi^{abc}_{ijk} | \hat{\mathcal{H}}^{(\mathrm{CCSD})} | \Phi_0 \rangle$$

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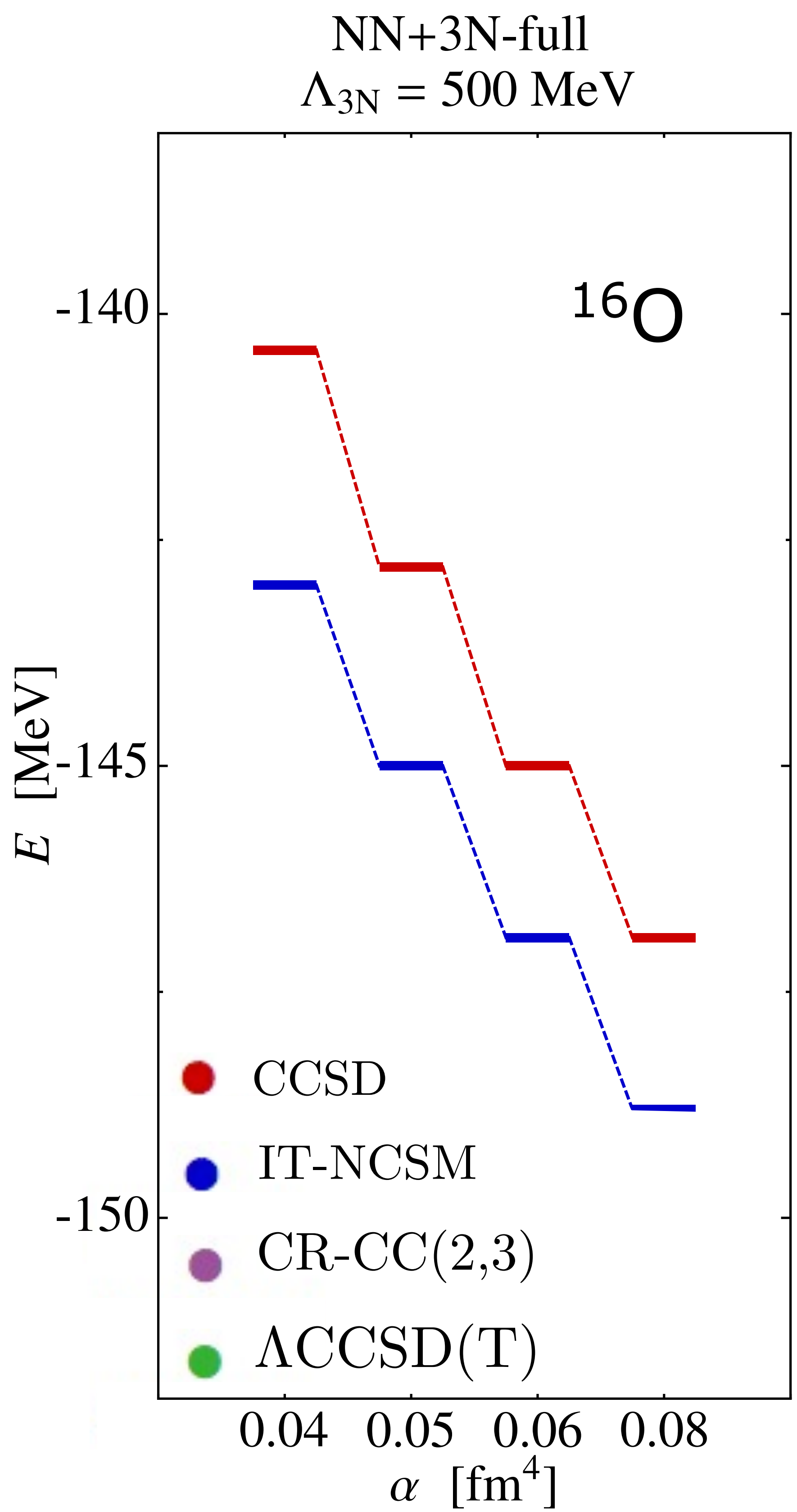
$$D^{abc}_{ijk} = - \sum_n \langle \Phi^{abc}_{ijk} | \hat{\mathcal{H}}^{(\mathrm{CCSD})}_n | \Phi^{abc}_{ijk} \rangle$$

- **CR-CC(2,3)** shows **excellent agreement** with IT-NCSM diagonalizations

CR-CC(2,3) vs. ΛCCSD(T) and IT-NCSM



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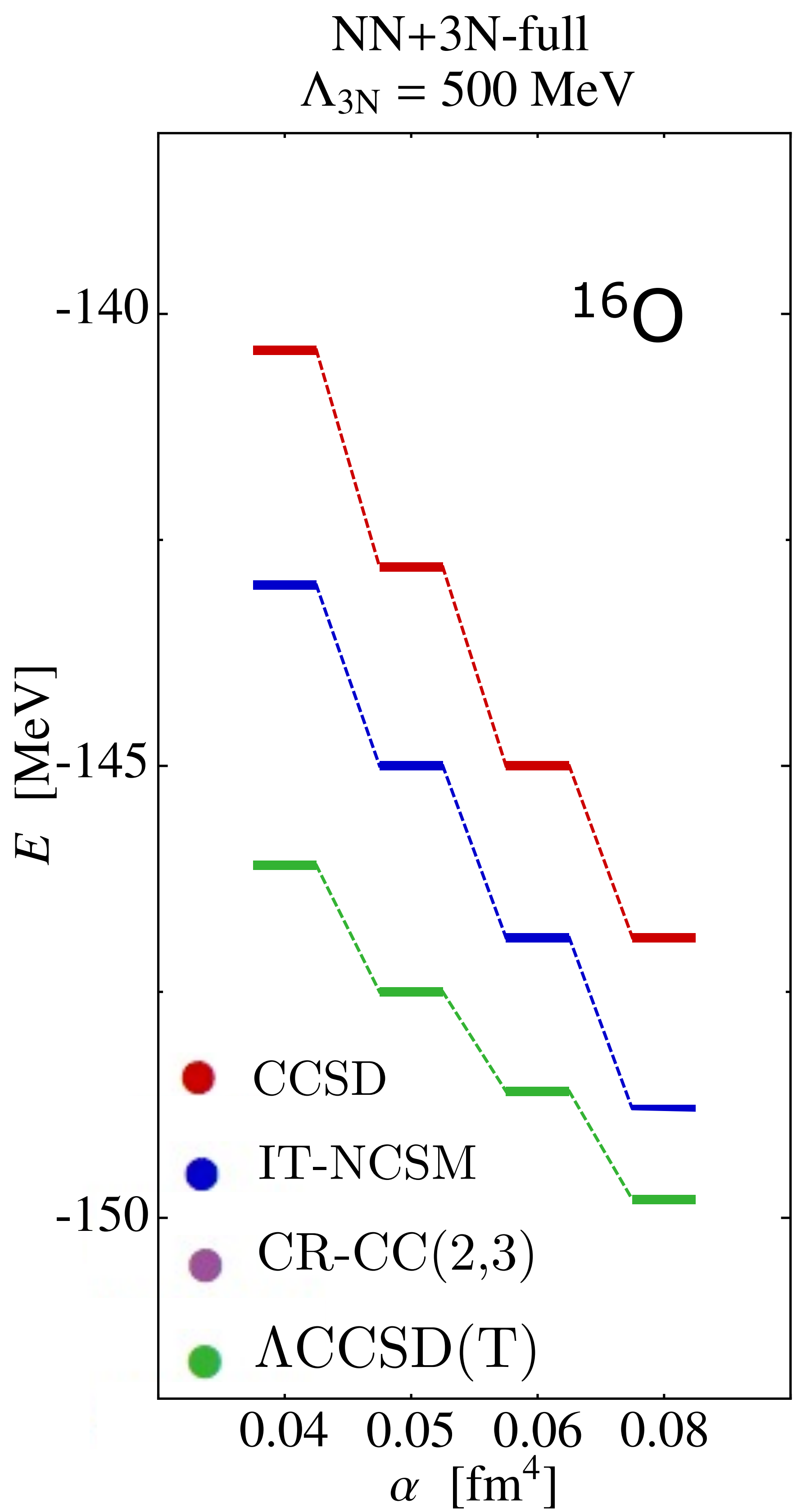

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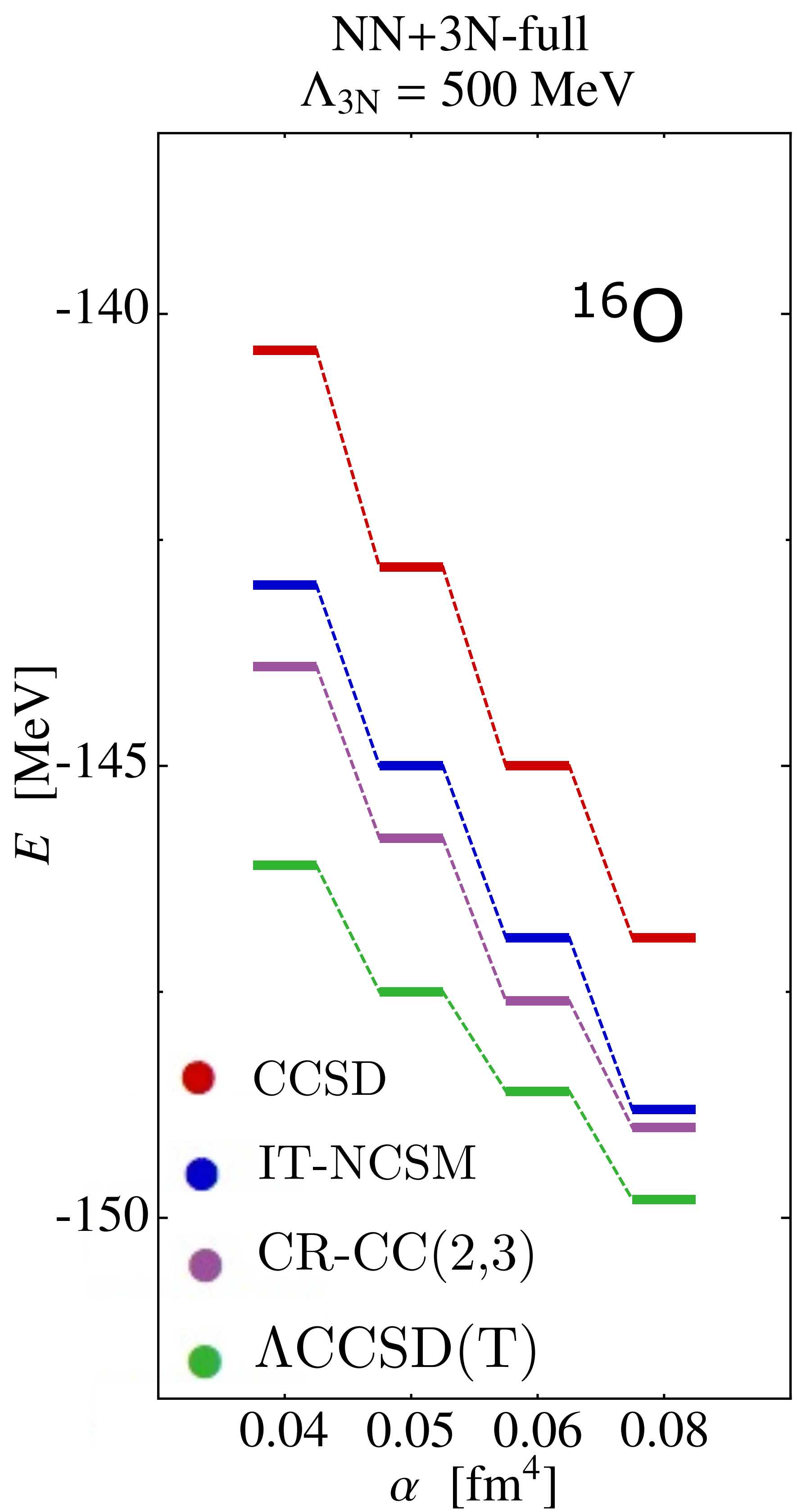

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$$\mathfrak{M}^{abc}_{ijk} = \langle \Phi^{abc}_{ijk} | \hat{\mathcal{H}}^{(\mathrm{CCSD})} | \Phi_0 \rangle$$

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$$D^{abc}_{ijk} = - \sum_n \langle \Phi^{abc}_{ijk} | \hat{\mathcal{H}}^{(\mathrm{CCSD})}_n | \Phi^{abc}_{ijk} \rangle$$

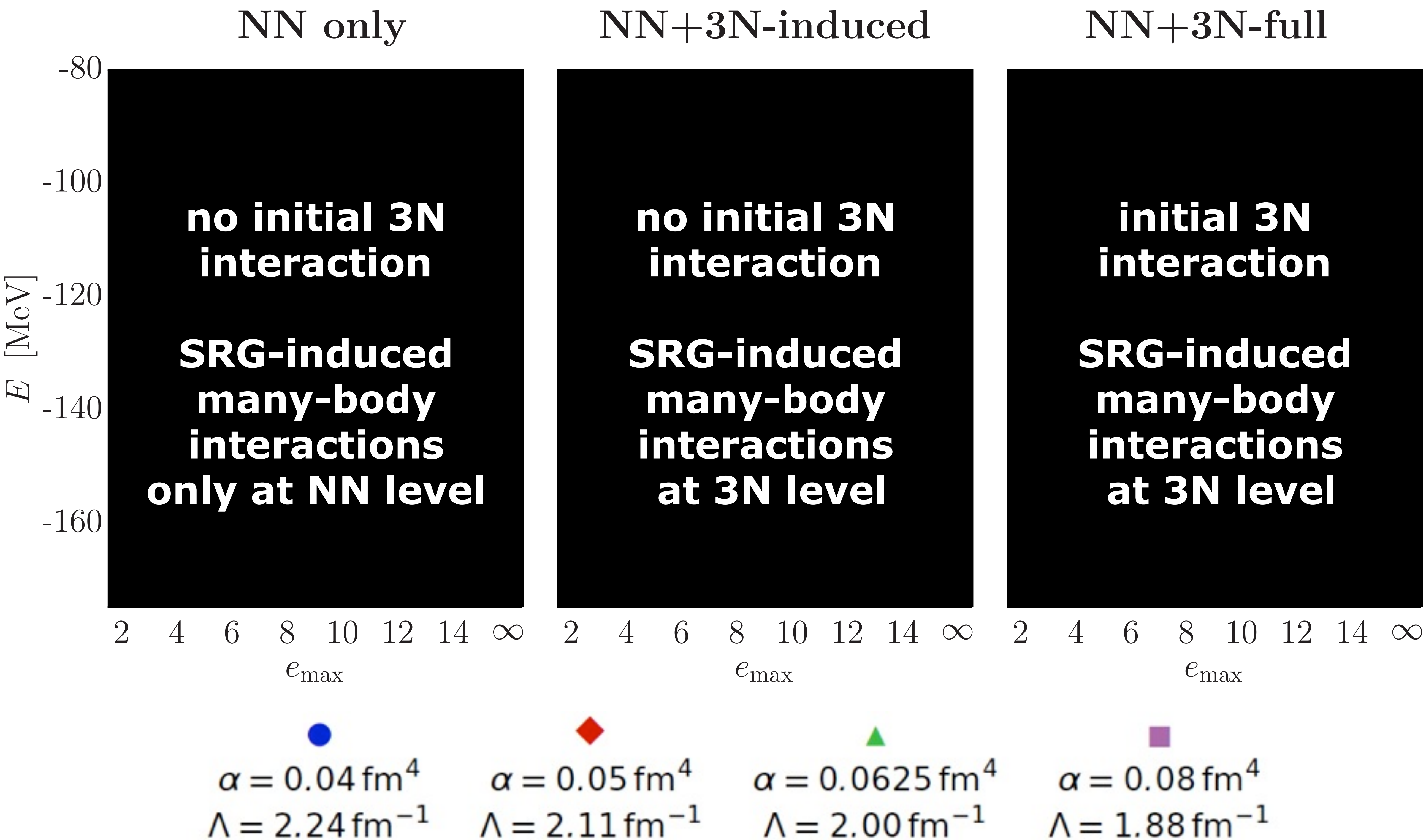
- **CR-CC(2,3)** shows **excellent agreement** with IT-NCSM diagonalizations

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

^{16}O: Reduced-Cutoff 3N Interaction



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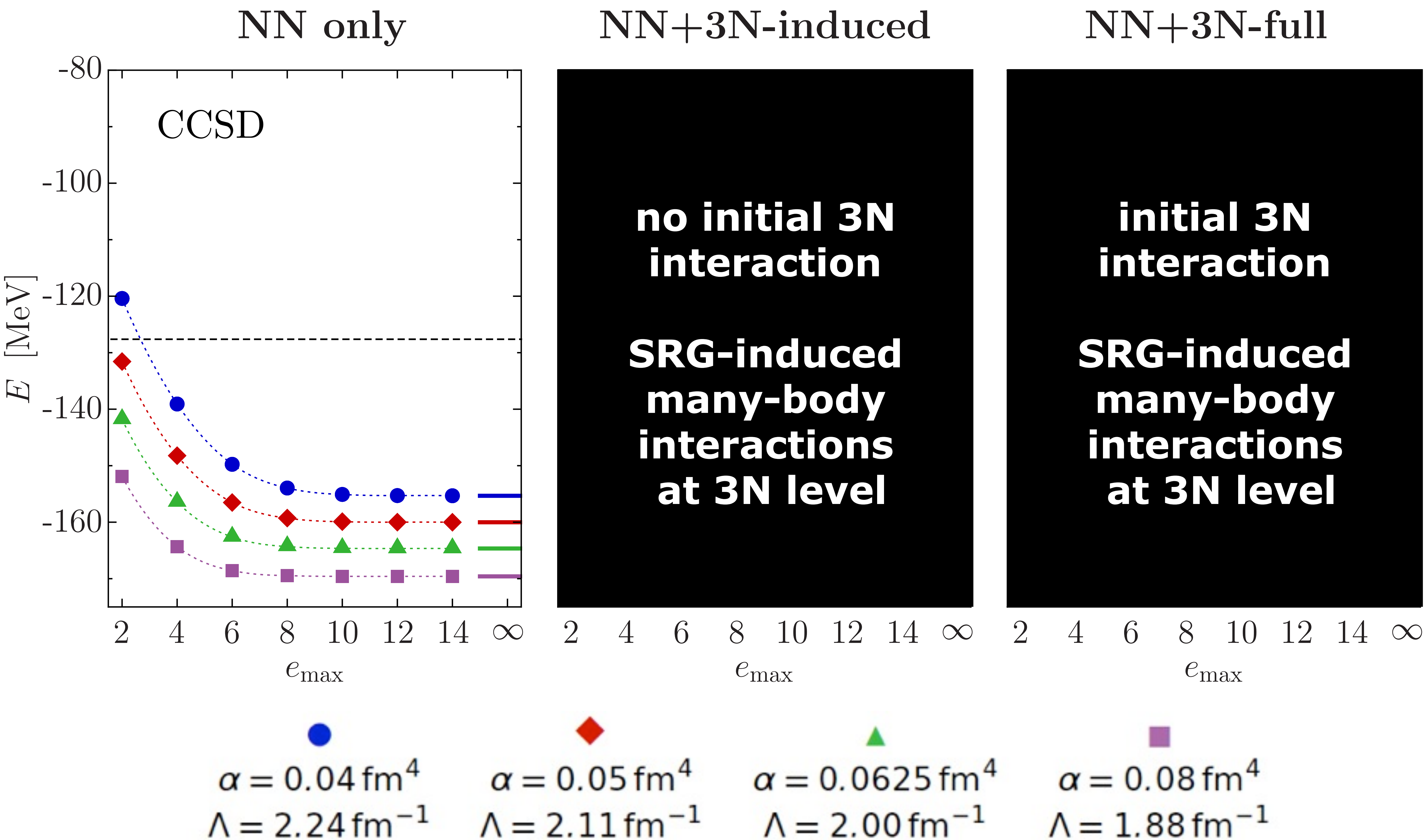

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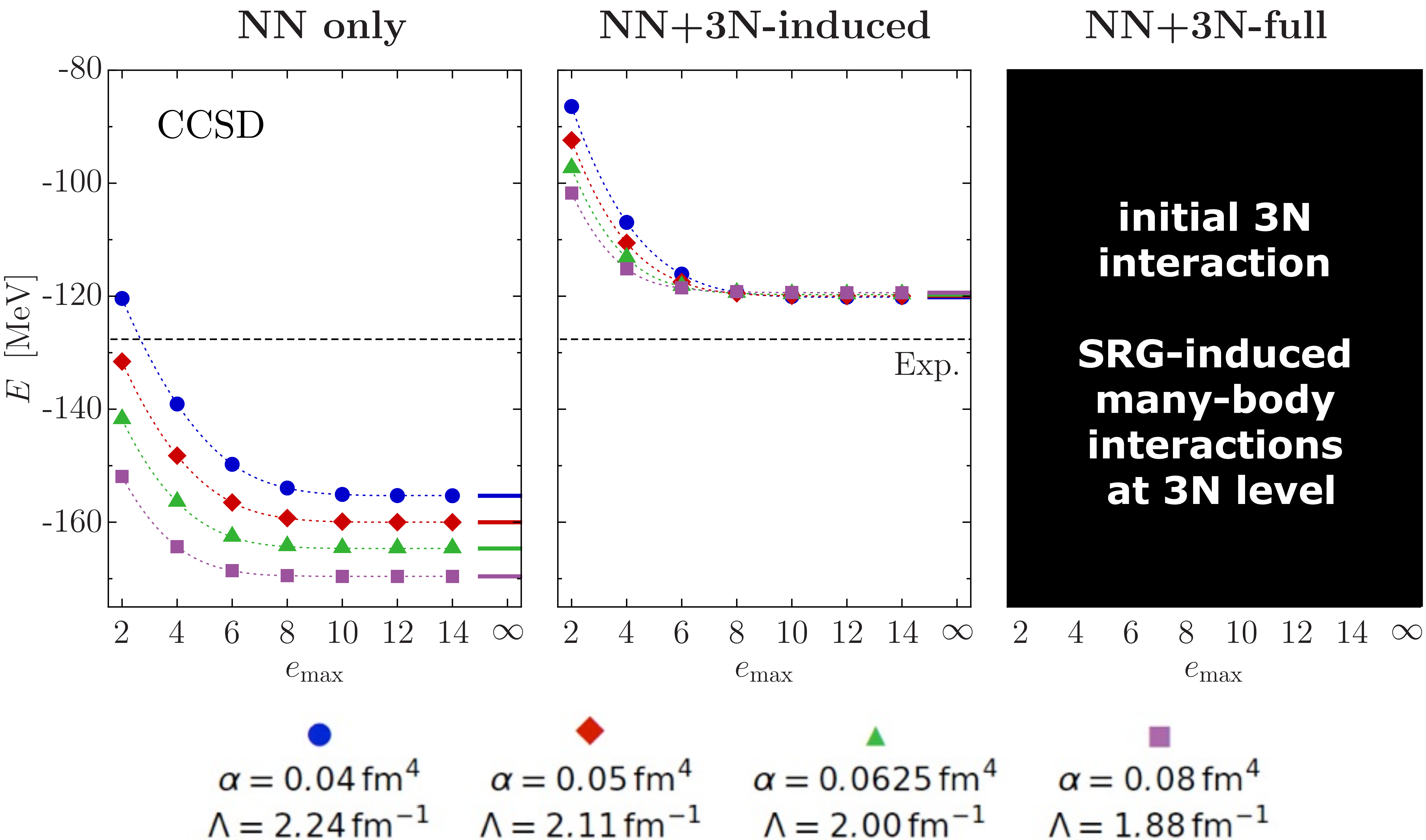

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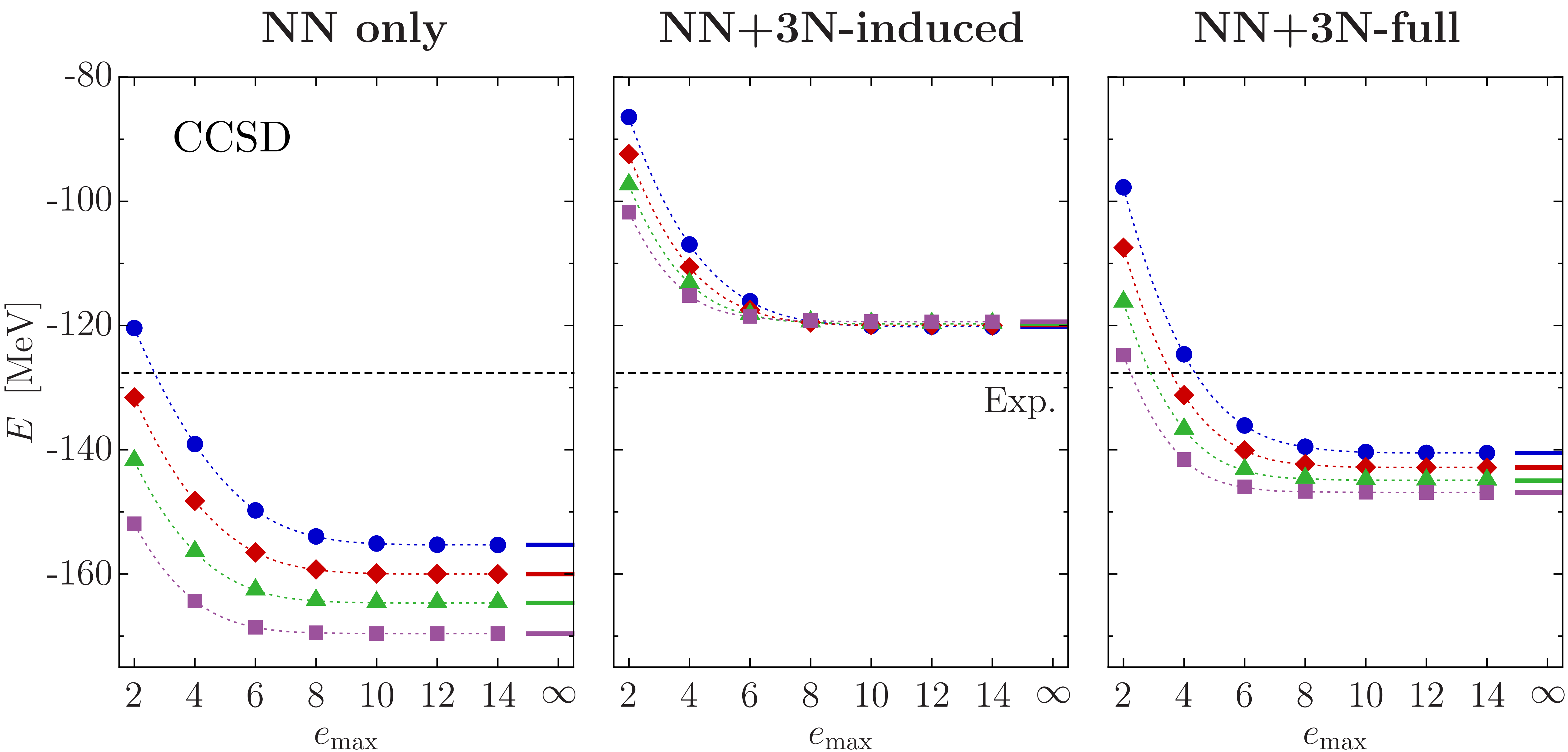

$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

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

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

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

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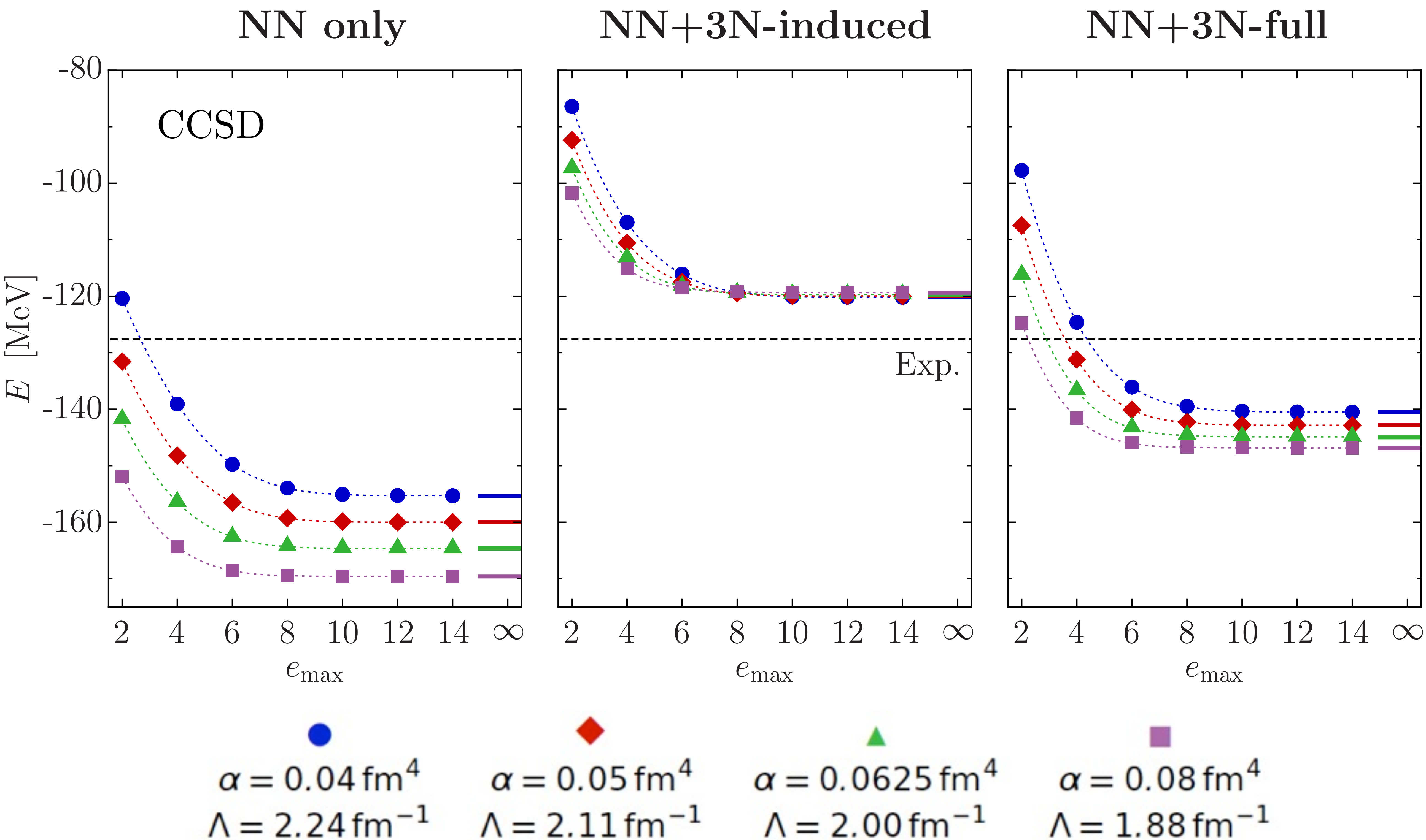

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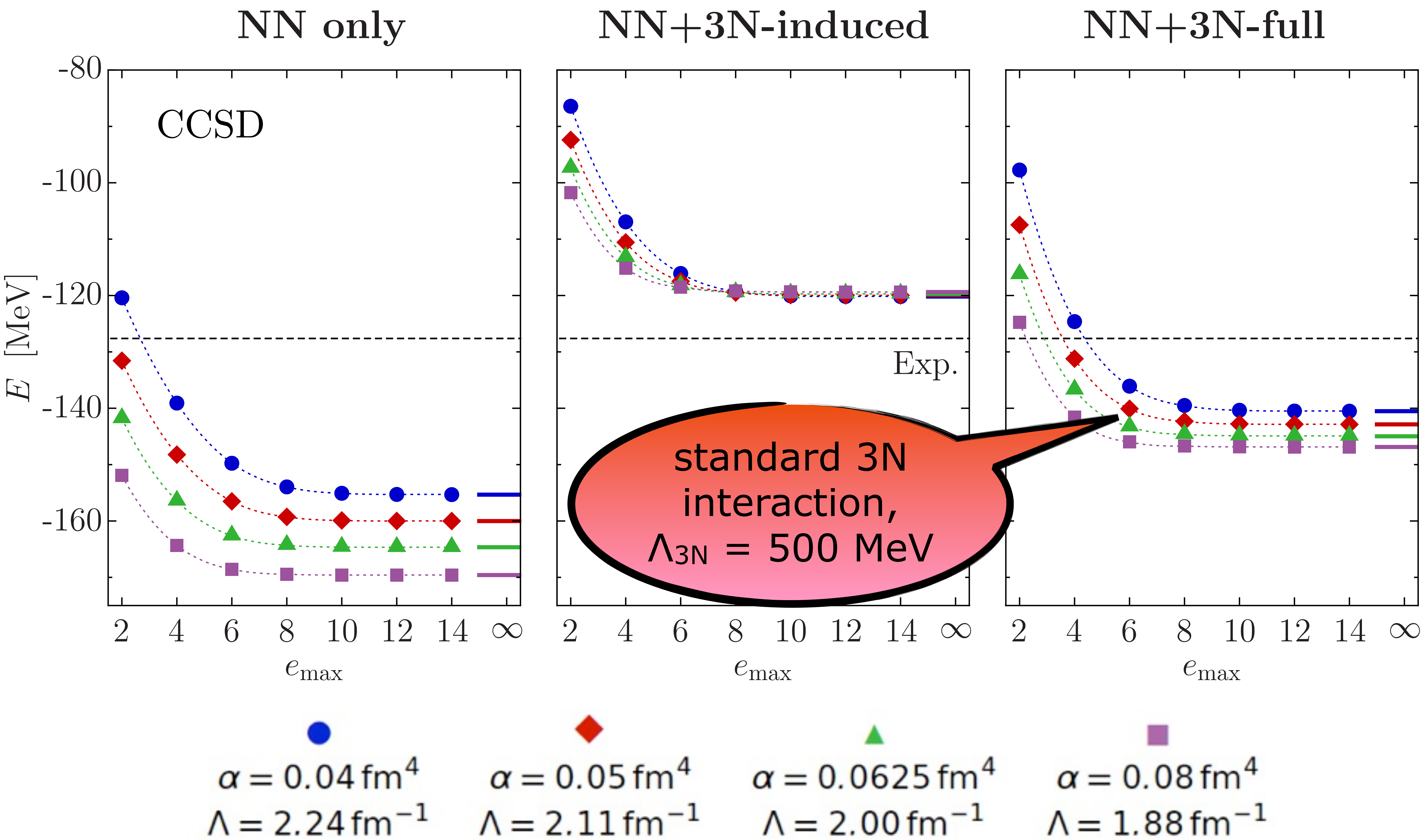
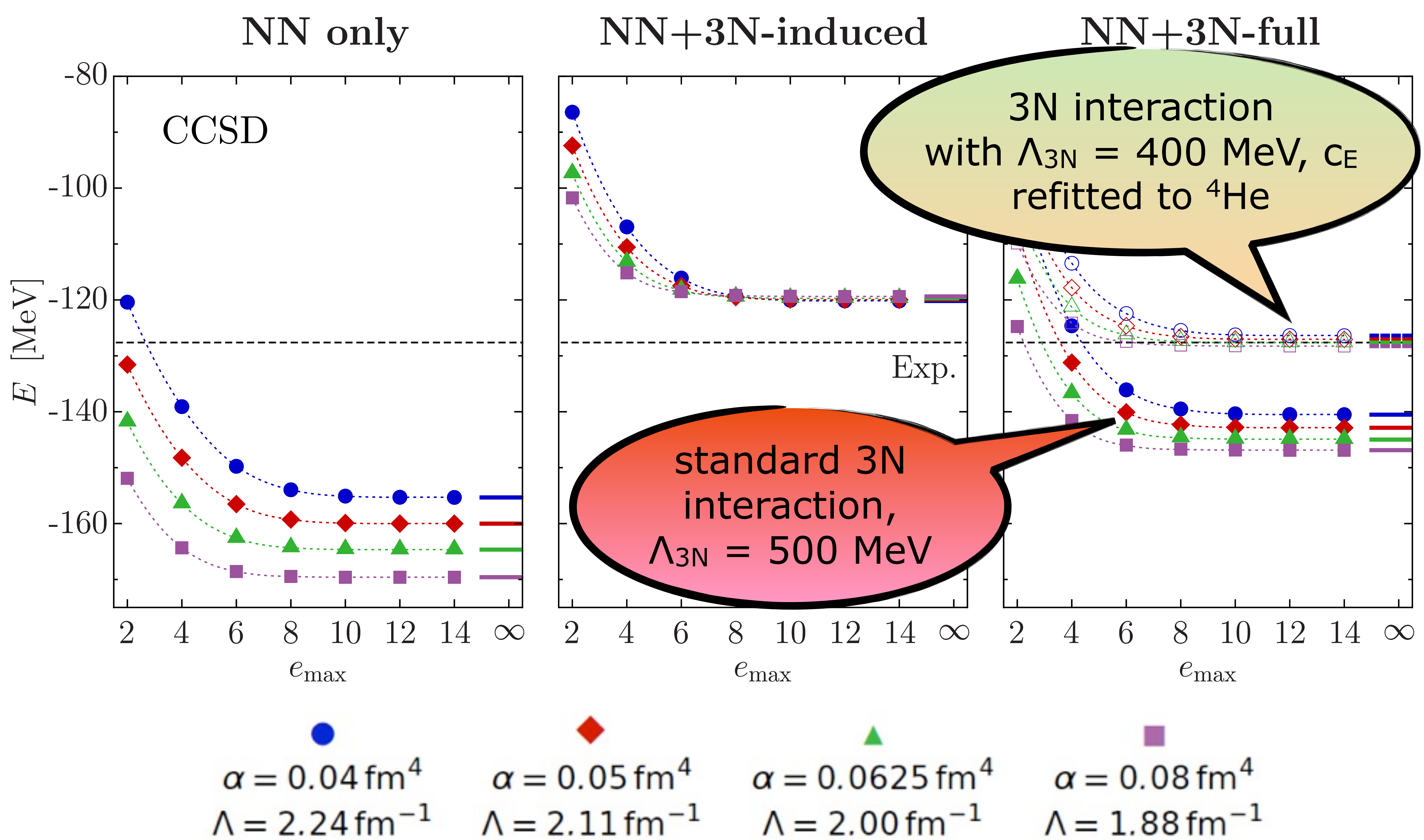
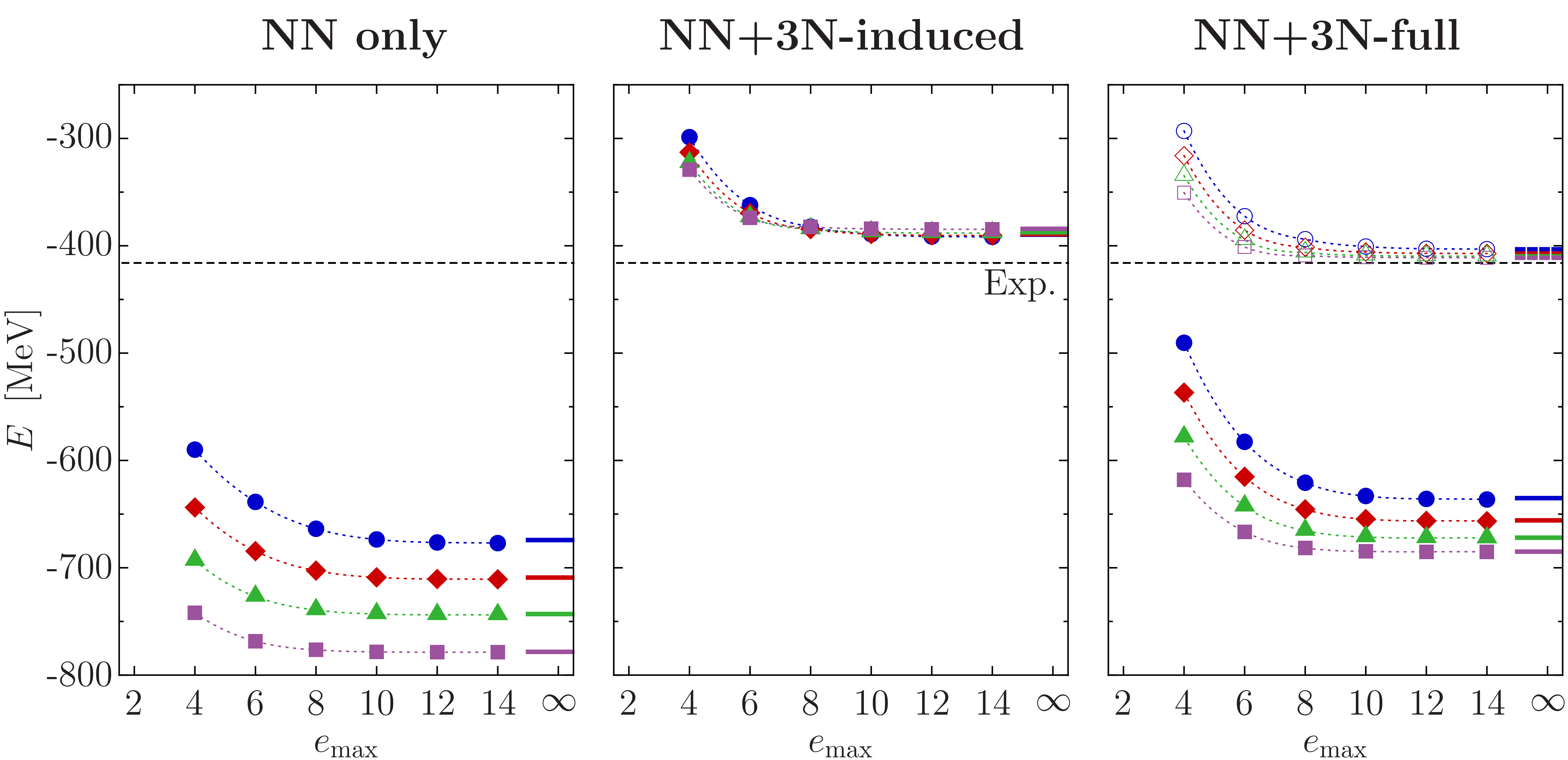


^{16}O: Reduced-Cutoff 3N Interaction



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



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

Normal-Ordered 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

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)

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

Normal-Ordered 3N Interaction

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

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

Normal-Ordered 3N Interaction

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

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

Normal-Ordered 3N Interaction

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

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

Normal-Ordered 3N Interaction

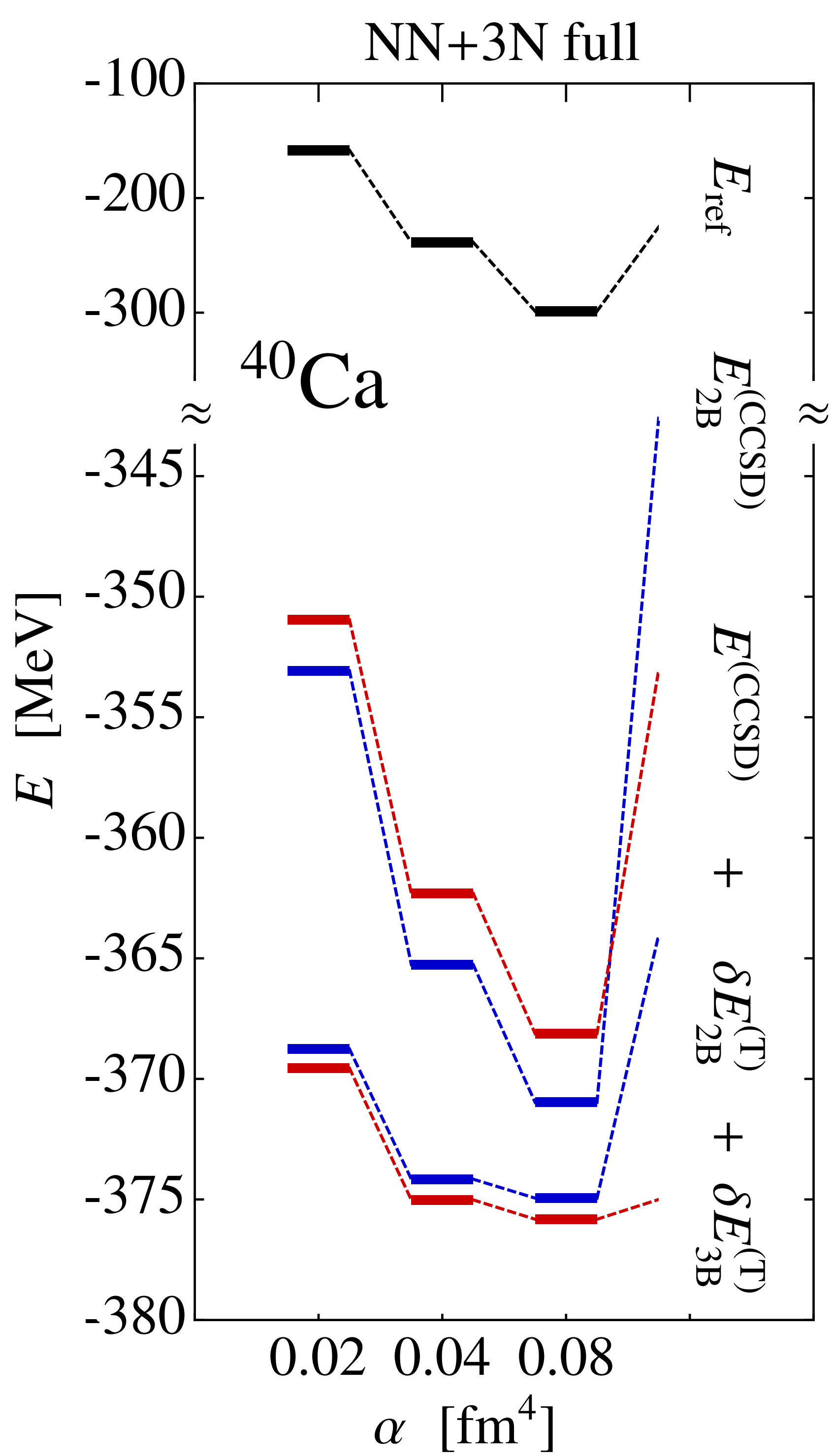
Avoid technical challenge of including explicit 3N interactions in many-body calculation

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

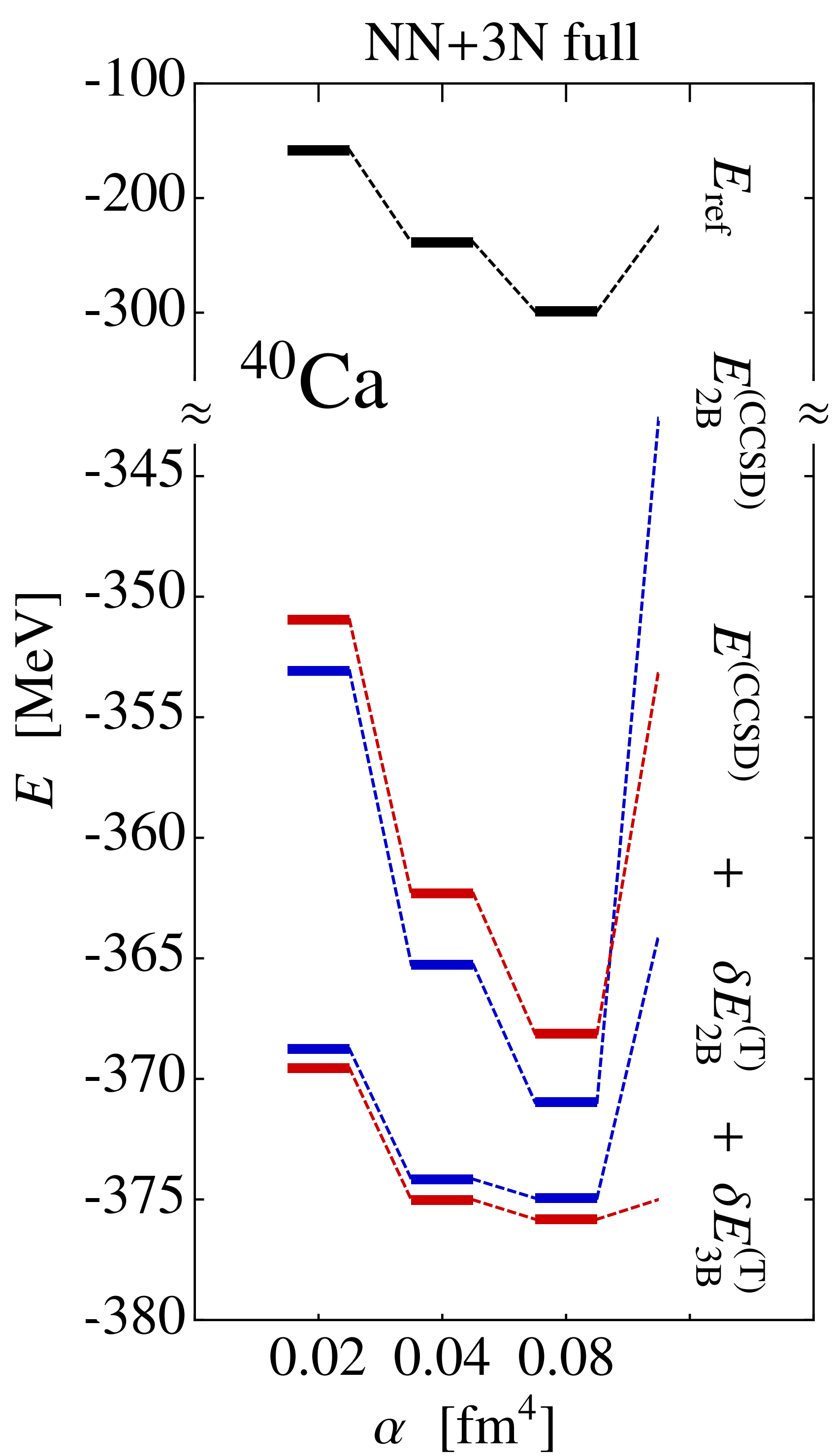
$$\hat{V}_{\mathrm{NO2B}} = W^{\mathrm{0B}} + \sum W^{\mathrm{1B}}_{\circ\circ}\; \hat{a}^{\dagger}_{\circ}\hat{a}_{\circ} + \sum W^{\mathrm{2B}}_{\circ\circ\circ\circ}\; \hat{a}^{\dagger}_{\circ}\hat{a}^{\dagger}_{\circ}\hat{a}_{\circ}\hat{a}_{\circ}$$

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

Benchmark NO2B

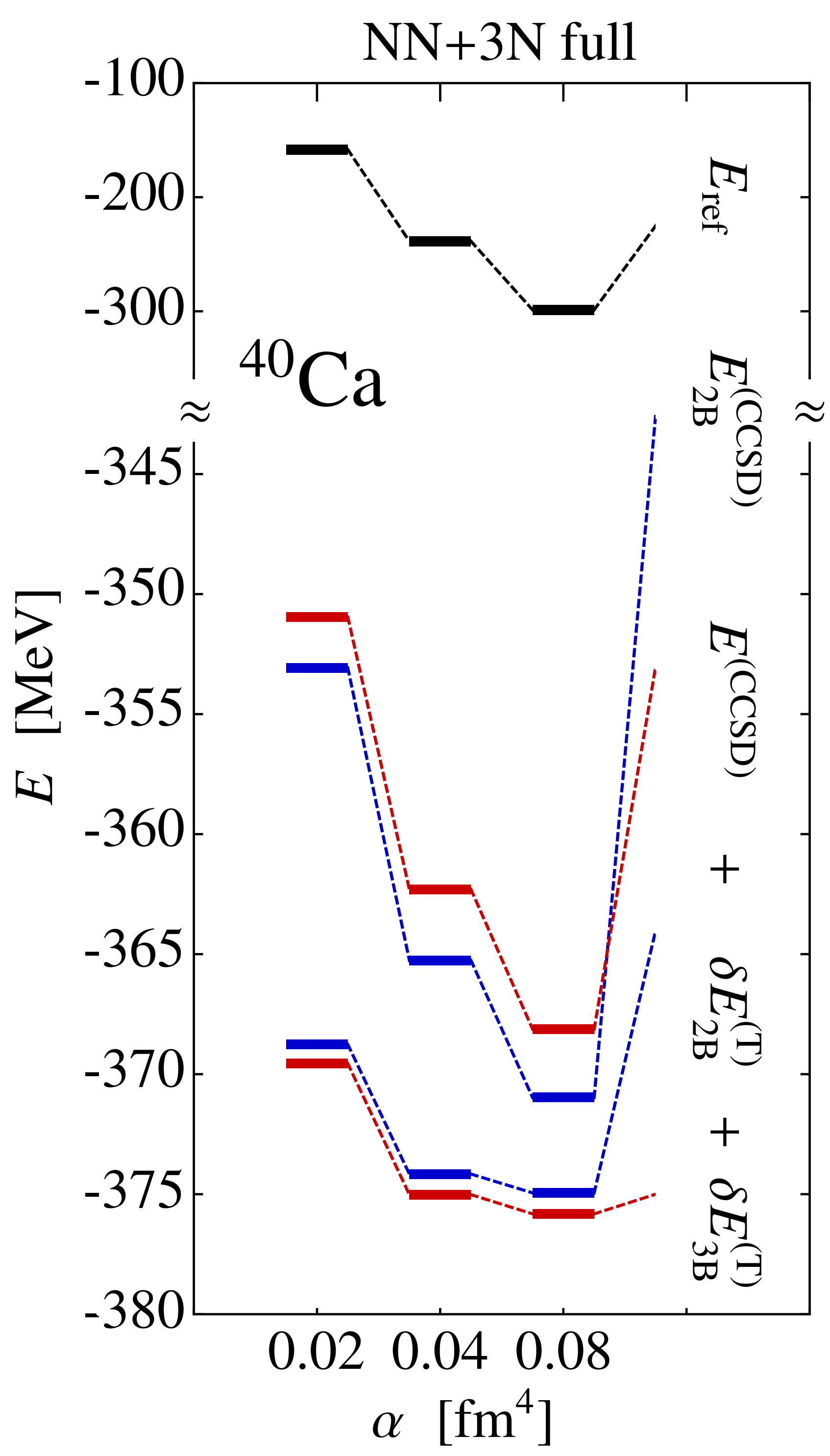


Benchmark NO2B



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

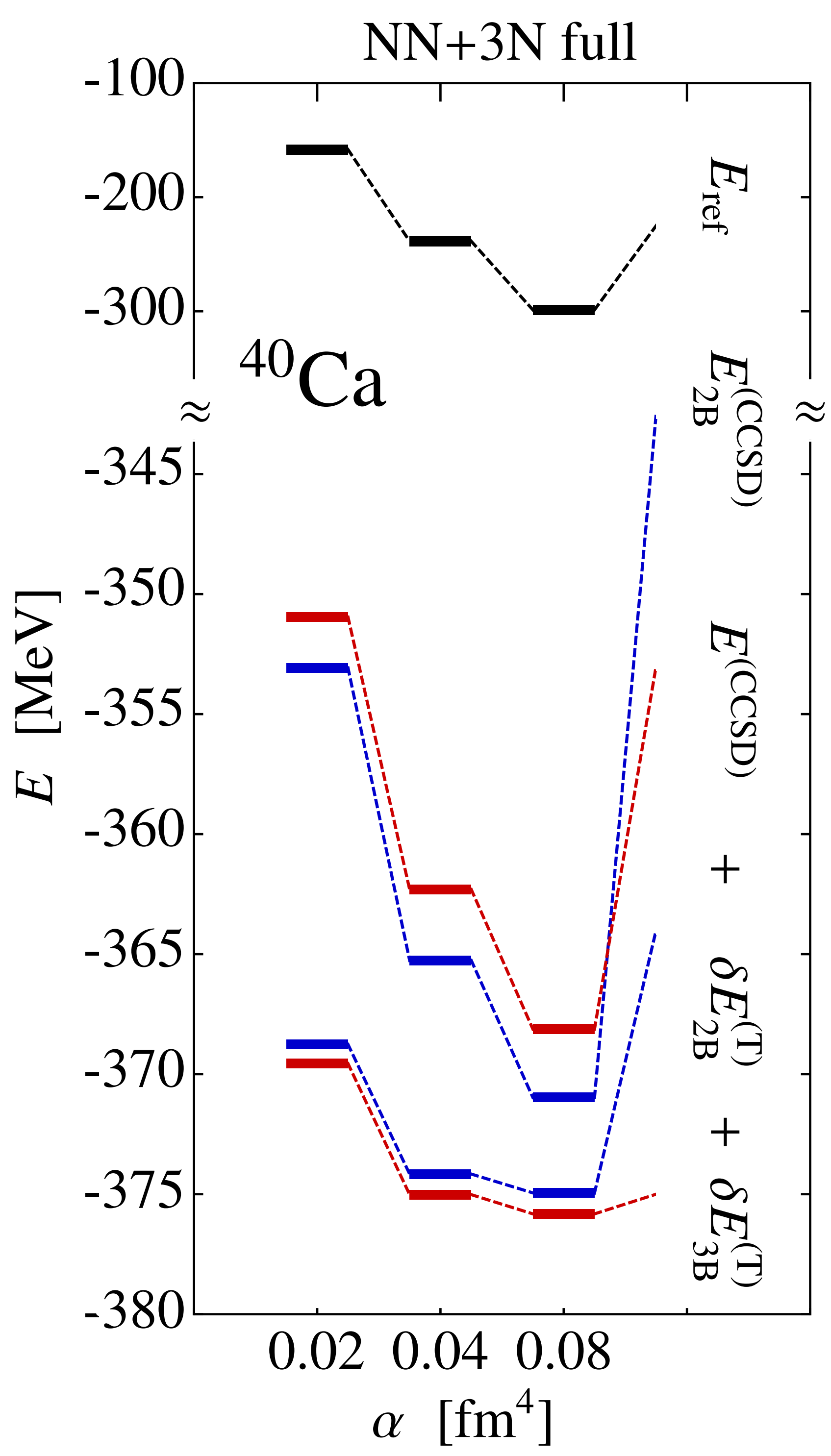
Benchmark NO2B



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

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

Benchmark NO2B

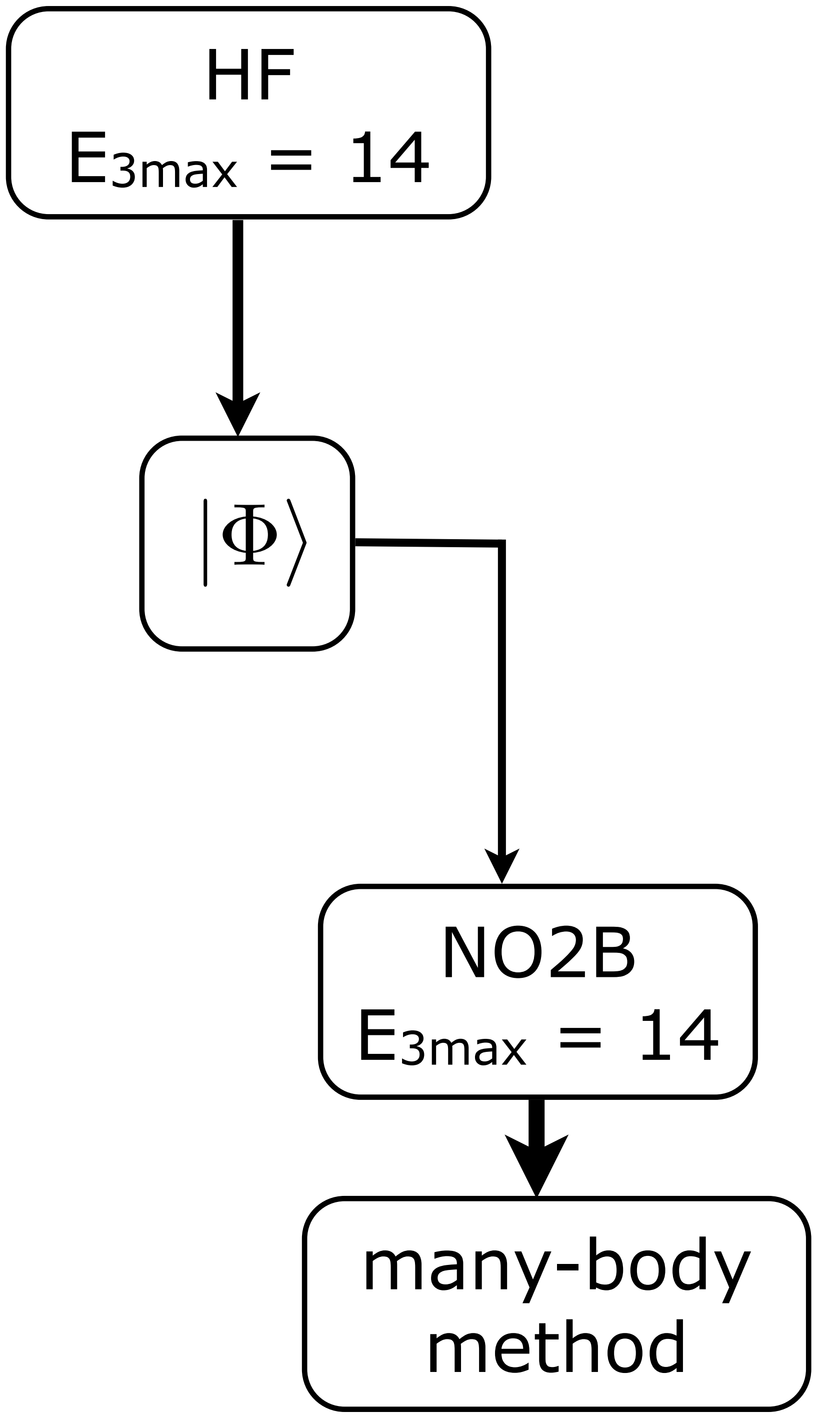


- Errors due to NO2B **< 1%**

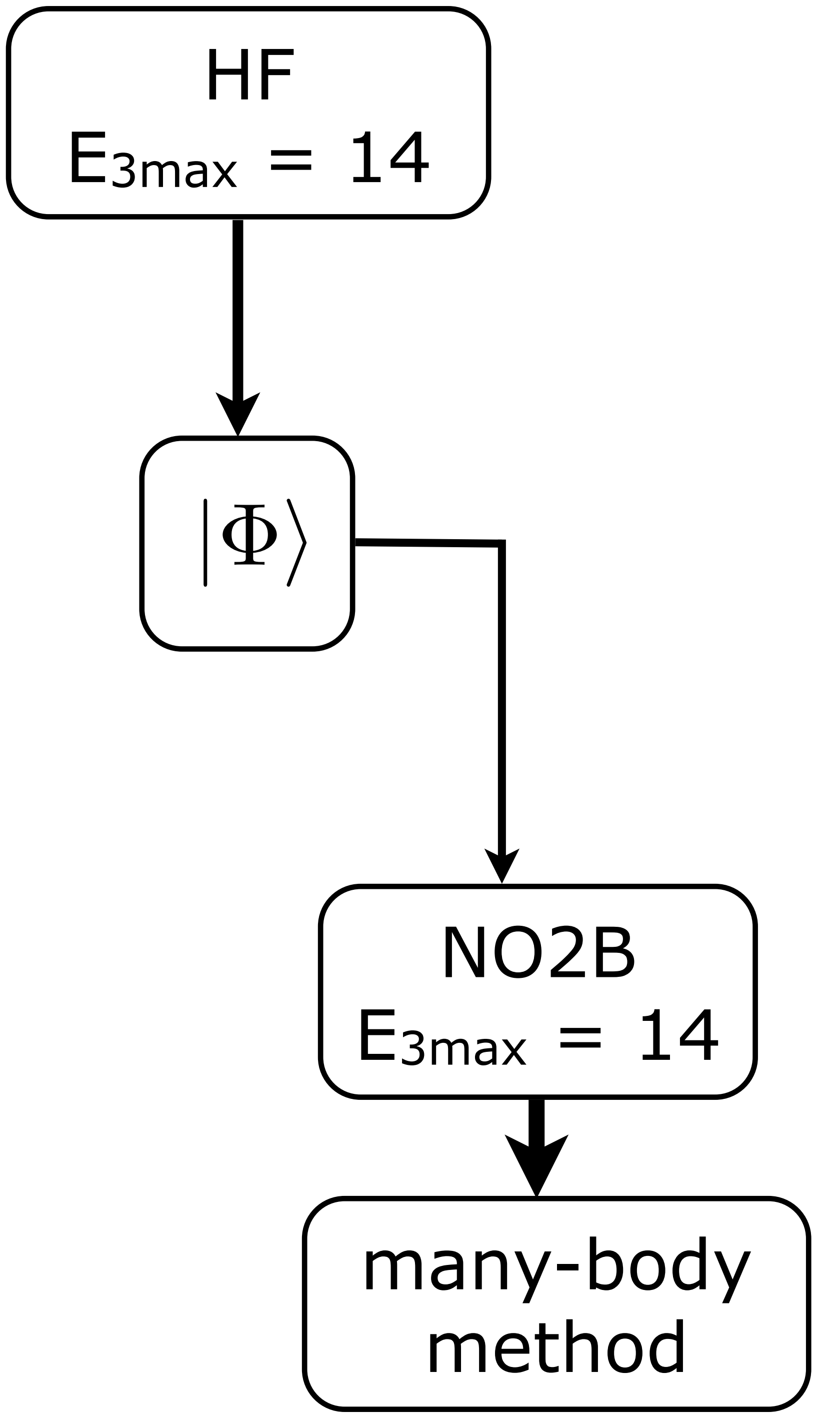
➡ NO2B is **efficient** and **accurate** way to include 3N interaction

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

Normal-Ordering Procedure



Normal-Ordering Procedure



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

restrict principal HO quantum numbers e_i in

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

according to

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

Normal-Ordering Procedure

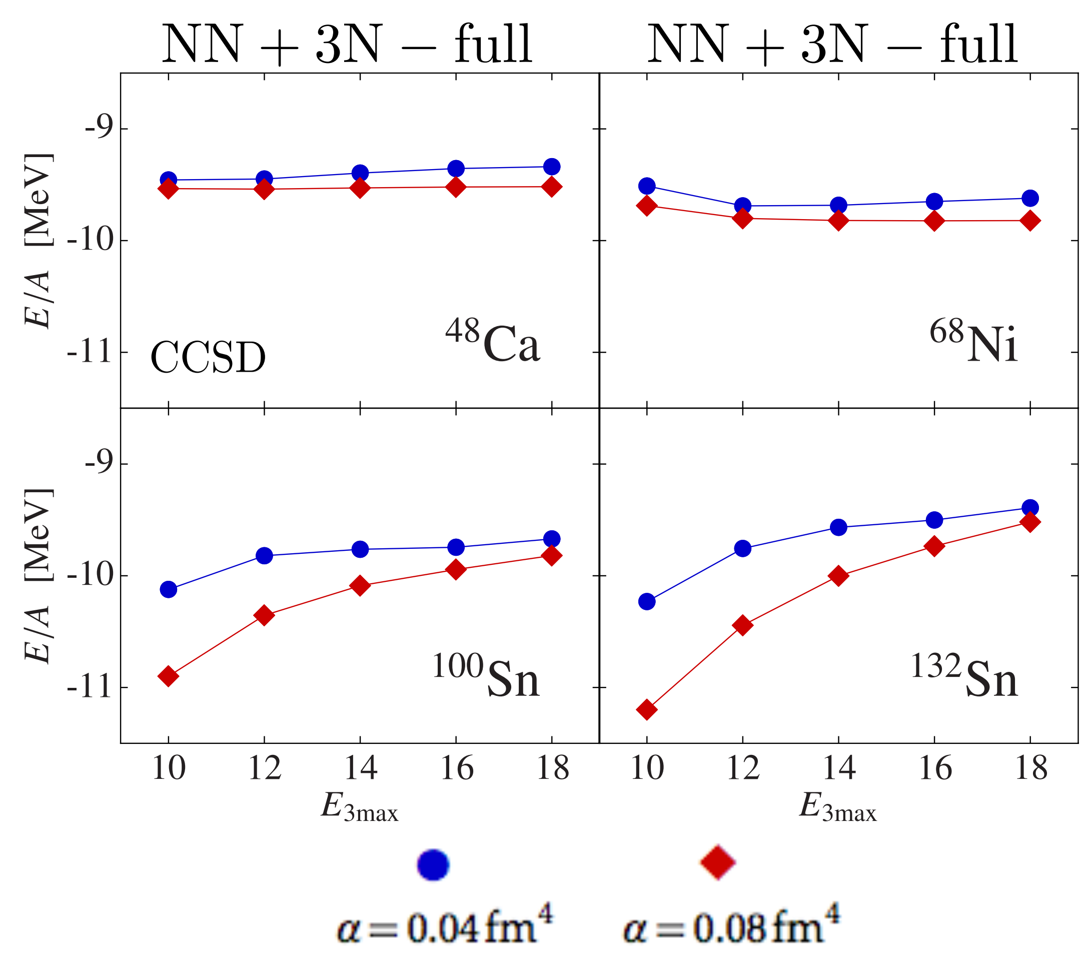
HF
$E_{3max} = 14$

$|\Phi\rangle$

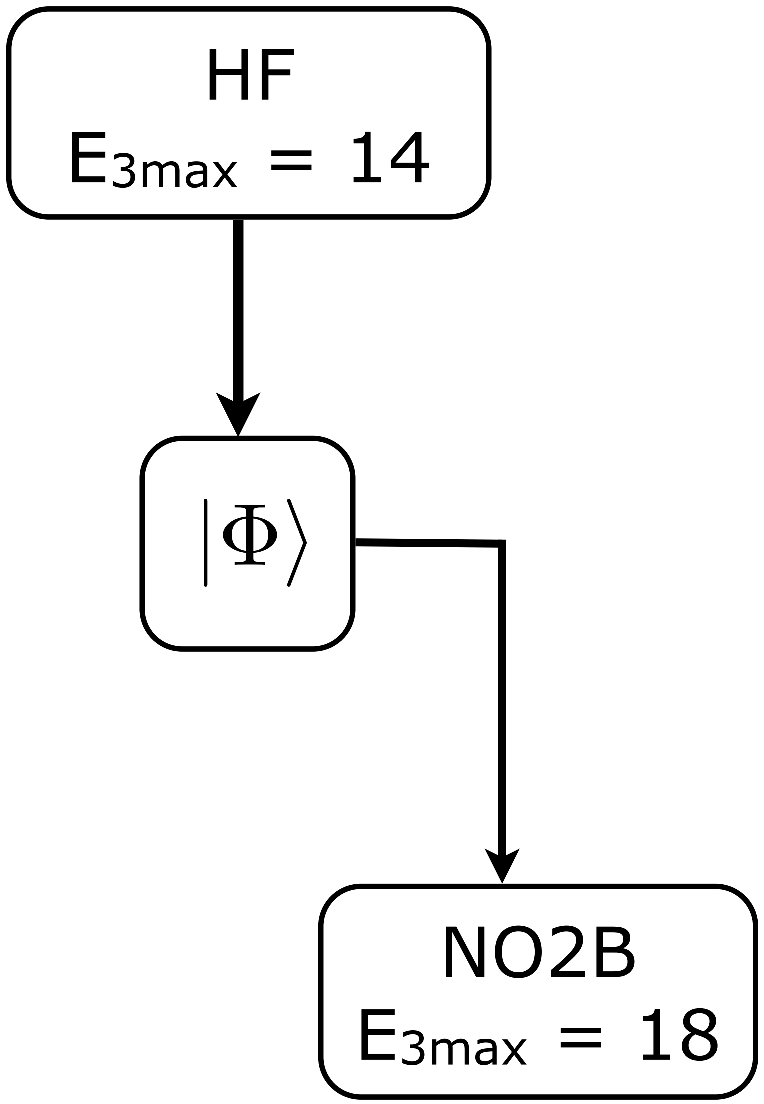
NO2B
$E_{3max} = 14$

many-body method

- heavy nuclei require **large E_{3max}**



Normal-Ordering Procedure



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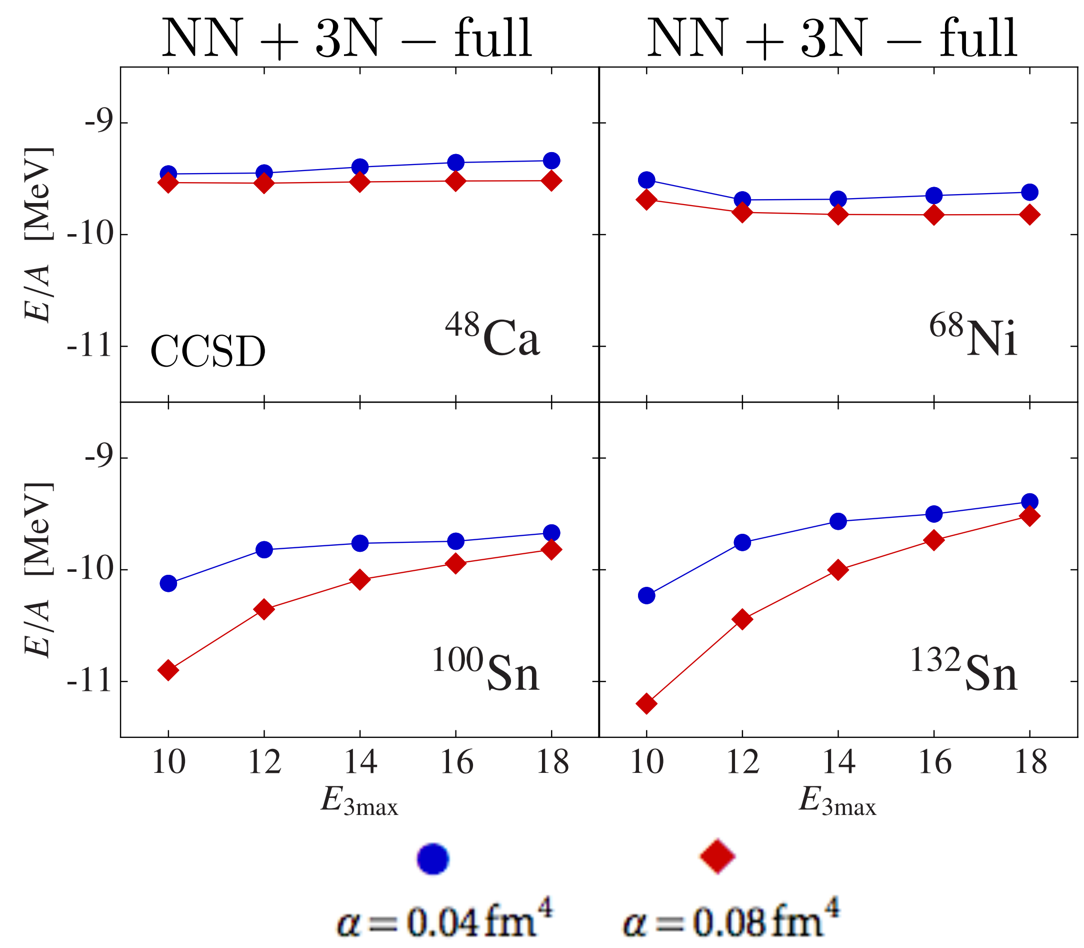
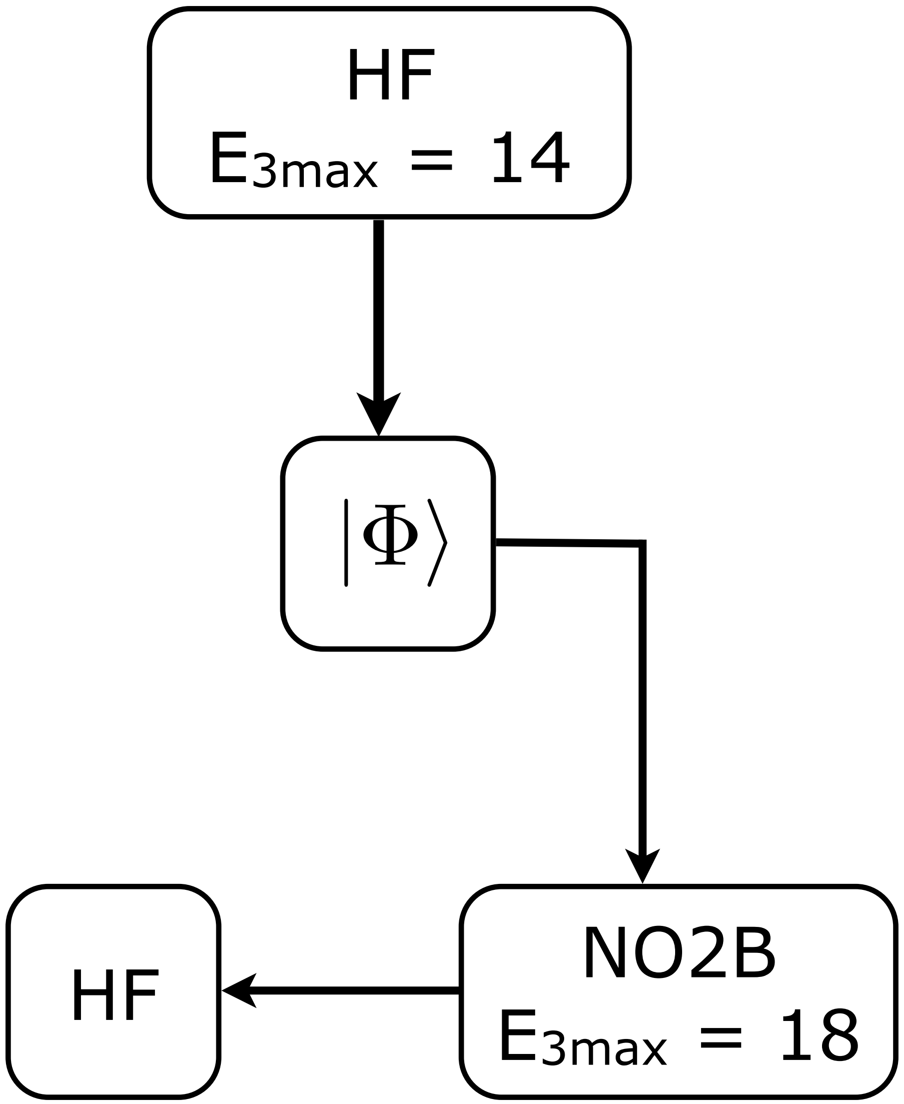


- simple protocol to **avoid using full sets** of large-E_{3max} matrix elements

Normal-Ordering Procedure



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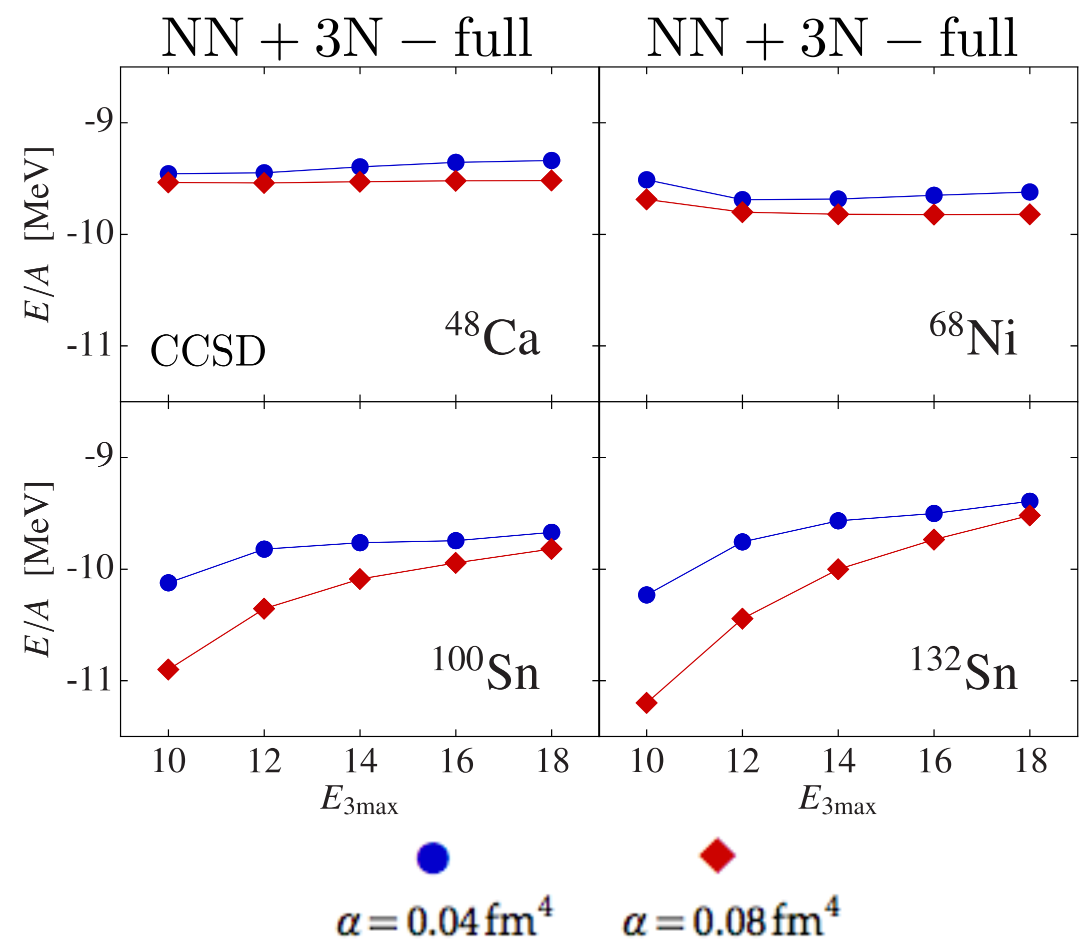

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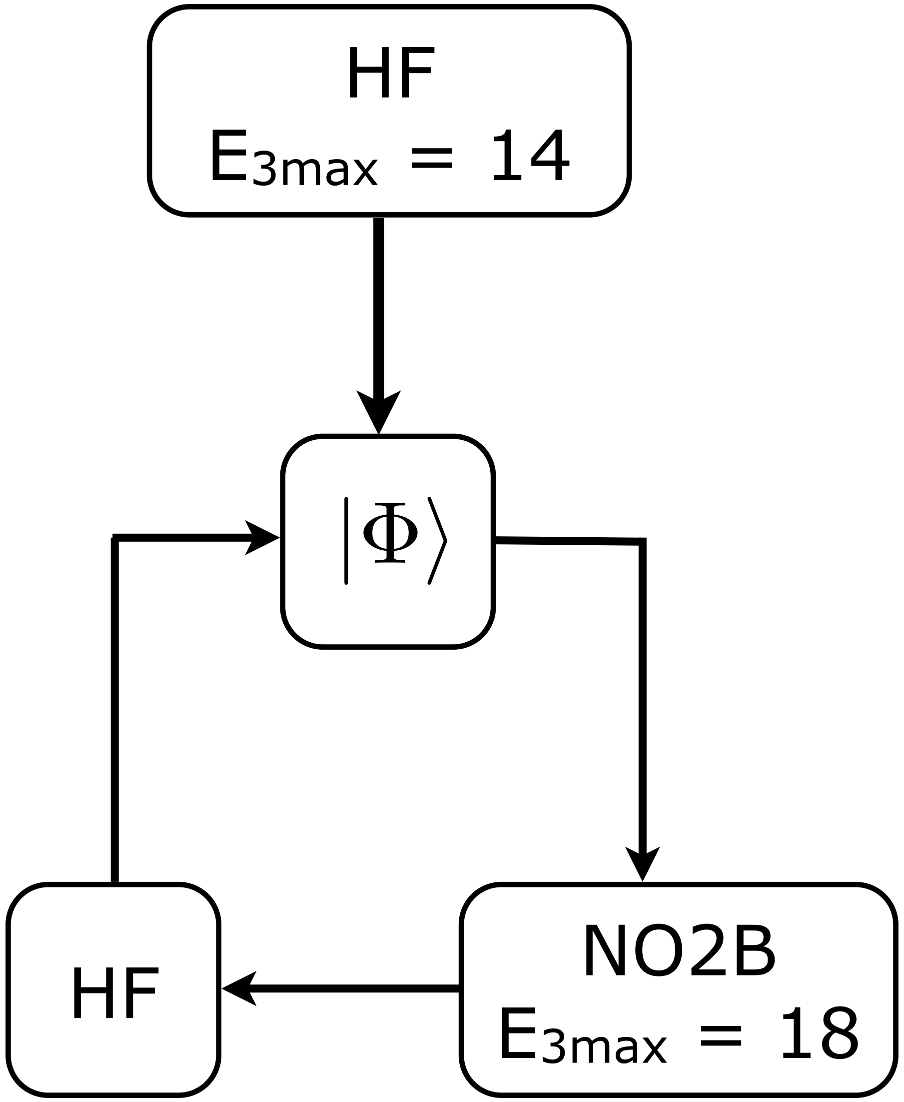

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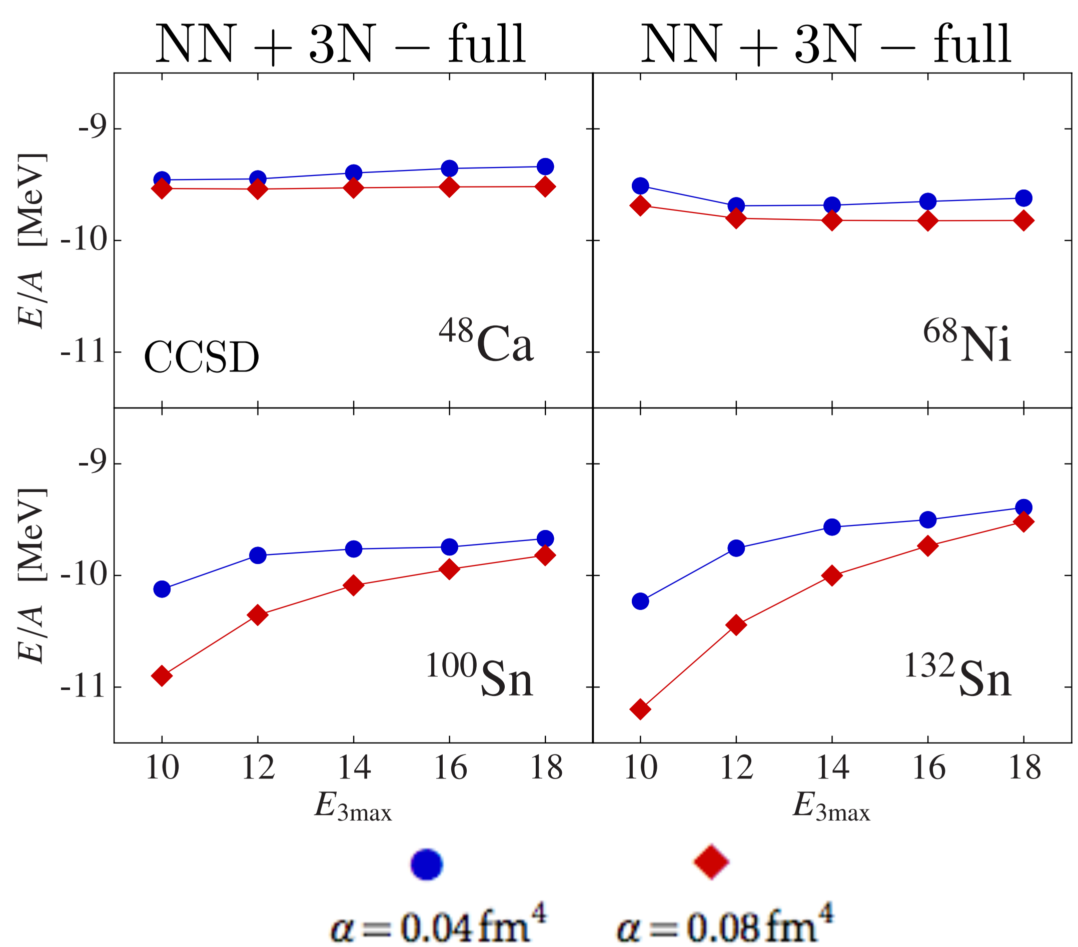

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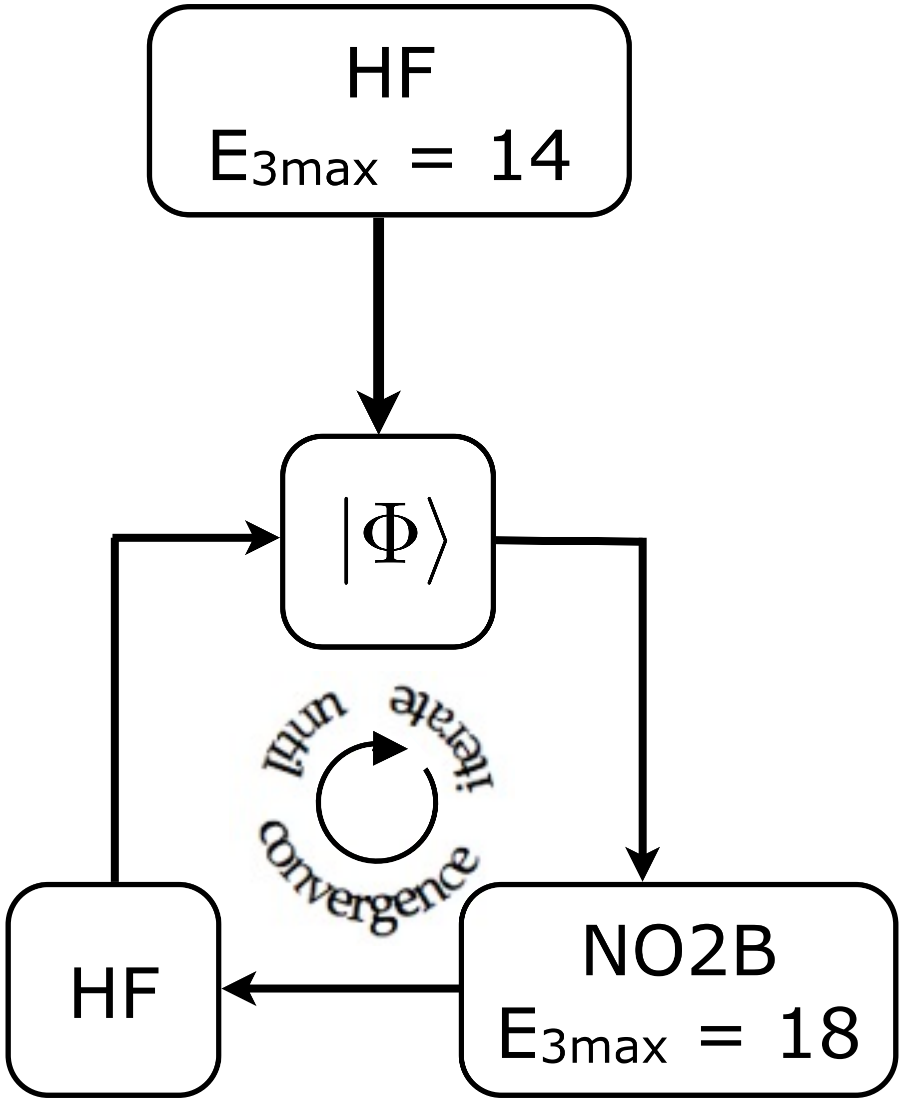

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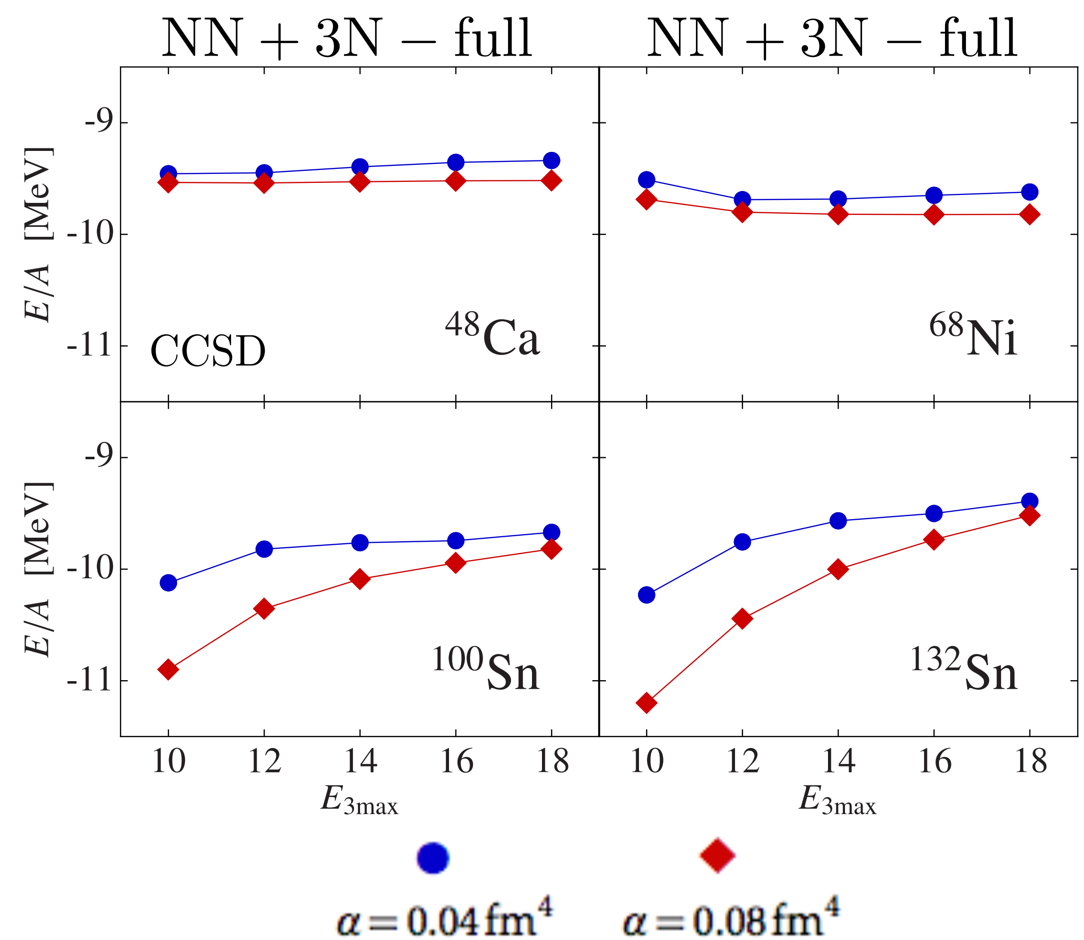

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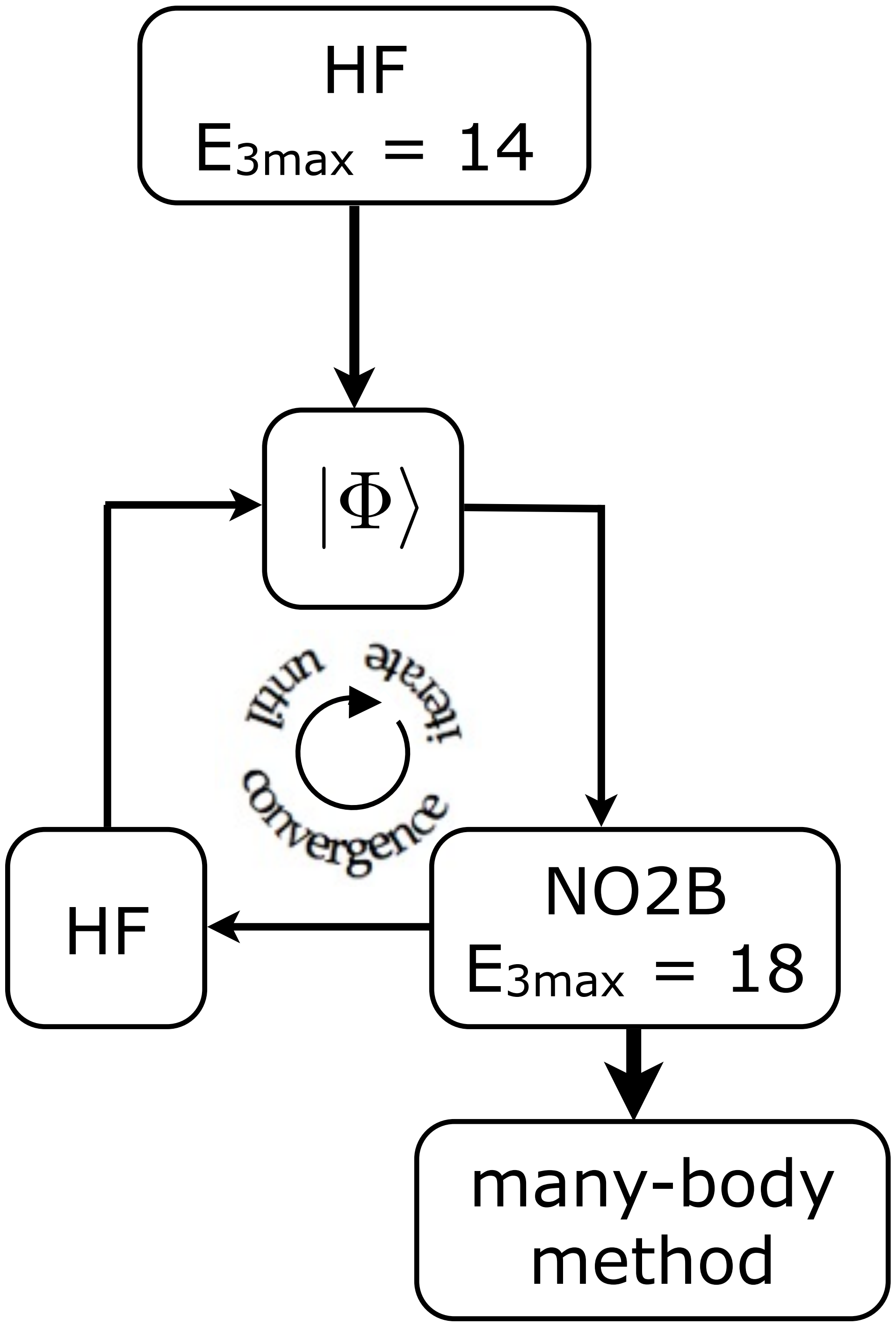

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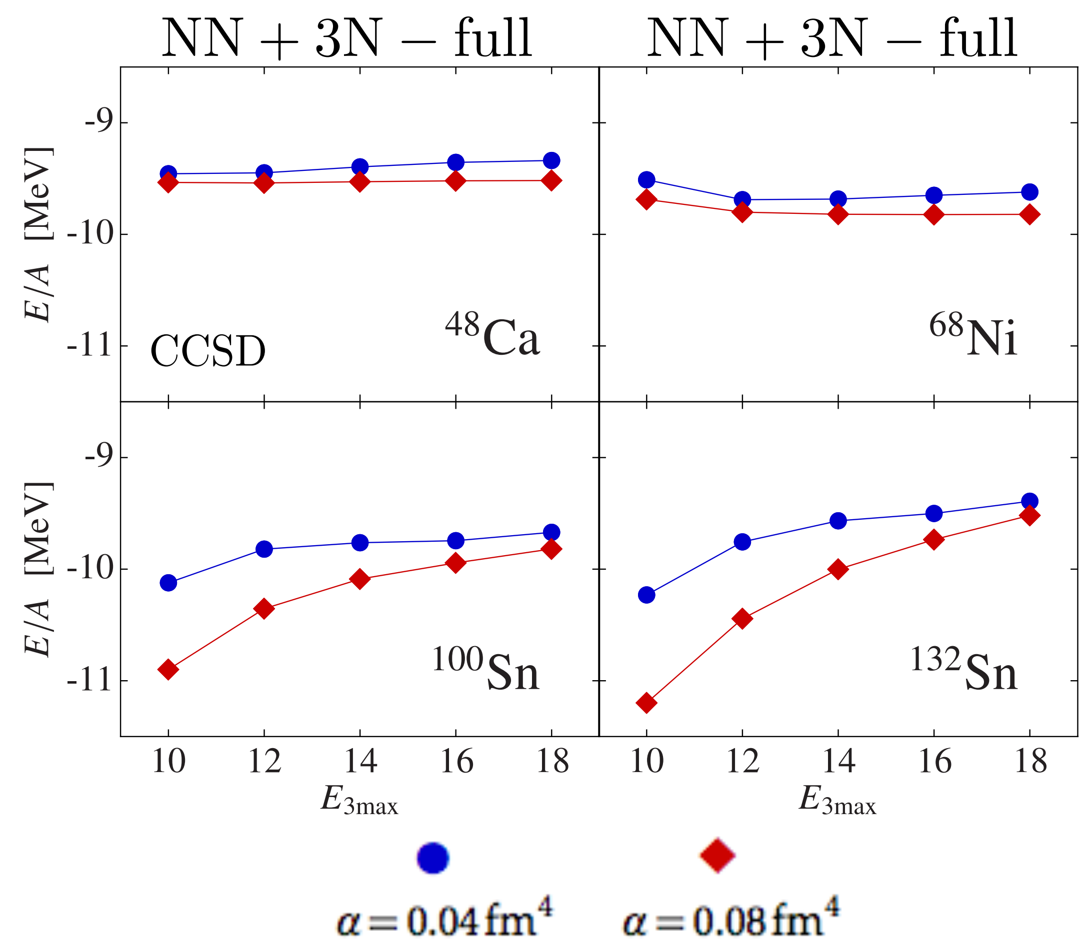

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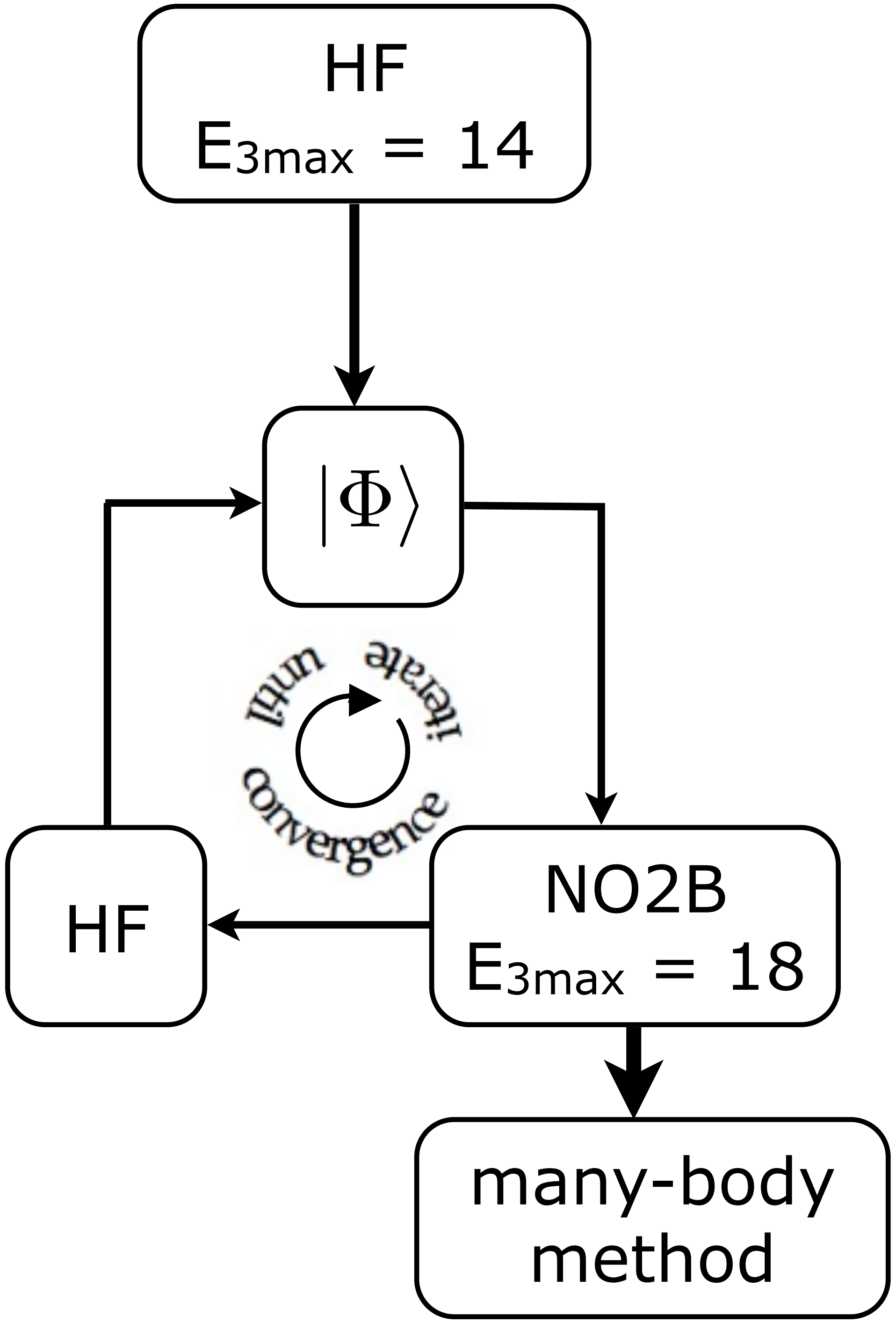

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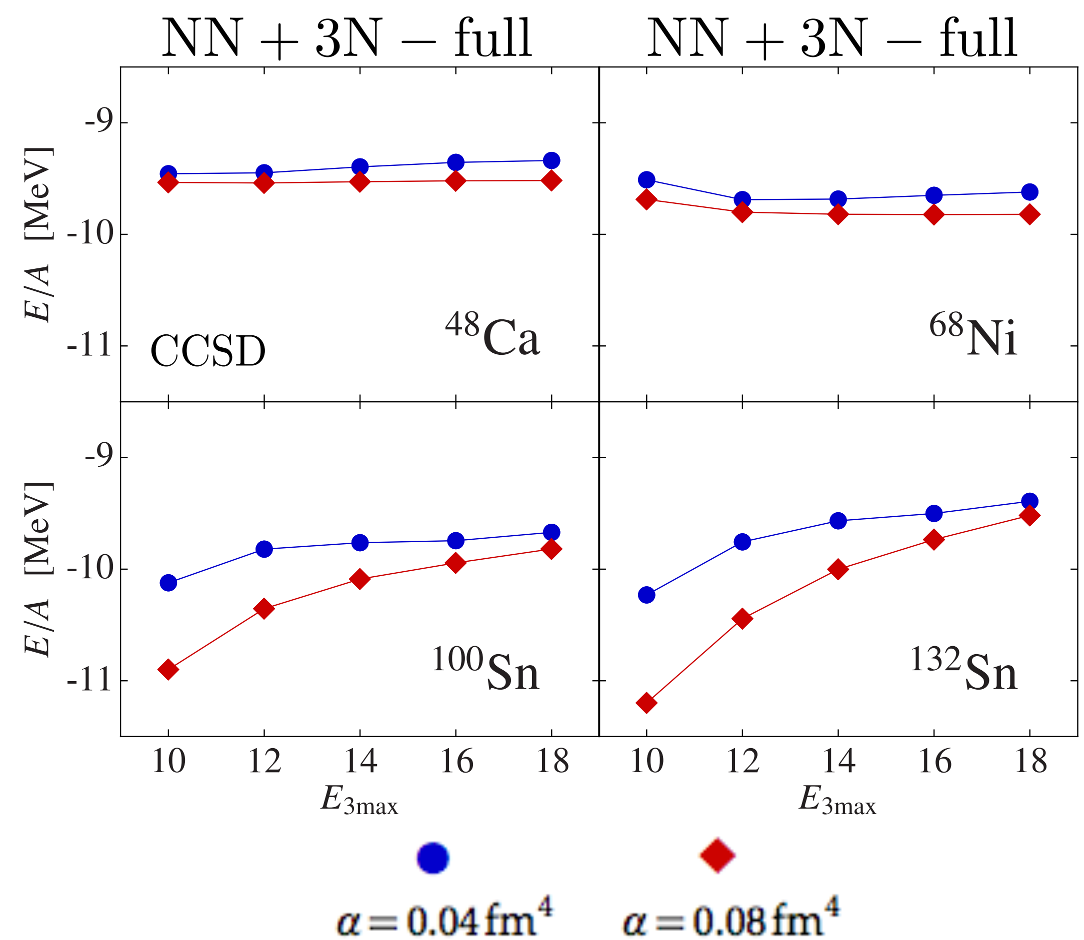
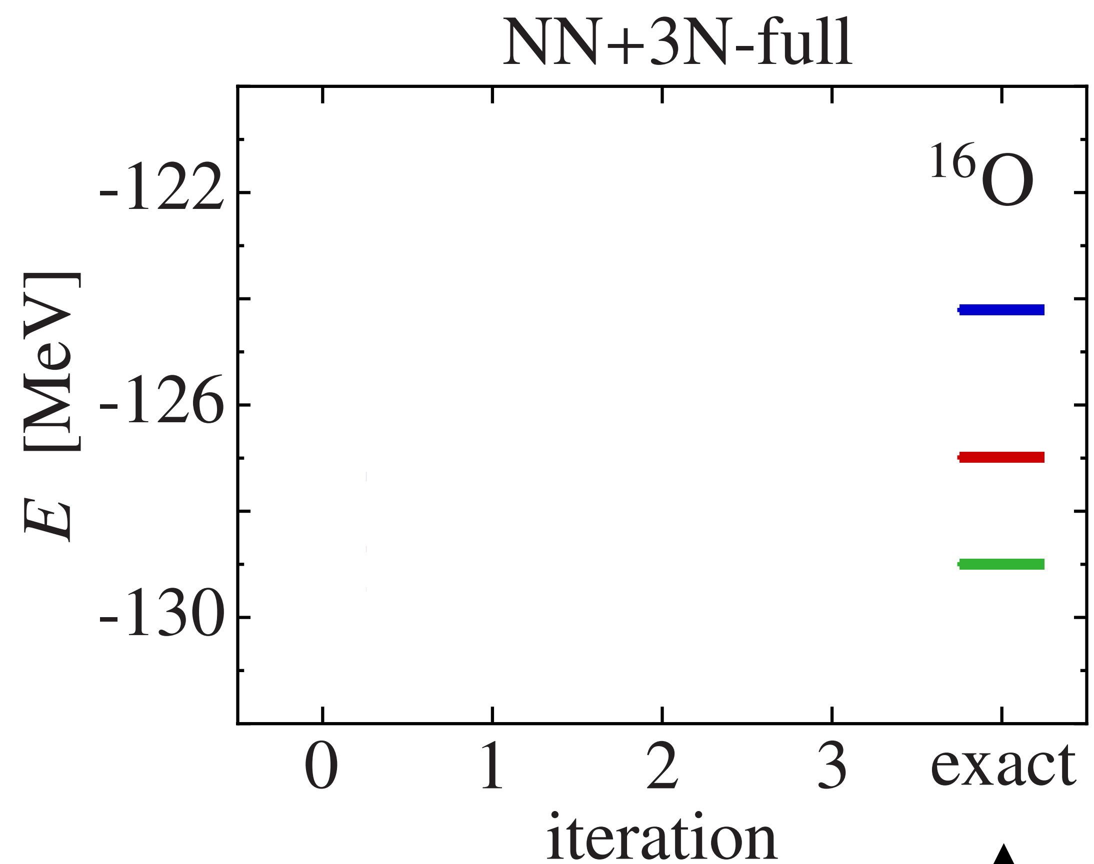


- simple protocol to **avoid using full sets** of large-E3max matrix elements
- large-E3max information enters via **NO2B**

Normal-Ordering Procedure

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



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

CCSD

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

Normal-Ordering Procedure

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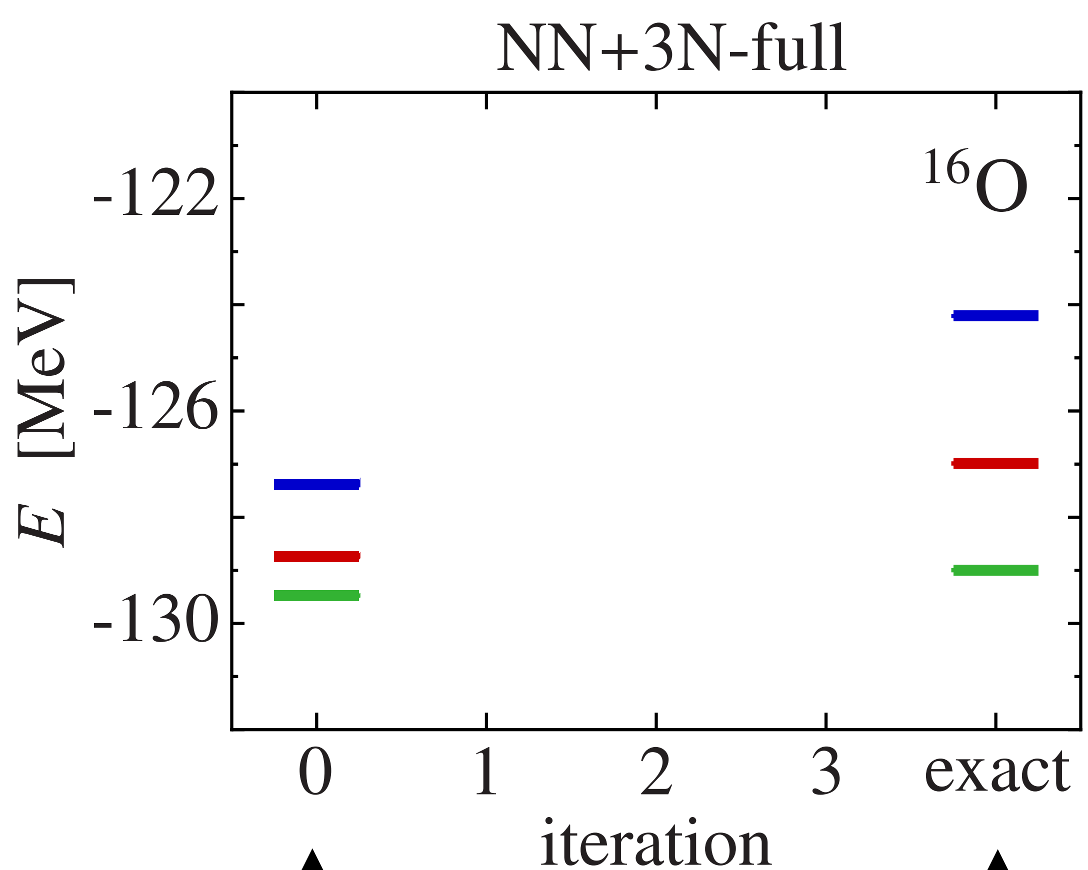
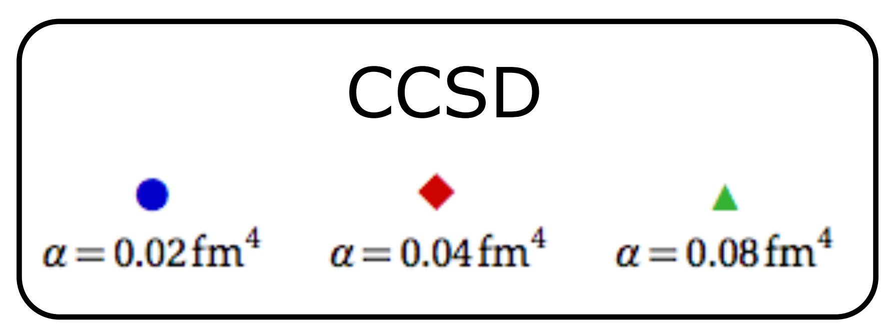


$|\Phi(E_{3\max} = 8)\rangle$

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



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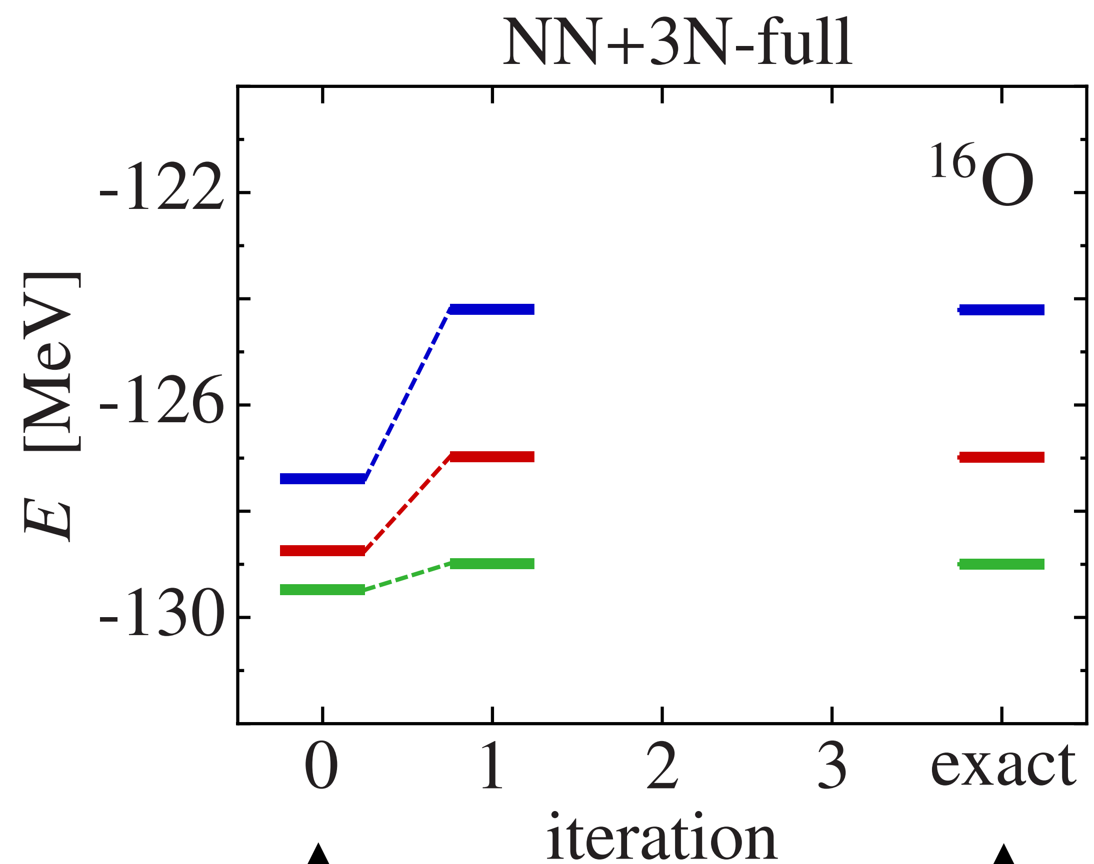
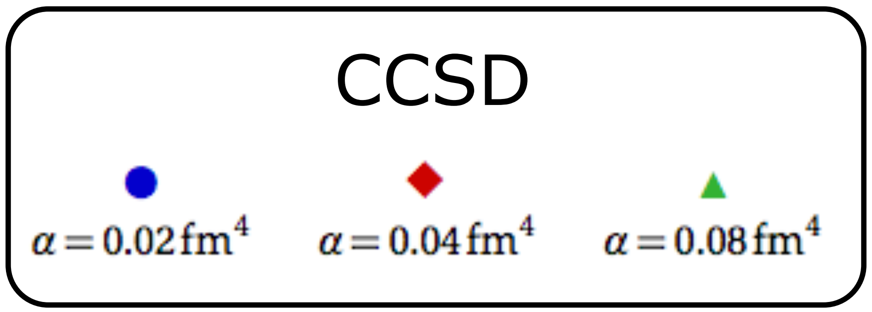


$$|\Phi(E_{3\max} = 8)\rangle$$

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



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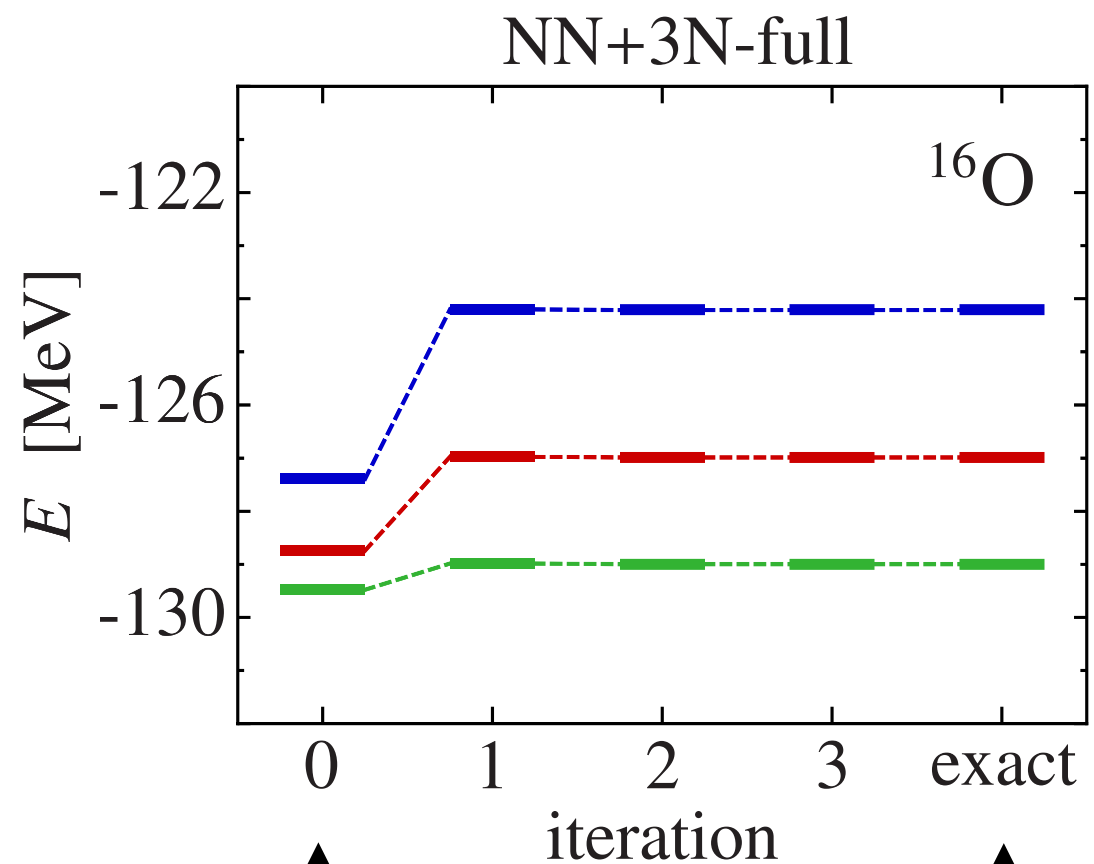

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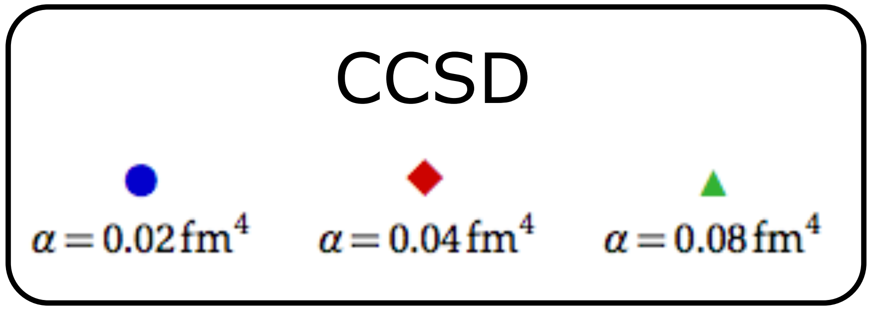

Normal-Ordering Procedure

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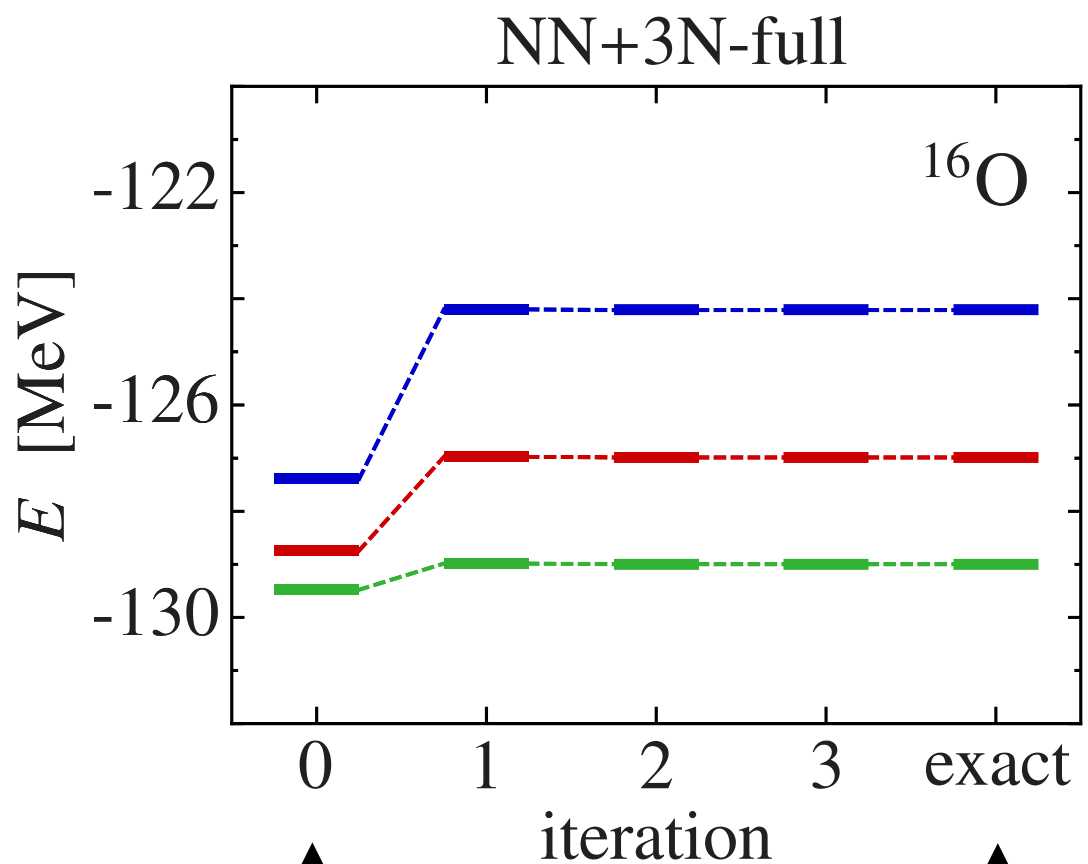

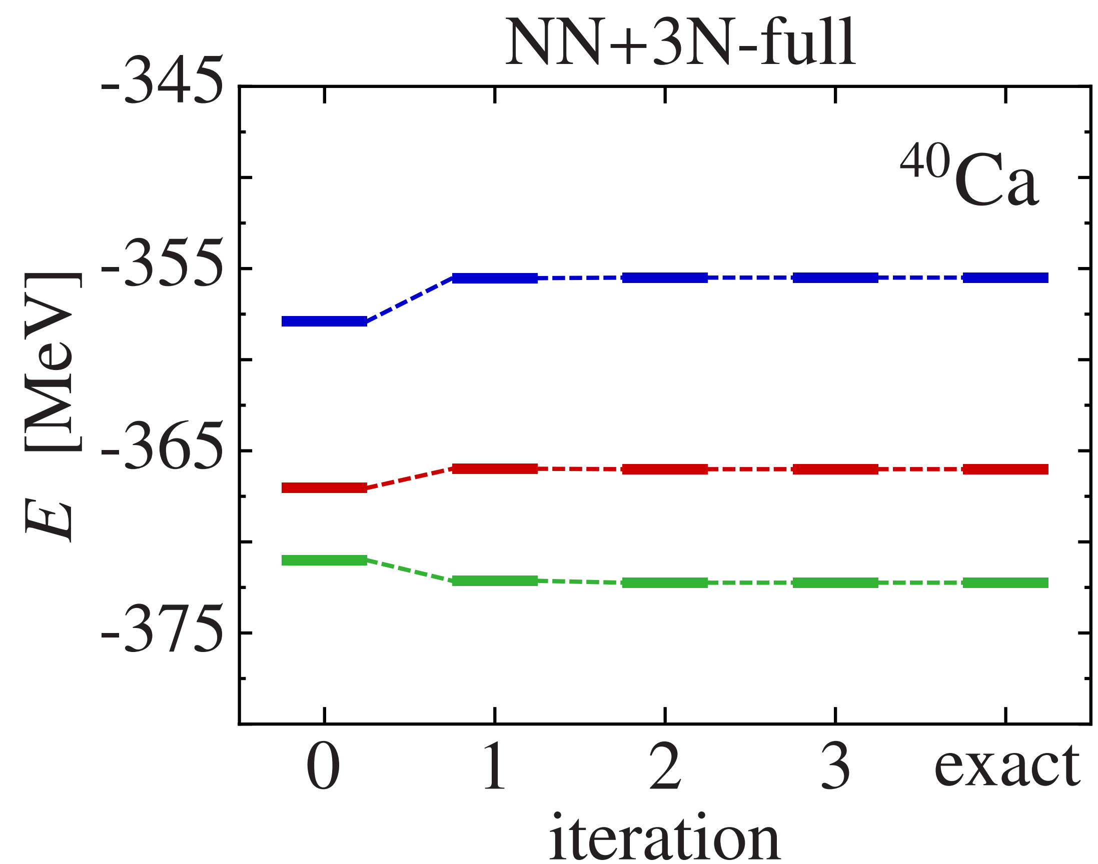

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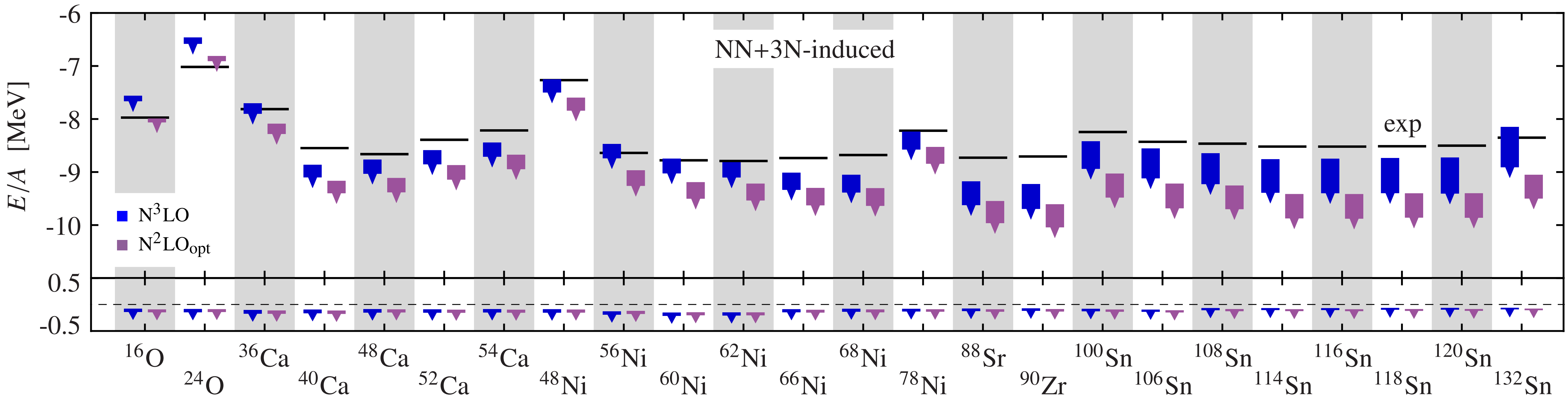
CCSD

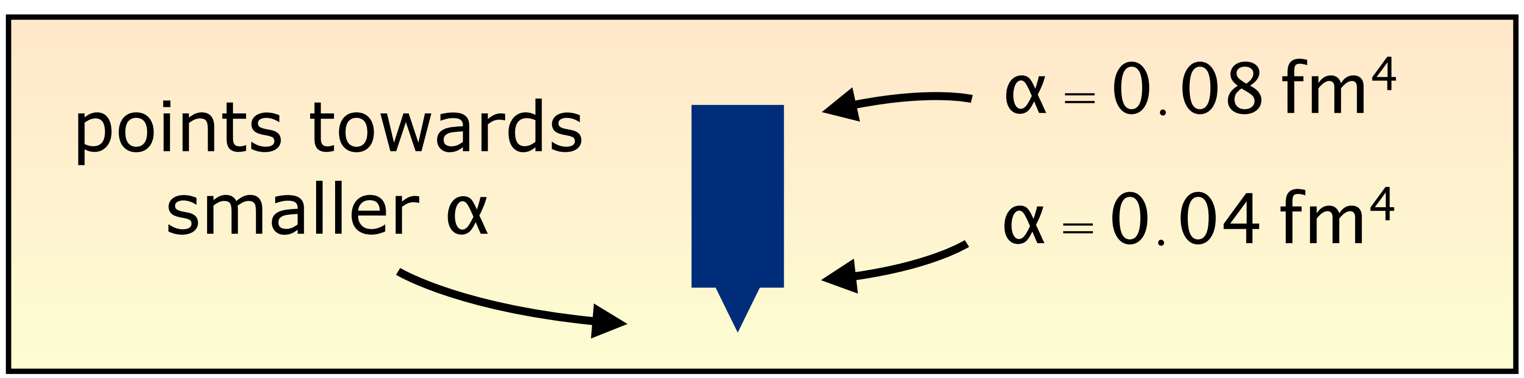
$\alpha = 0.02\,\text{fm}^4$ $\alpha = 0.04\,\text{fm}^4$ $\alpha = 0.08\,\text{fm}^4$

Heavy Nuclei

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

Heavy Nuclei from Chiral Interactions





CR-CC(2,3)

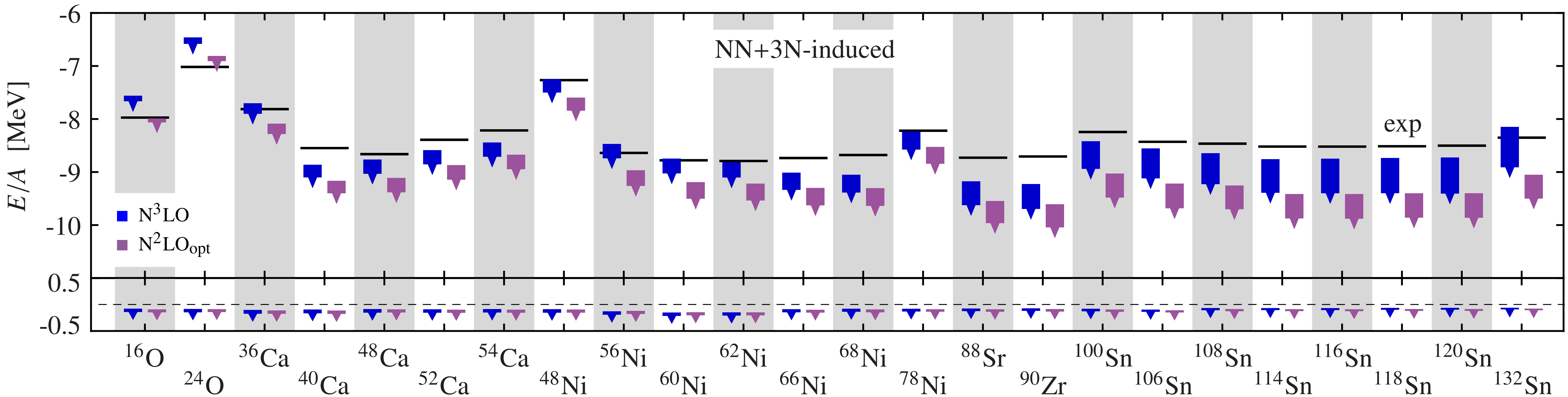
HF basis

$\hbar\Omega = 24$ MeV

$E_{3\max} = 18$

$e_{\max} = 12$

Heavy Nuclei from Chiral Interactions



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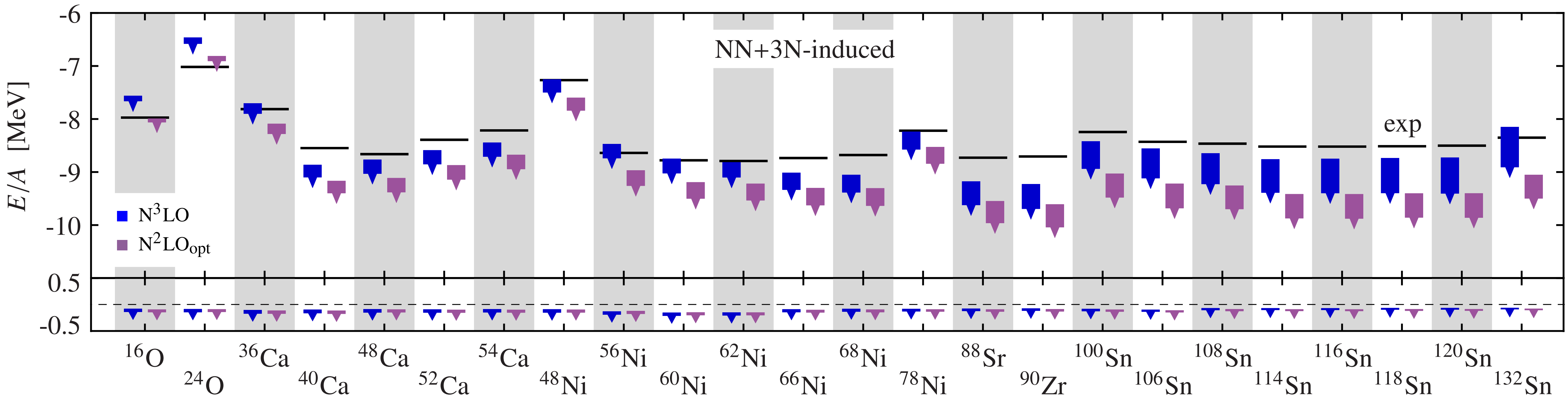
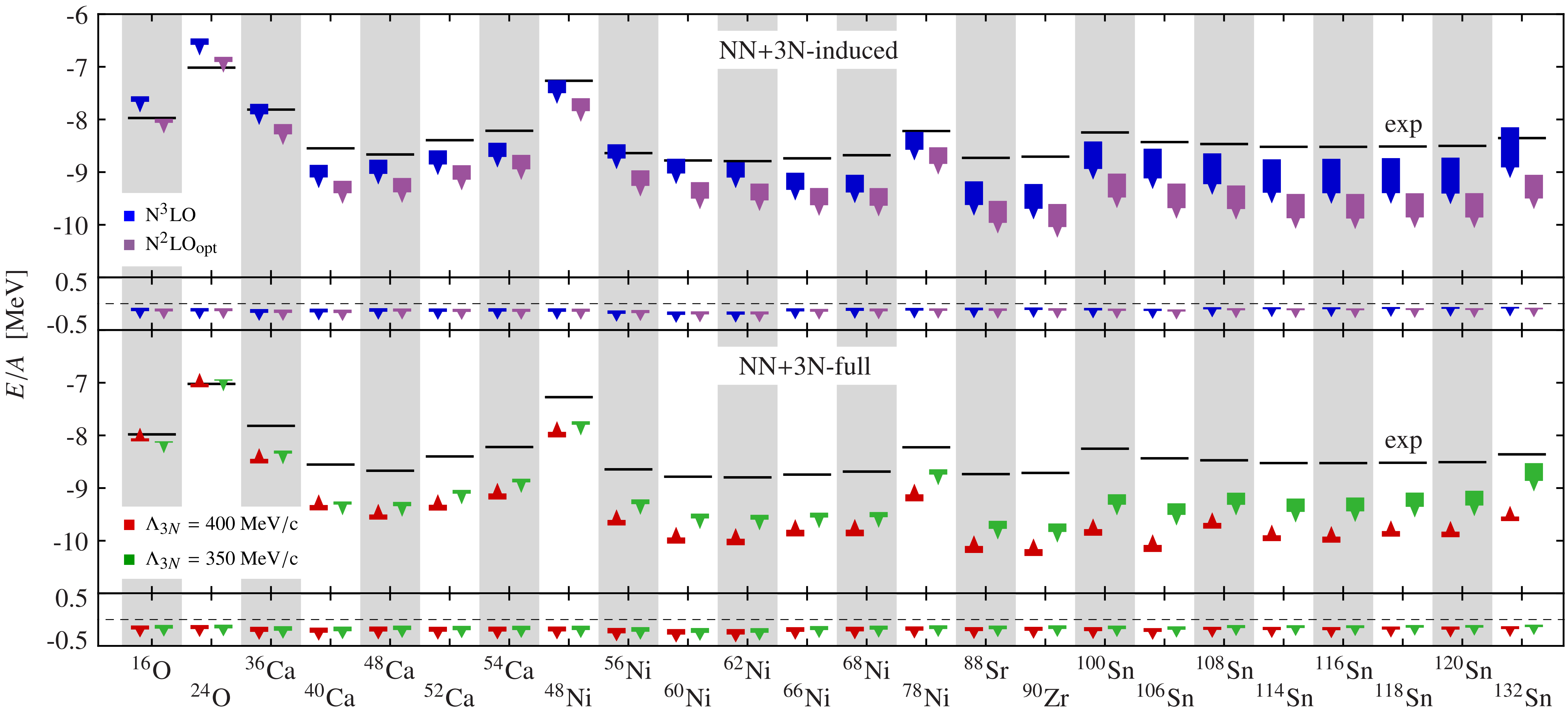


- NN+3N-induced: **strong** SRG-induced **4N**, ... interactions

Heavy Nuclei from Chiral Interactions



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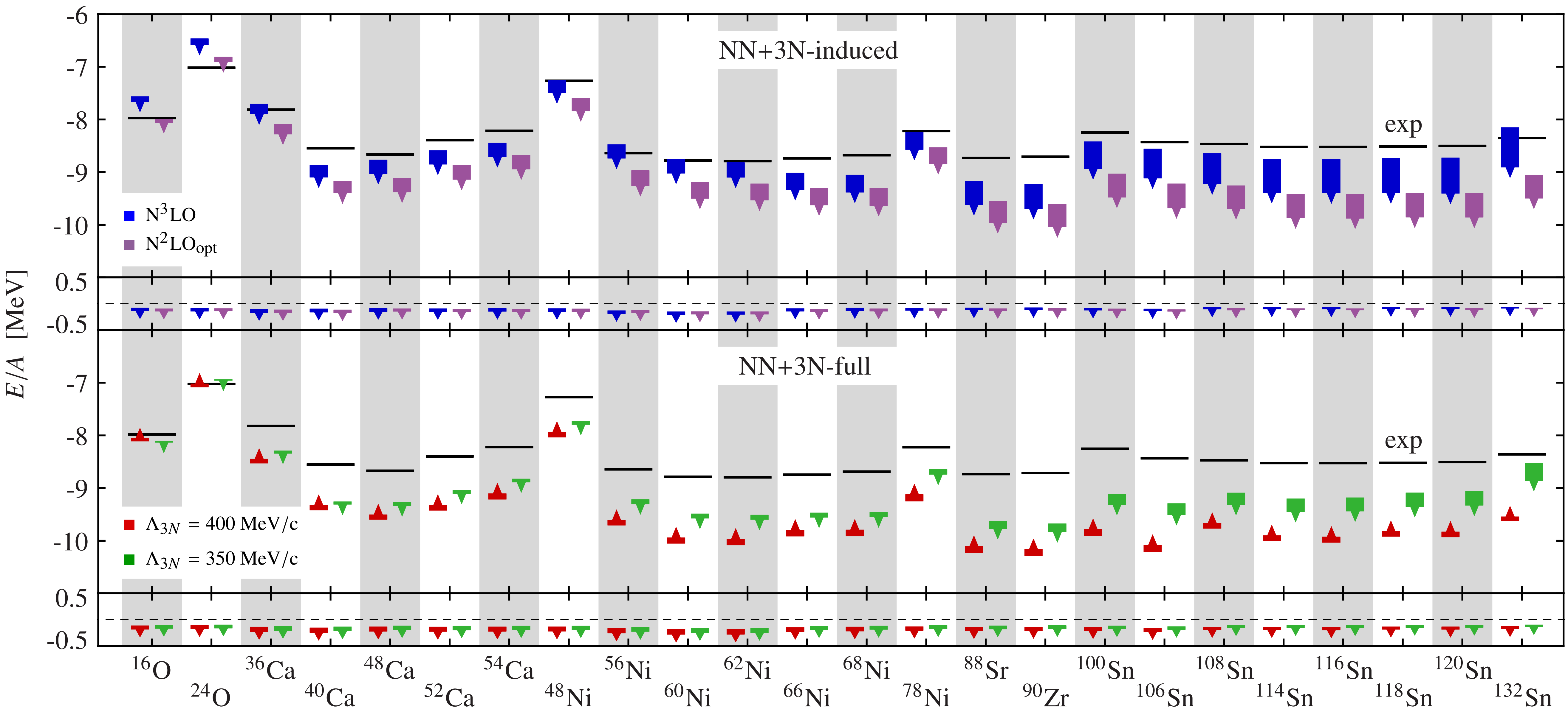
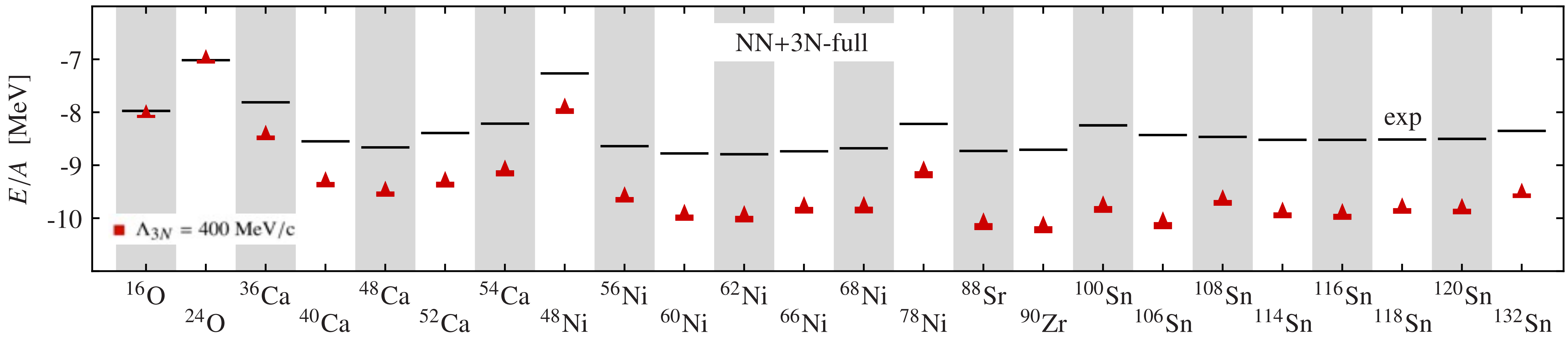
Heavy Nuclei from Chiral Interactions

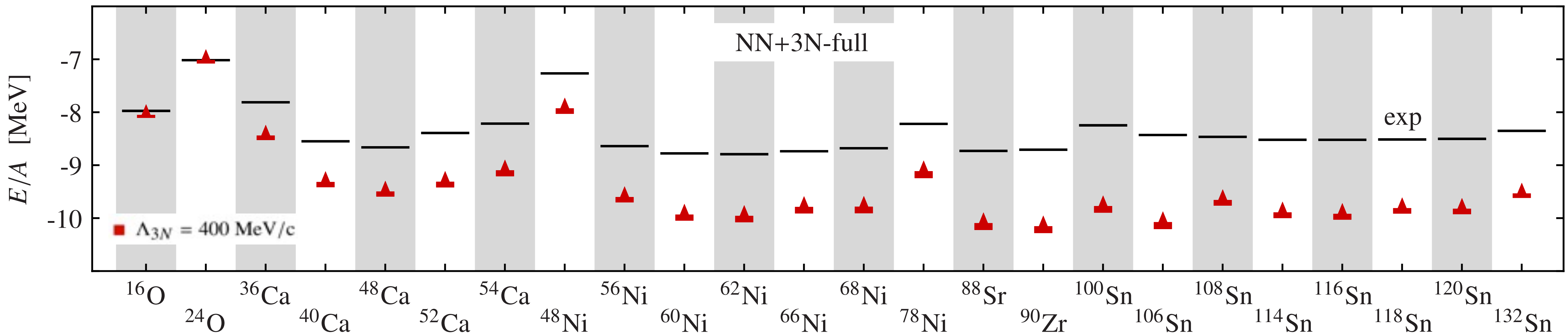


- NN+3N-induced: **strong** SRG-induced **4N**, ... interactions
- NN+3N-full: **cancellation** of SRG-induced **4N**, ... interactions

Heavy Nuclei from Chiral Interactions

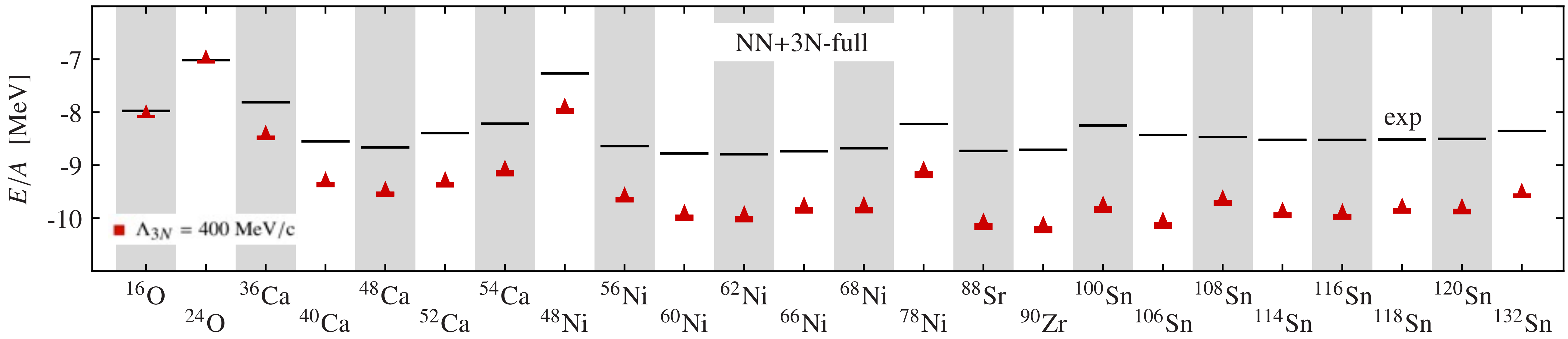


Heavy Nuclei from Chiral Interactions



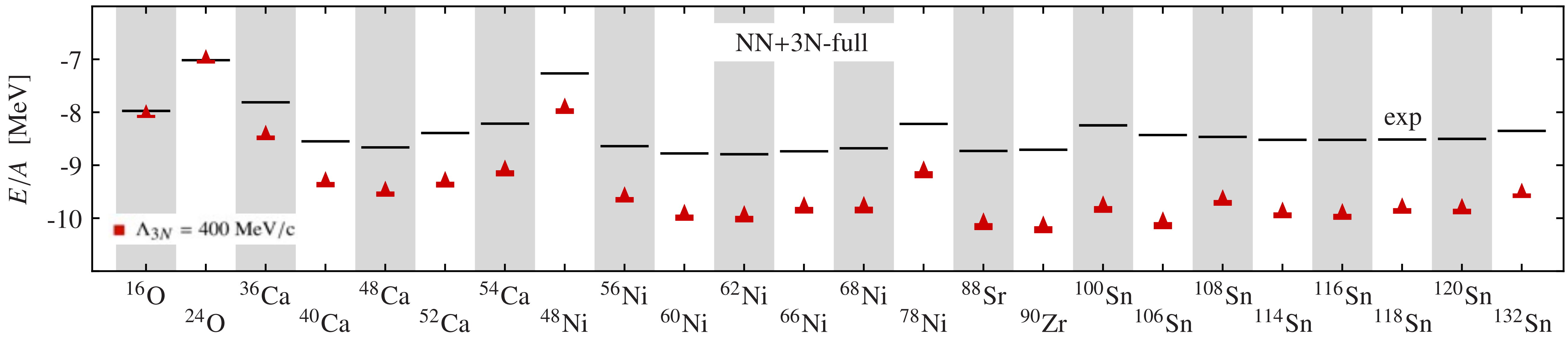
- Hamiltonian fixed in **A≤4** systems

Heavy Nuclei from Chiral Interactions



- Hamiltonian fixed in **A≤4** systems
- **current** chiral Hamiltonians capable of describing the **experimental trend** of binding energies

Heavy Nuclei from Chiral Interactions



- Hamiltonian fixed in **A≤4** systems
- **current** chiral Hamiltonians capable of describing the **experimental trend** of binding energies
- systematic overbinding ⇒ still **deficiencies**
  - **consistent 3N** interaction at N^{3}LO, and **4N** interaction
  - SRG-induced **4N, ...** interactions

3N Forces - Status and Needs

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➡ need **alternative renormalization scheme** with **less induced many-body interactions** beyond the 3N level

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

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Thanks for your attention!

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