Coupled-Cluster Theory

for

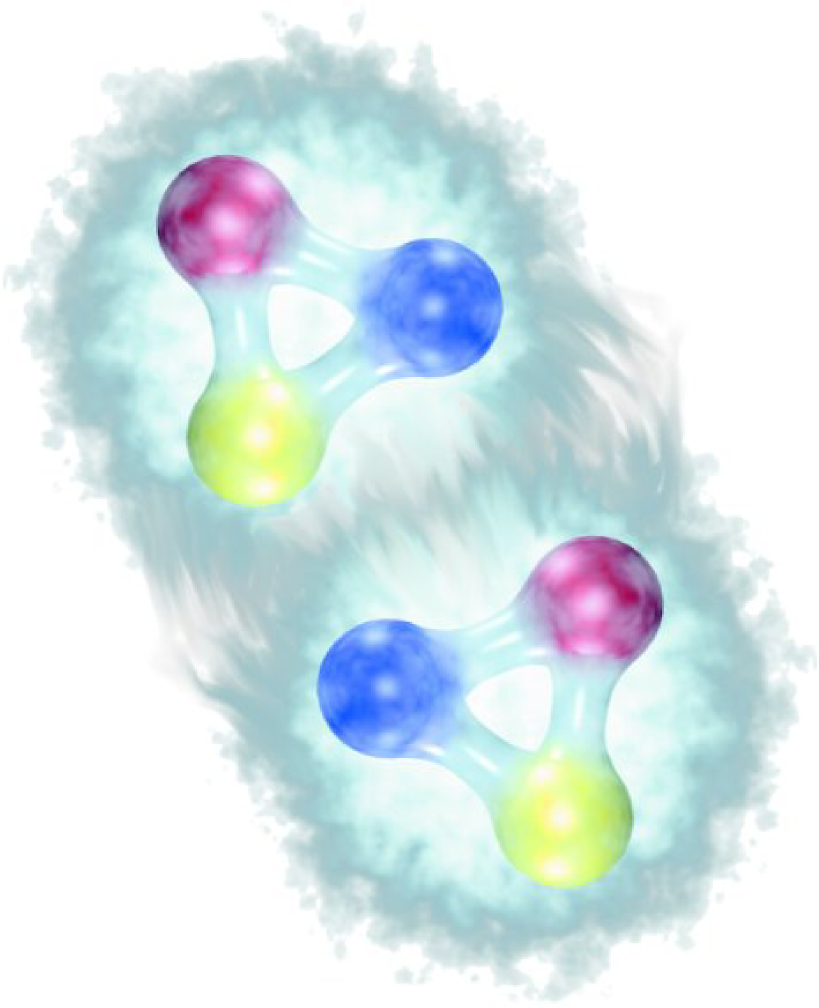
Nuclear Structure

Sven Binder

INSTITUT FÜR KERNPHYSIK

TECHNISCHE UNIVERSITÄT DARMSTADT

Nuclear Interactions from Chiral EFT



Nuclear Interactions from Chiral EFT

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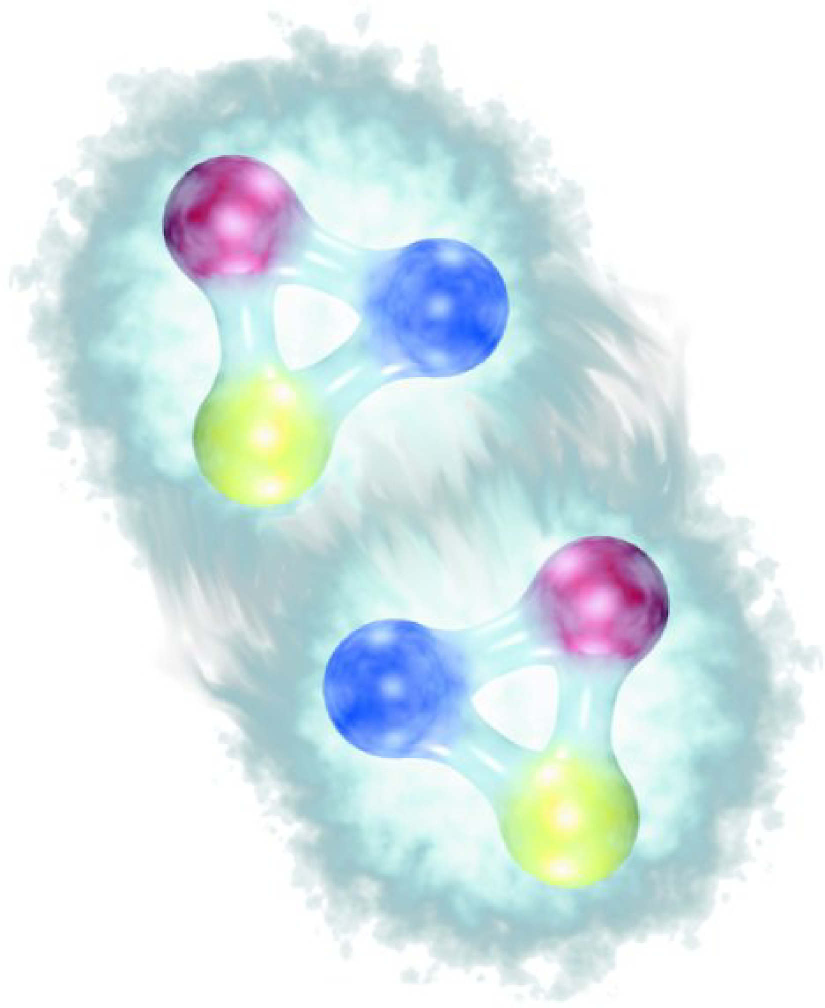

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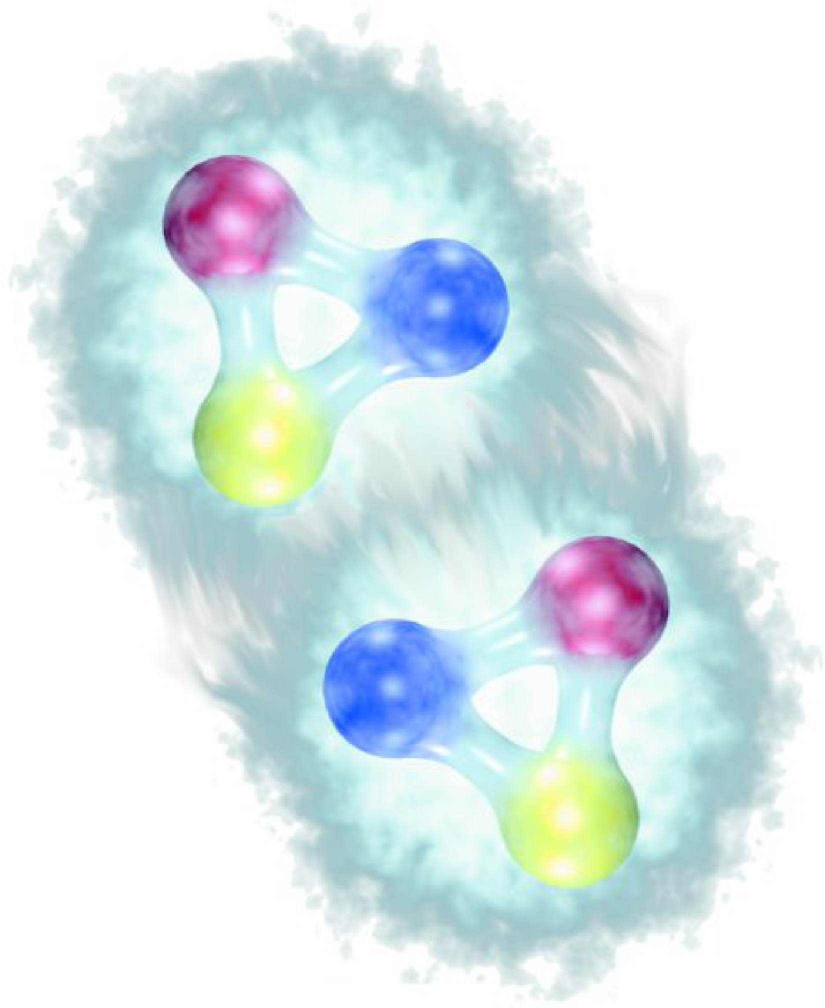

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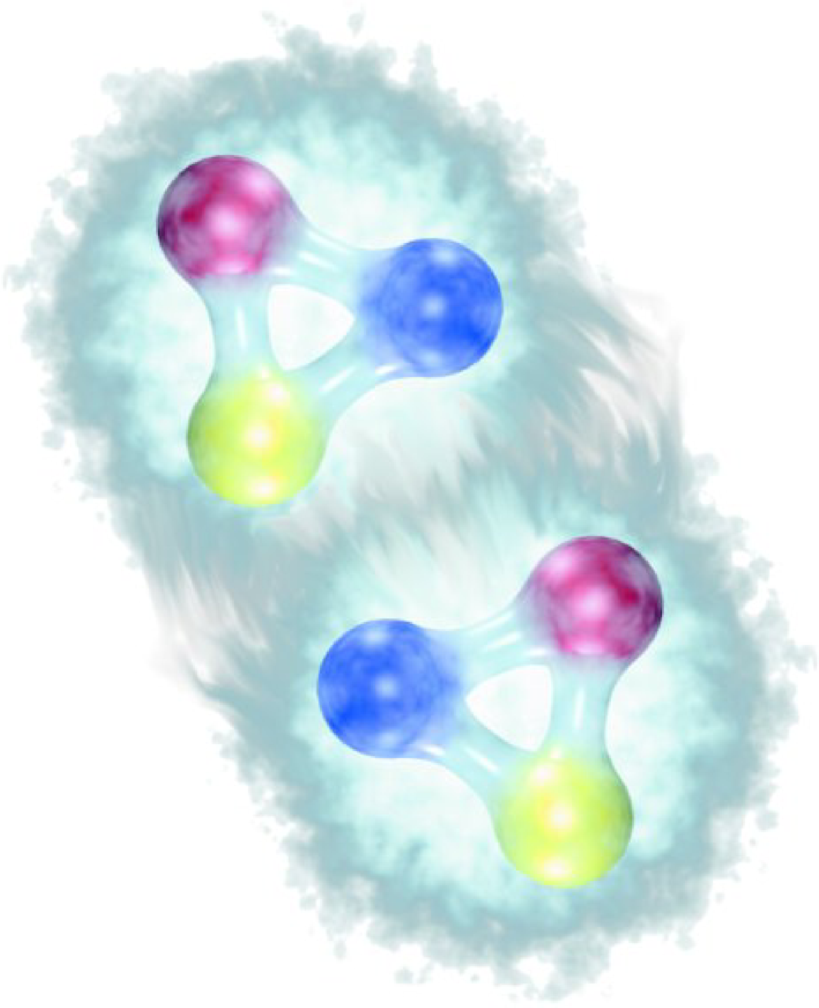

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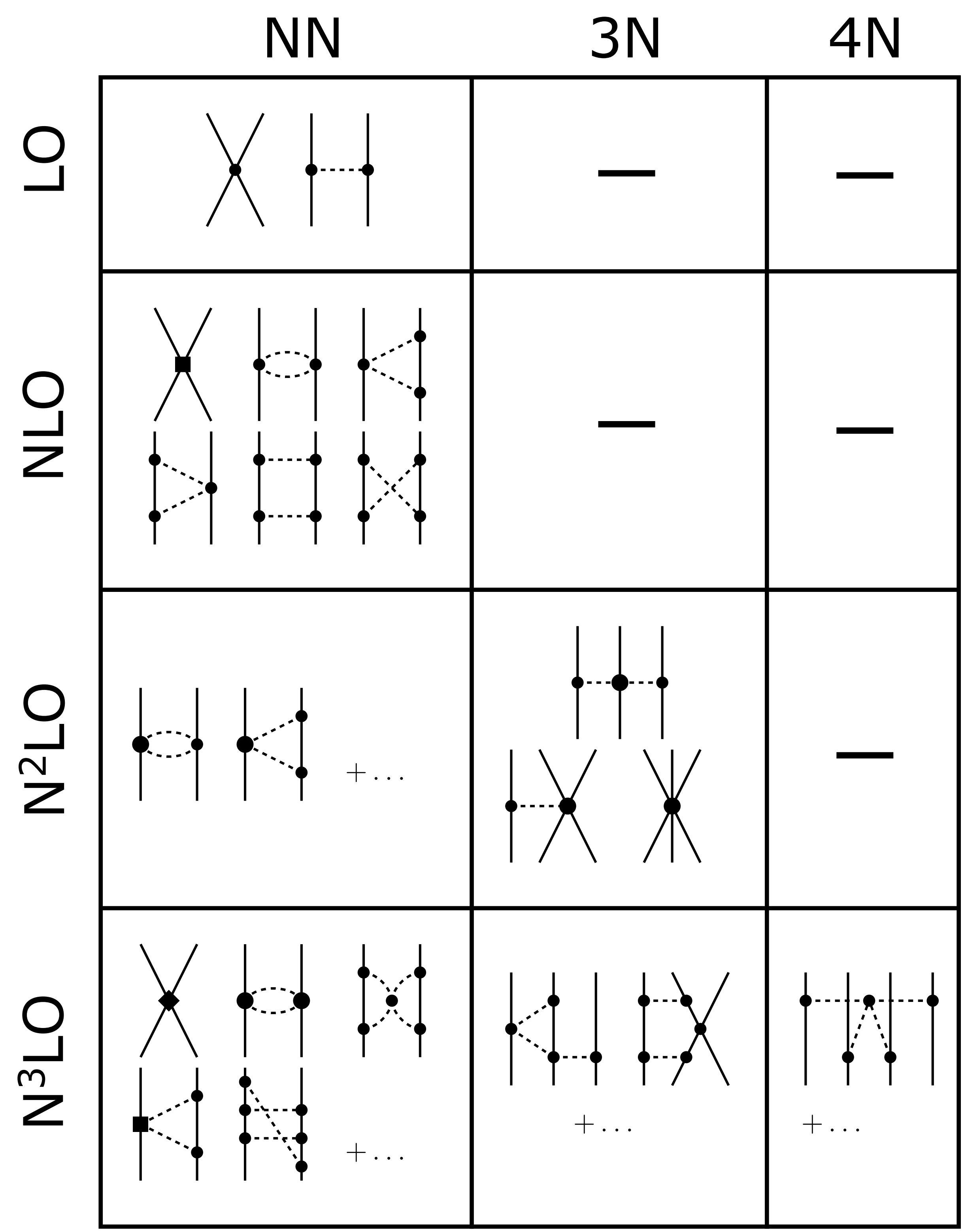

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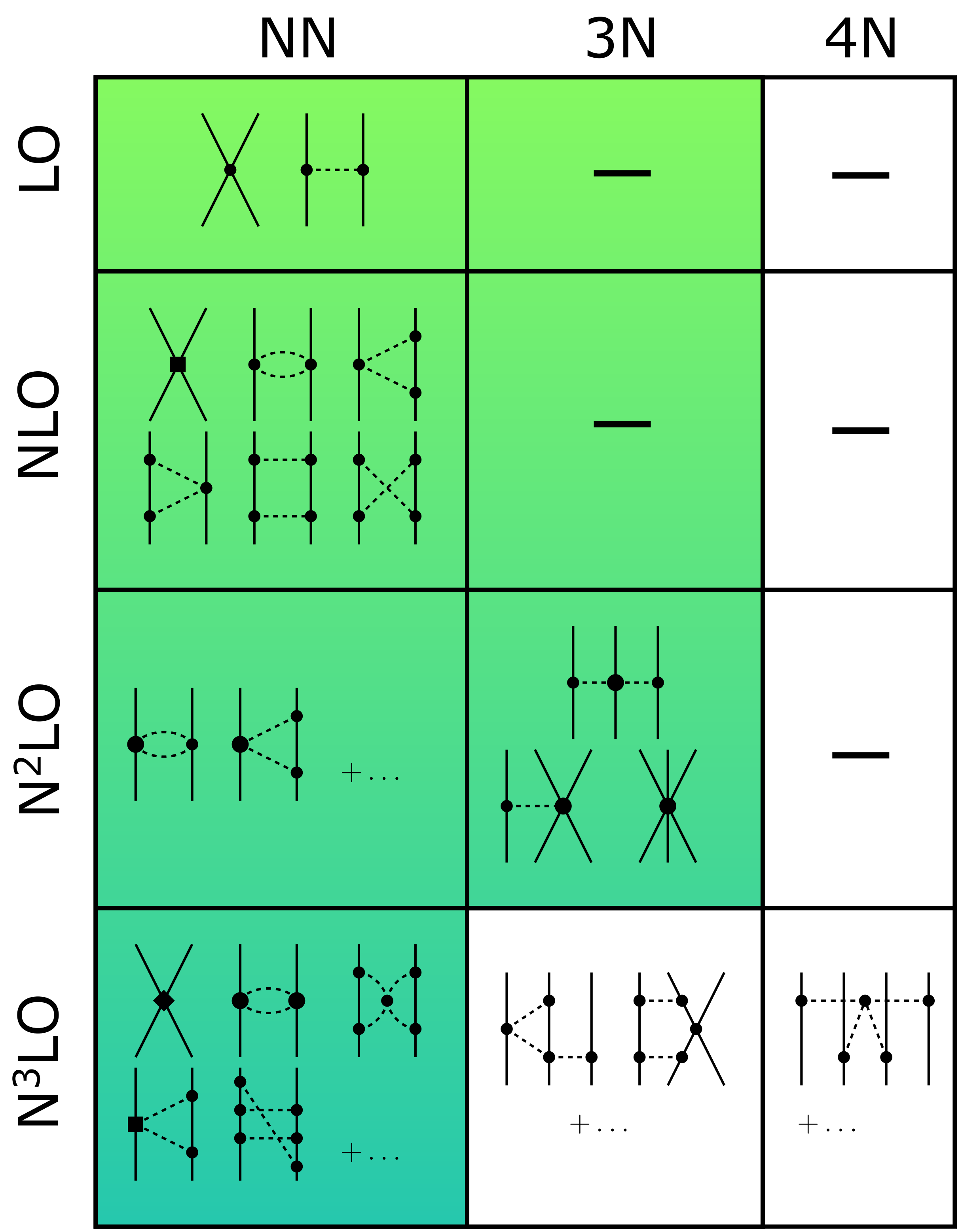

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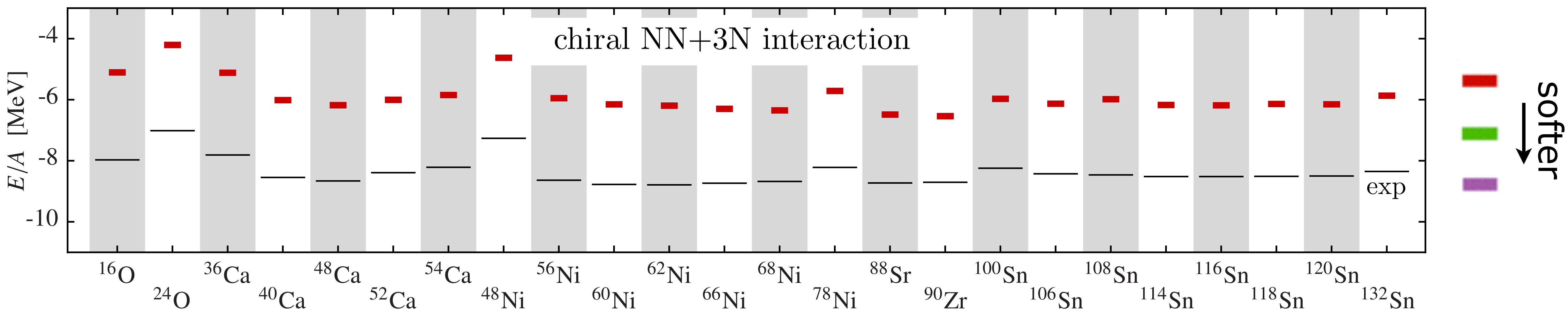

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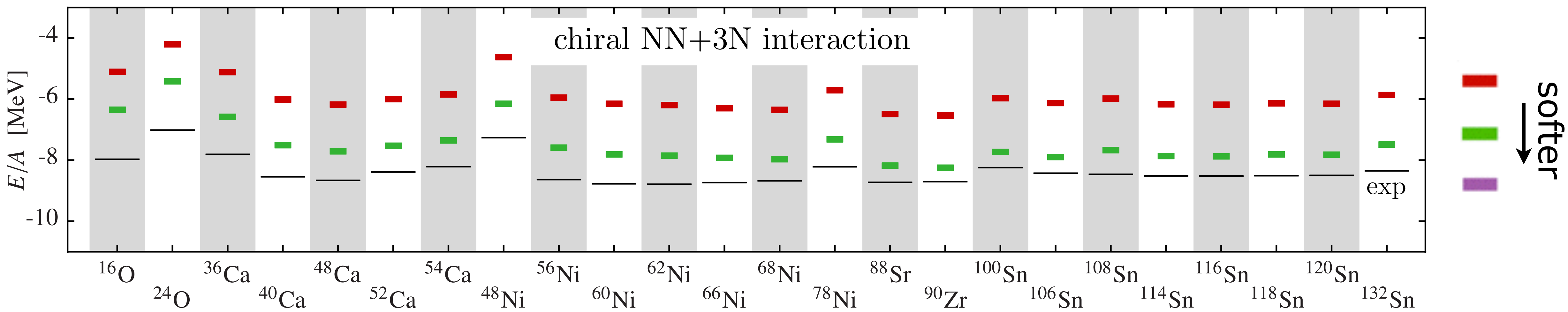

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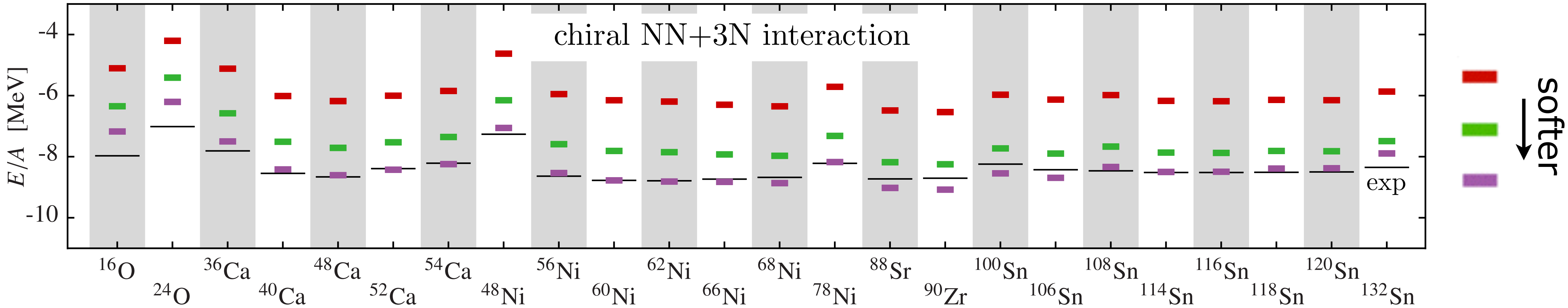

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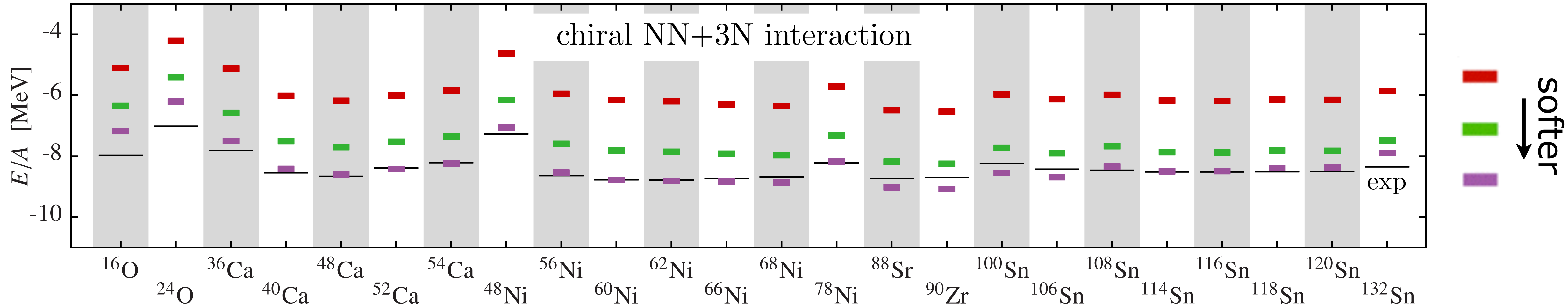

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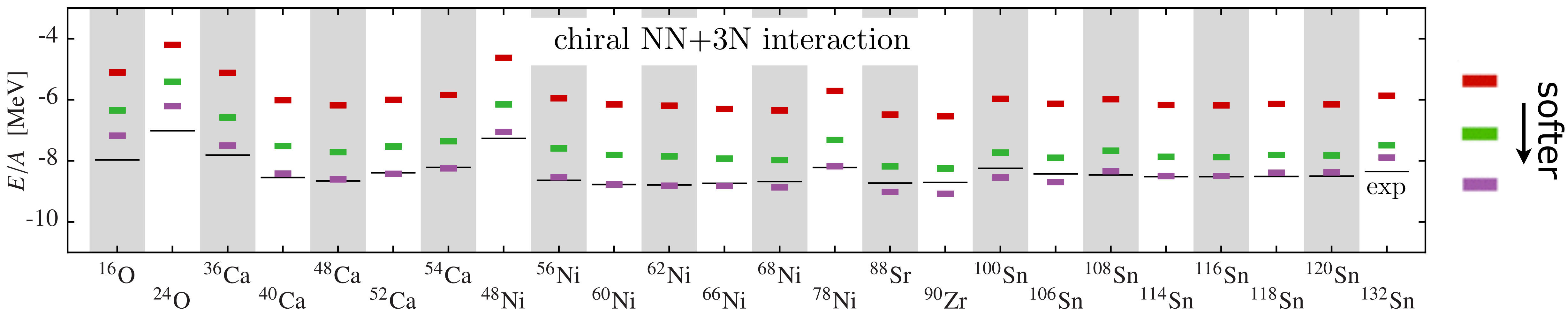

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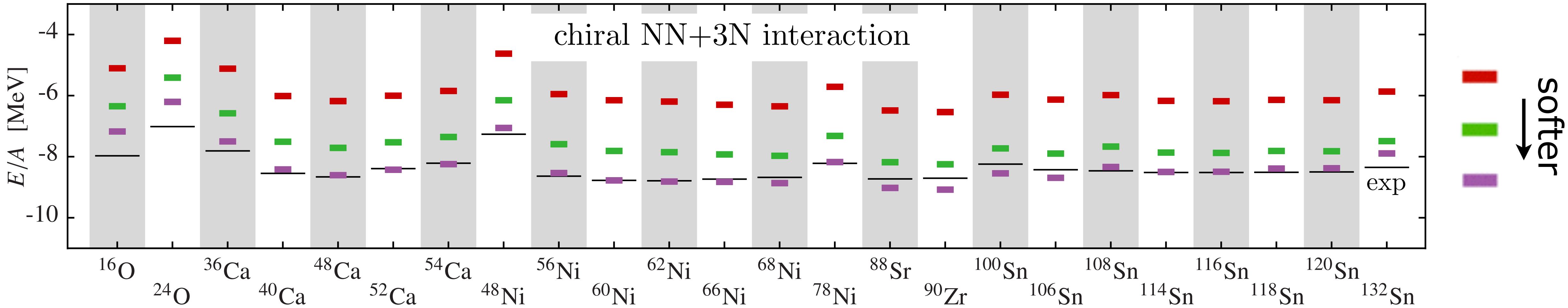

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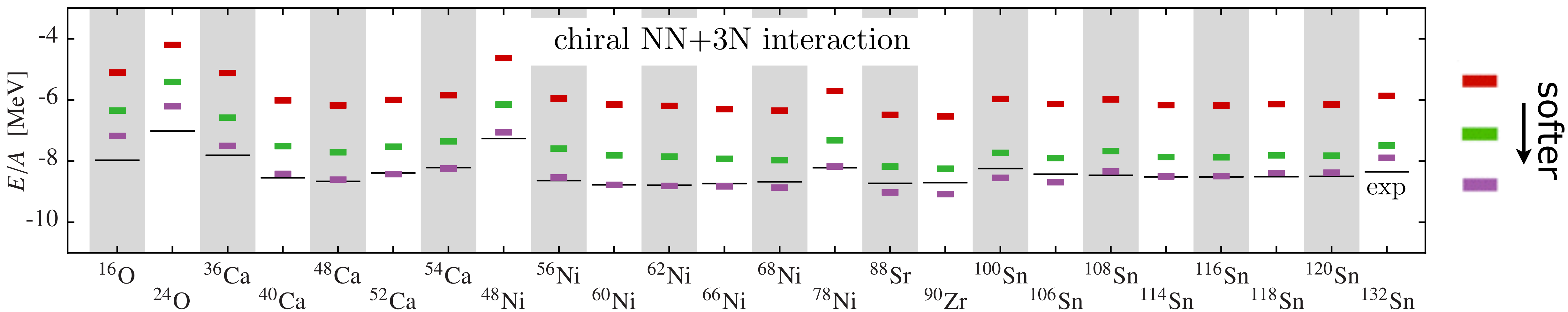

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Ab Initio

approaches
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---

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

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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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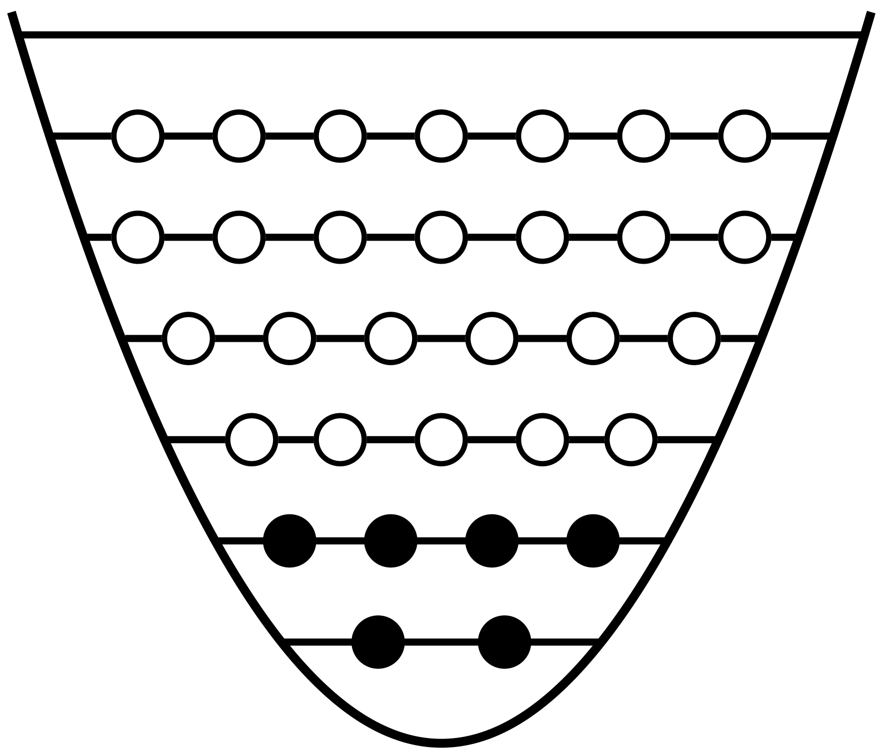

$|\Phi_0\rangle$

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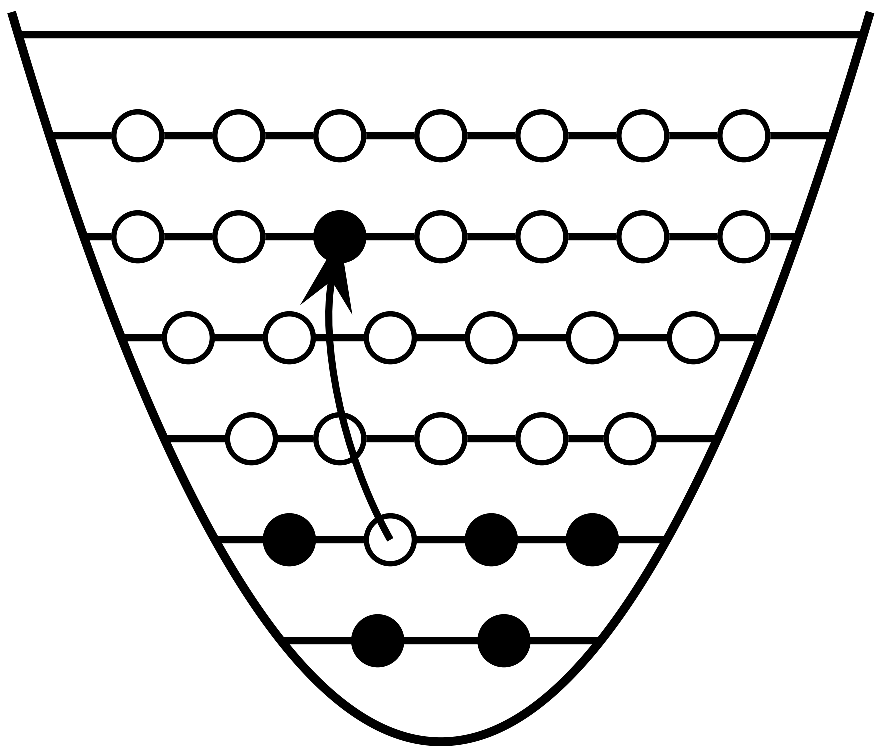

$$\hat{T}_1 \, |\Phi_0\rangle$$

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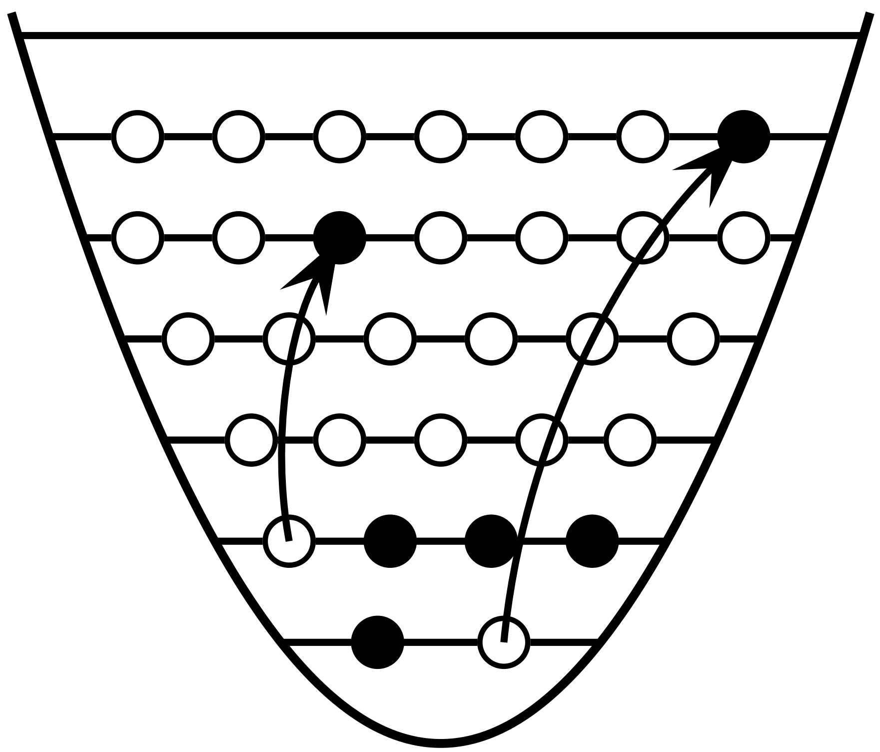

$\hat{T}_2 \left|\Phi_0\right\rangle$

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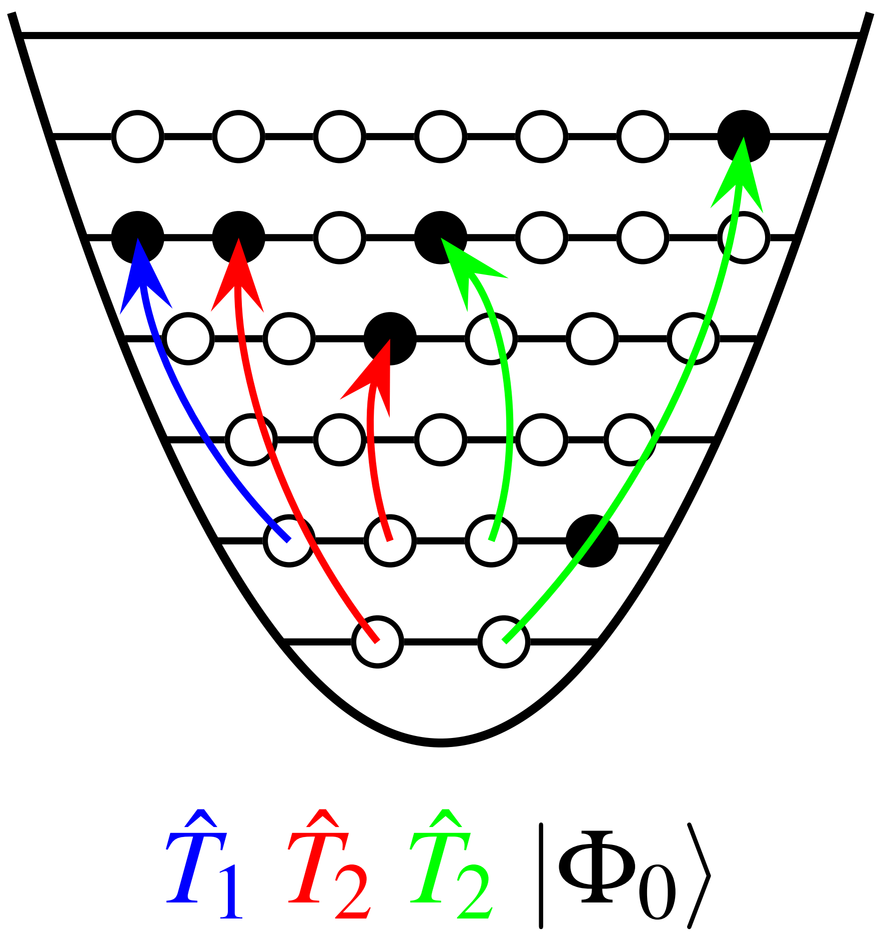

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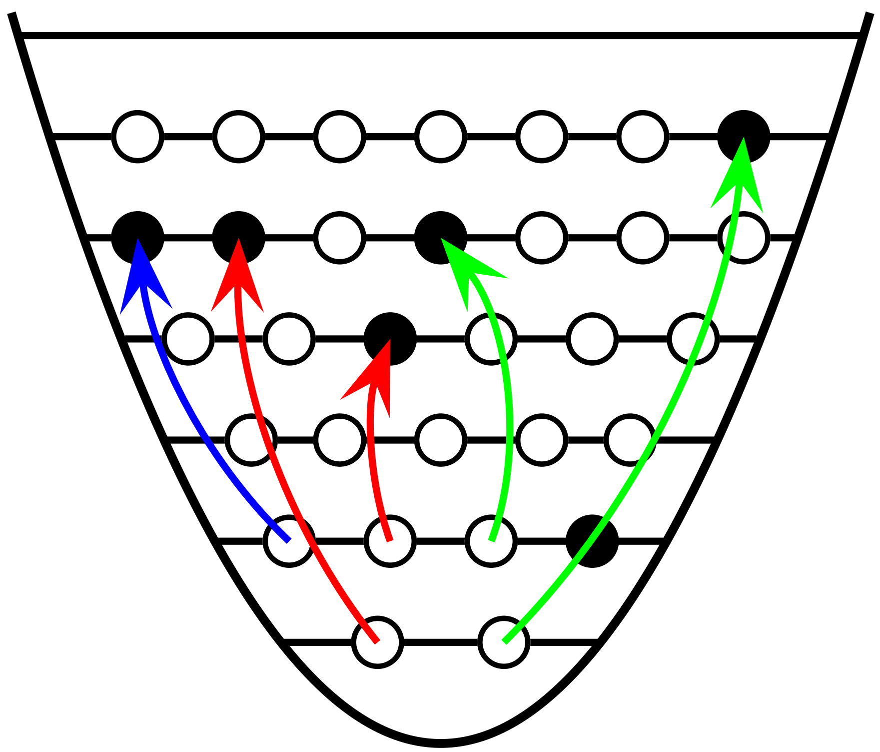

$$\hat{T}_1 \, \hat{T}_2 \, \hat{T}_2 \, |\Phi_0\rangle$$

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- CCSD equations

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

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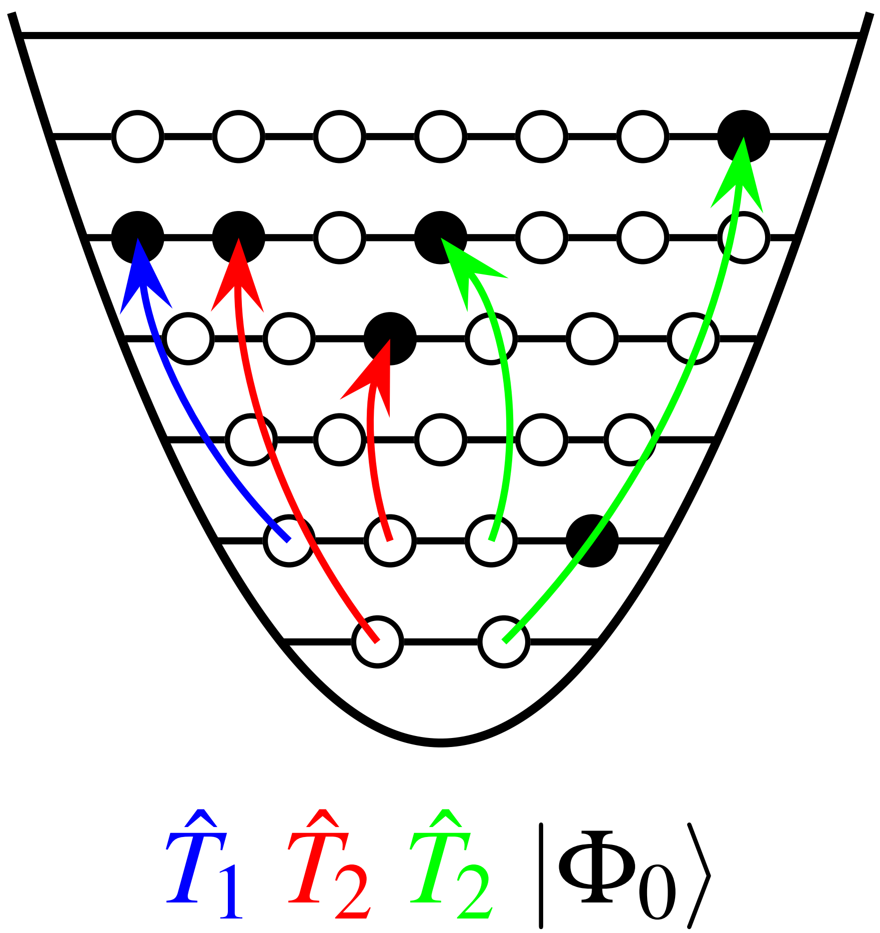

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- Coupled system of **nonlinear equations**, dimension ~ 10^8

Coupled-Cluster Equations

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

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$$0 = \langle\Phi_{ij}^{ab}|\Big[\hat{H}_N\Big(\mathbb{1} + \hat{T}_1 + \hat{T}_2 + \tfrac{1}{2!}\hat{T}_1^2 + \hat{T}_1\hat{T}_2 + \tfrac{1}{2!}\hat{T}_2^2 + \tfrac{1}{3!}\hat{T}_1^3 + \tfrac{1}{2!}\hat{T}_1^2\hat{T}_2 + \tfrac{1}{4!}\hat{T}_1^4\Big)\Big]_C|\Phi_0\rangle$$

Coupled-Cluster Equations

$$
\begin{aligned}
0 = {} & v_{ij}^{ab} + \hat{P}_{ab} \sum_{c} f_{c}^{b}\, t_{ij}^{ac} - \hat{P}_{ij} \sum_{k} f_{j}^{k}\, t_{ik}^{ab} + \tfrac{1}{2} \sum_{cd} v_{cd}^{ab}\, t_{ij}^{cd} + \tfrac{1}{2} \sum_{k} v_{ij}^{kl}\, t_{kl}^{ab} + \hat{P}_{ab} \hat{P}_{ij} \sum_{ck} v_{cj}^{kb}\, t_{ik}^{ac} \\
& + \tfrac{1}{4} \sum_{cdkl} v_{cd}^{kl}\, t_{ij}^{cd}\, t_{kl}^{ab} + \hat{P}_{ij} \sum_{cdkl} v_{cd}^{kl}\, t_{ik}^{ac}\, t_{jl}^{bd} - \tfrac{1}{2}\, \hat{P}_{ij} \sum_{cdkl} v_{cd}^{kl}\, t_{ik}^{dc}\, t_{lj}^{ab} - \tfrac{1}{2}\, \hat{P}_{ab} \sum_{cdkl} v_{cd}^{kl}\, t_{lk}^{ac}\, t_{ij}^{db} \\
& + \hat{P}_{ij} \sum_{c} v_{cj}^{ab}\, t_{i}^{c} - \hat{P}_{ab} \sum_{k} v_{ij}^{kb}\, t_{k}^{a} - \hat{P}_{ij} \sum_{ck} f_{c}^{k}\, t_{kj}^{ab}\, t_{i}^{c} - \hat{P}_{ab} \sum_{ck} f_{c}^{k}\, t_{ij}^{cb}\, t_{k}^{a} \\
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$$

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- Exploit **spherical symmetry** for closed-shell nuclei, use spherical tensor operator formulation

$$\hat{T}_1 = \sum_{ai} t_i^a \left\{ \hat{a}_a^\dagger \otimes \hat{\tilde{a}}_i \right\}_0^{(0)}$$

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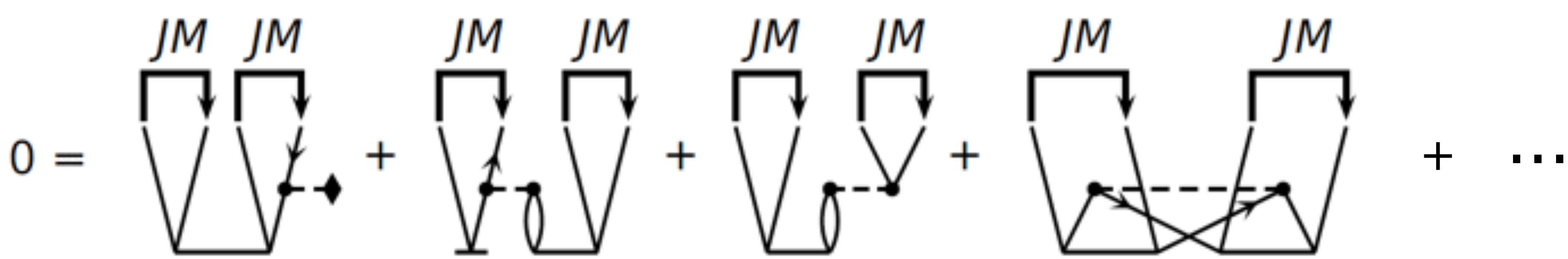
- **Angular-momentum coupling** of external lines



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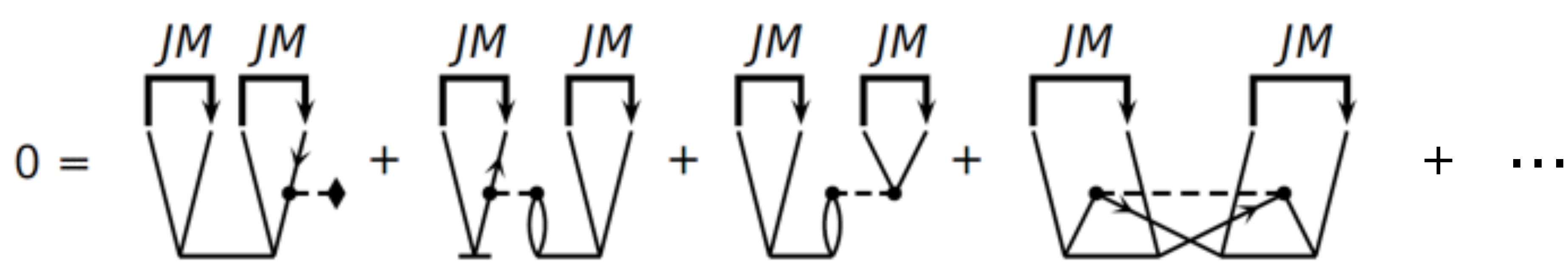
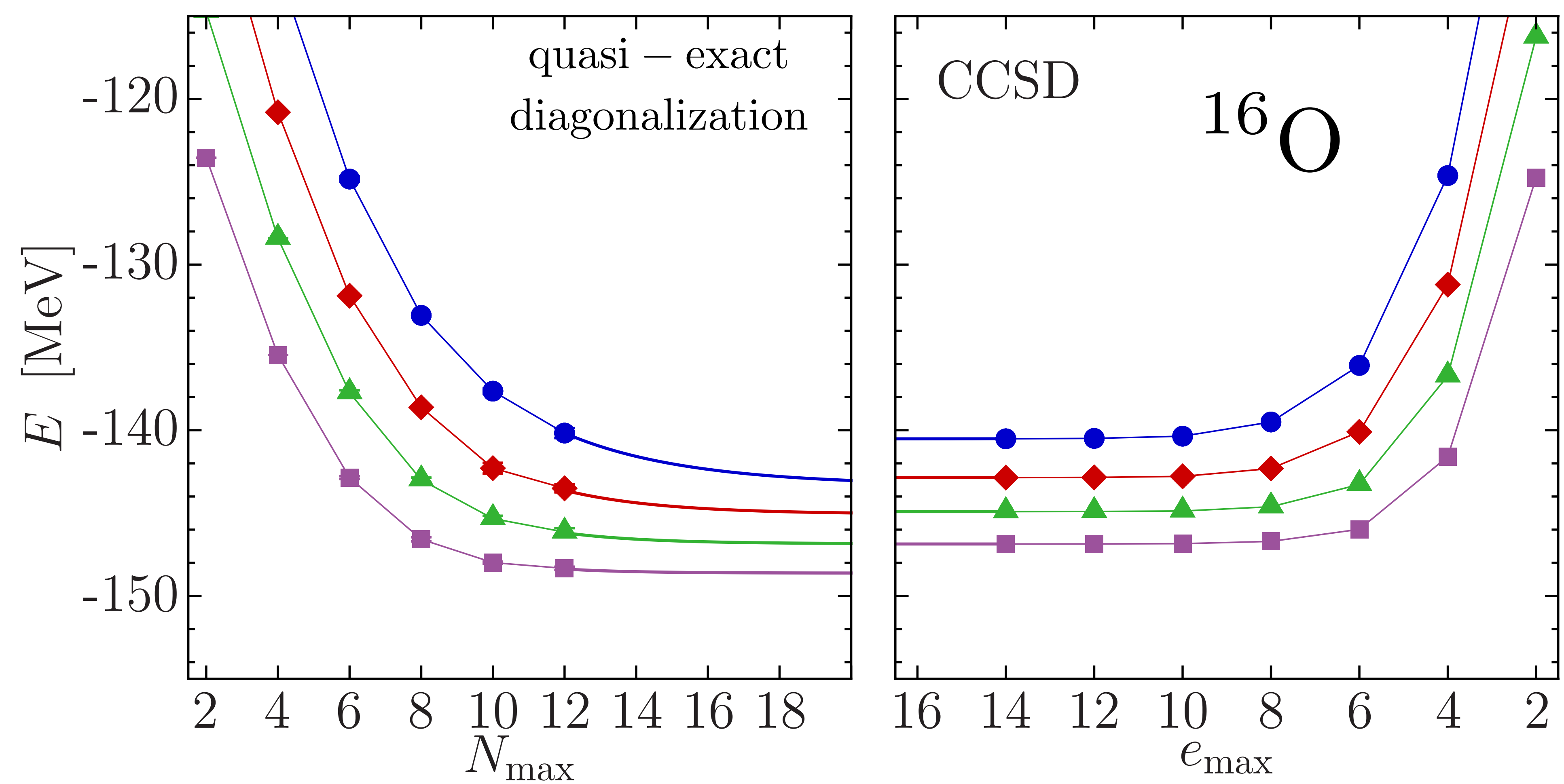


- Express Coupled-Cluster equations in terms of

$$\langle \overset{JM}{pq} | \hat{v} | \overset{JM}{rs} \rangle \;, \qquad \langle \overset{JM}{ab} | \hat{t}_2 | \overset{JM}{ij} \rangle \;, \qquad \langle \overbrace{p | \hat{f} | q}^{00} \rangle$$

^{16}O: Exact Diagonalization vs. CCSD

chiral NN+3N interaction



softer ⟶

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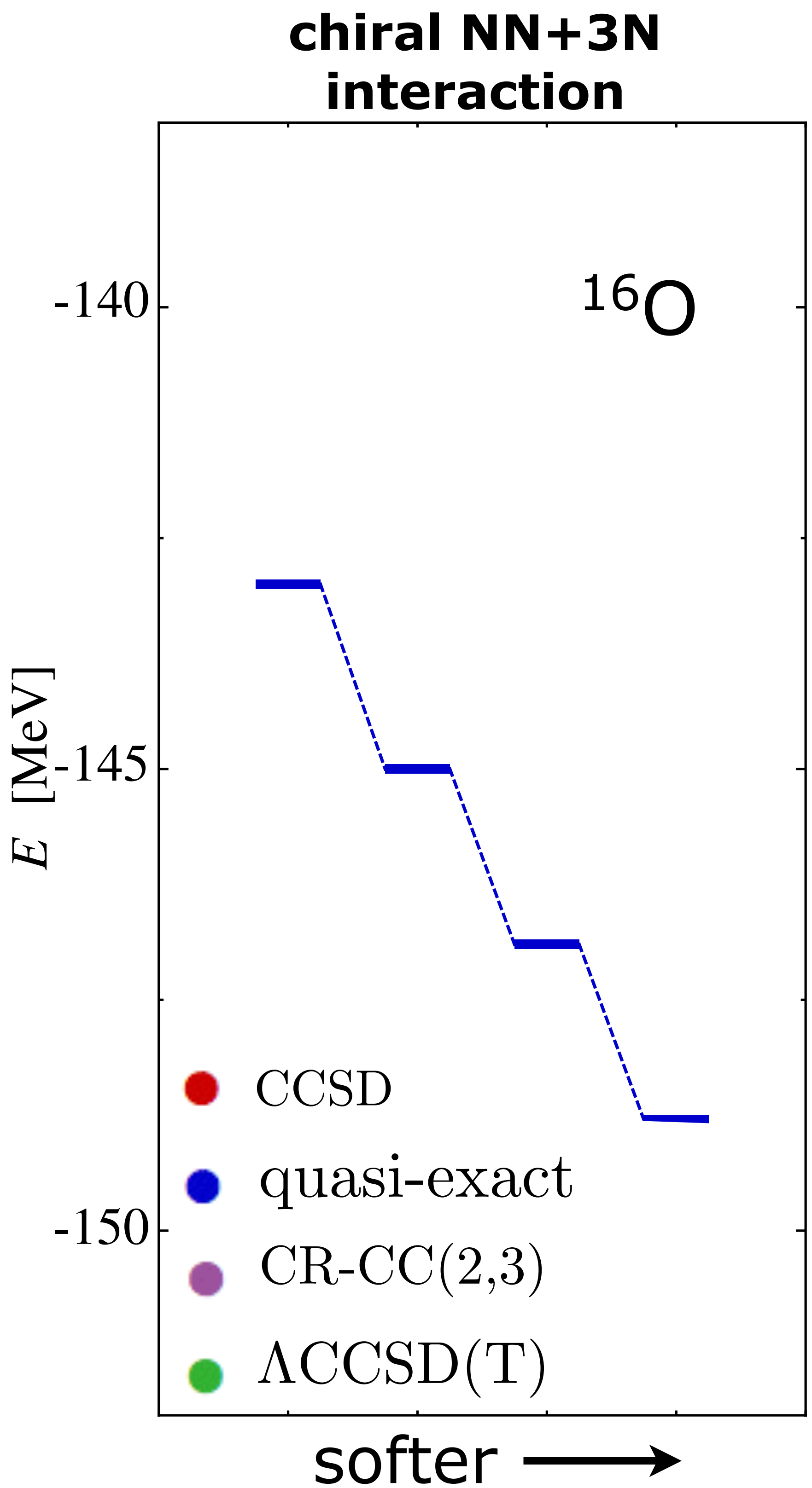
CR-CC(2,3)

"Left-Eigenstate Completely Renormalized Coupled-Cluster Method with Singles, Doubles, and Non-Iterative Triples Excitations"

Coupled-Cluster Methods



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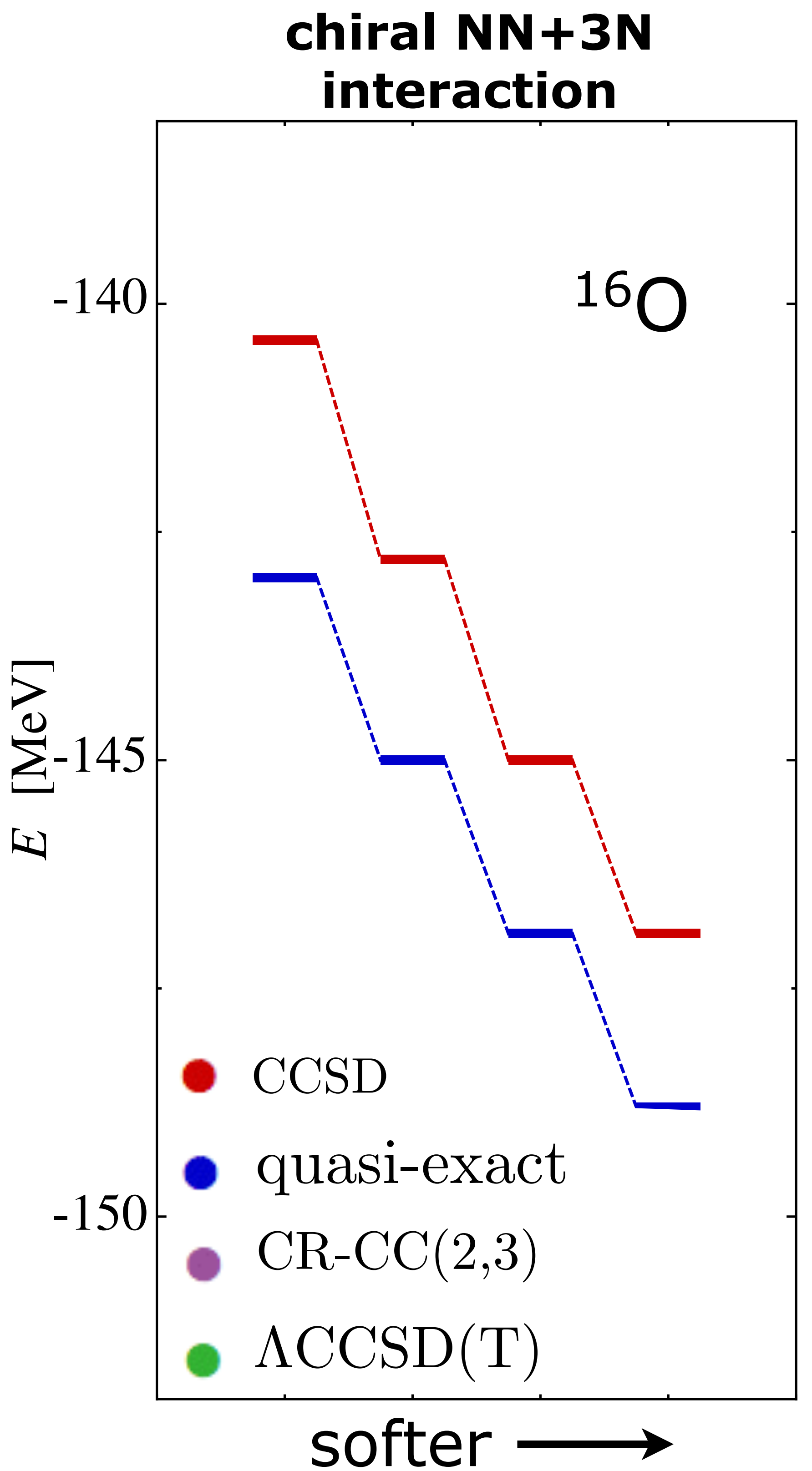

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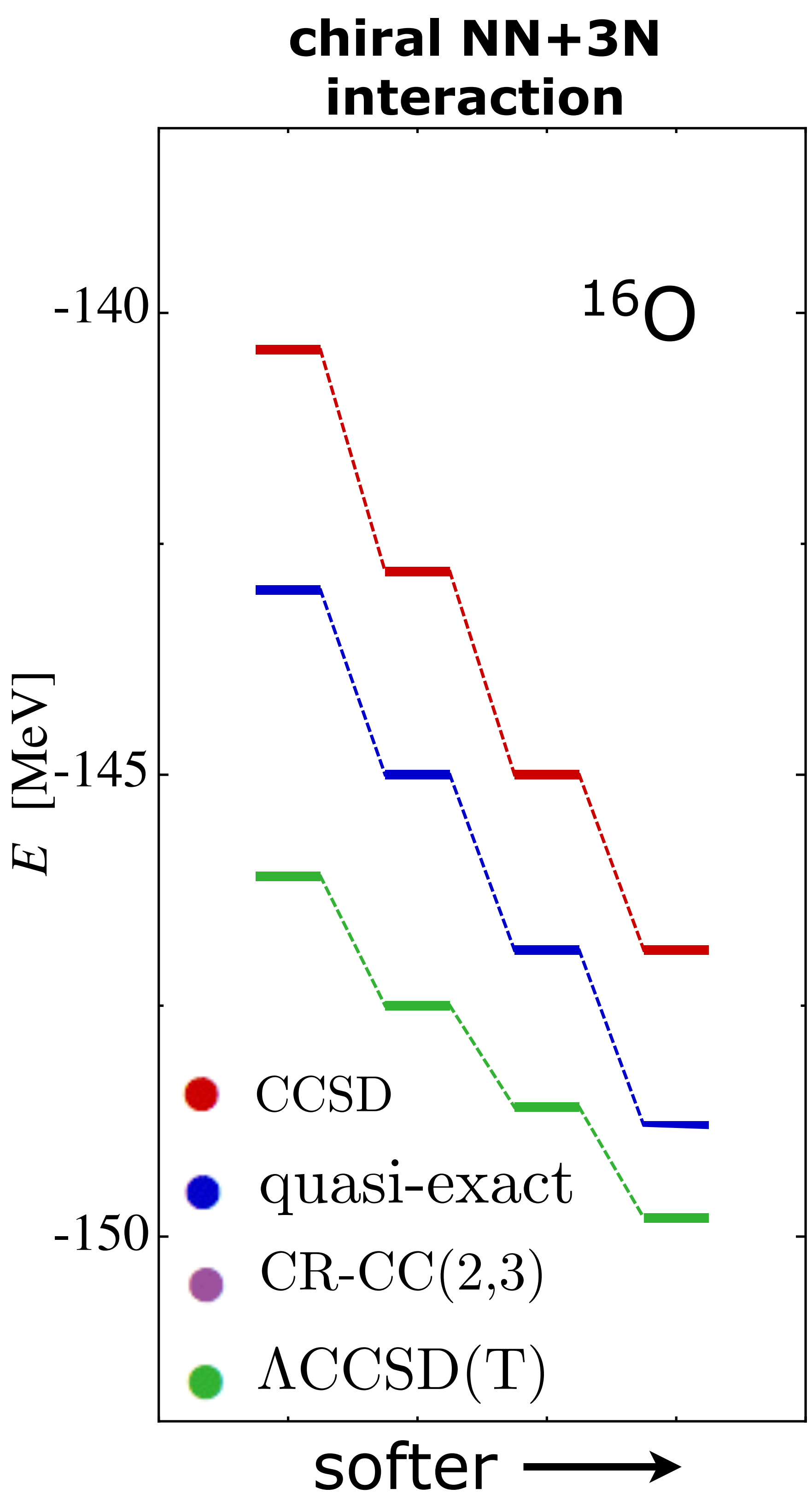

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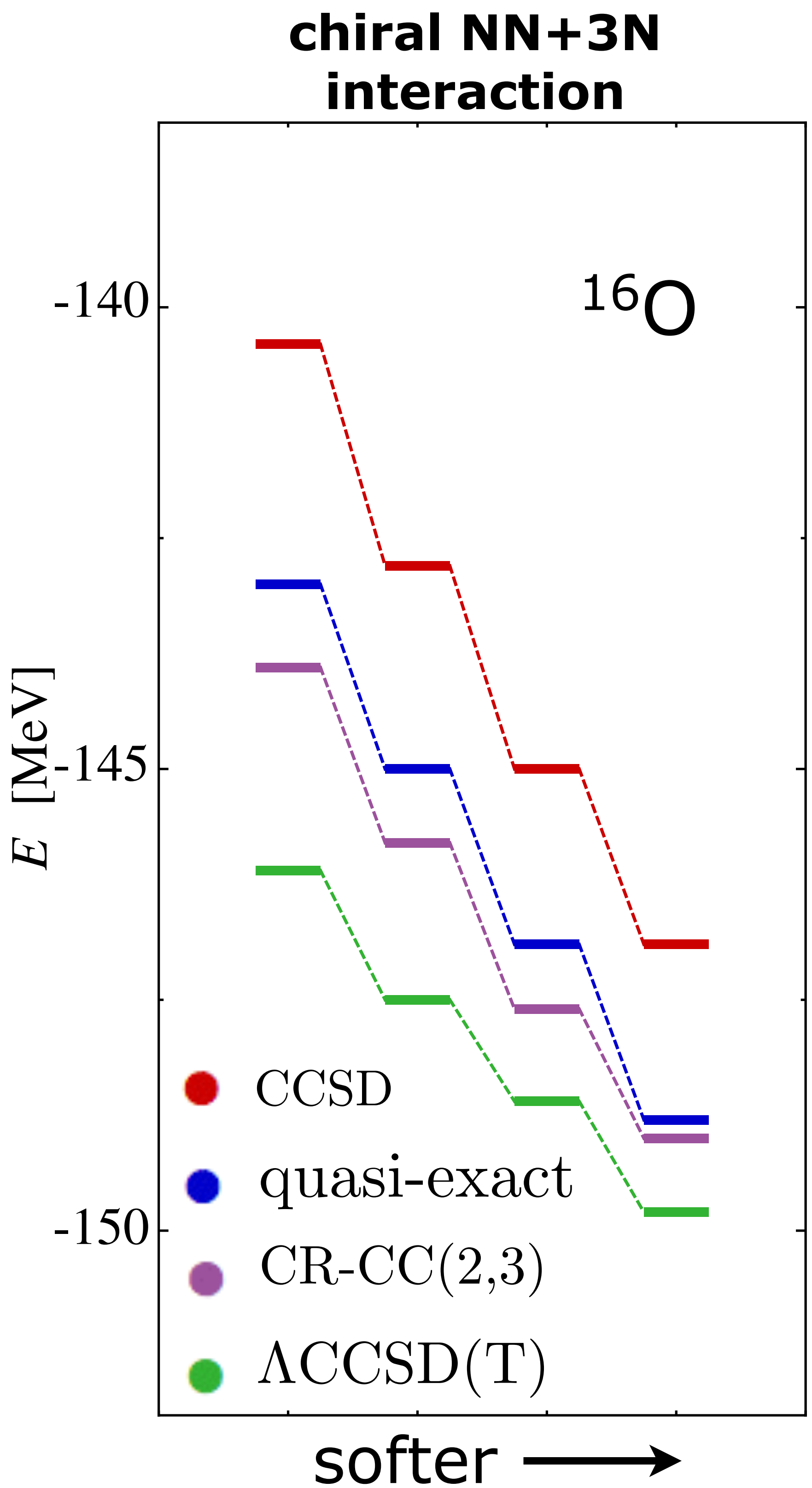

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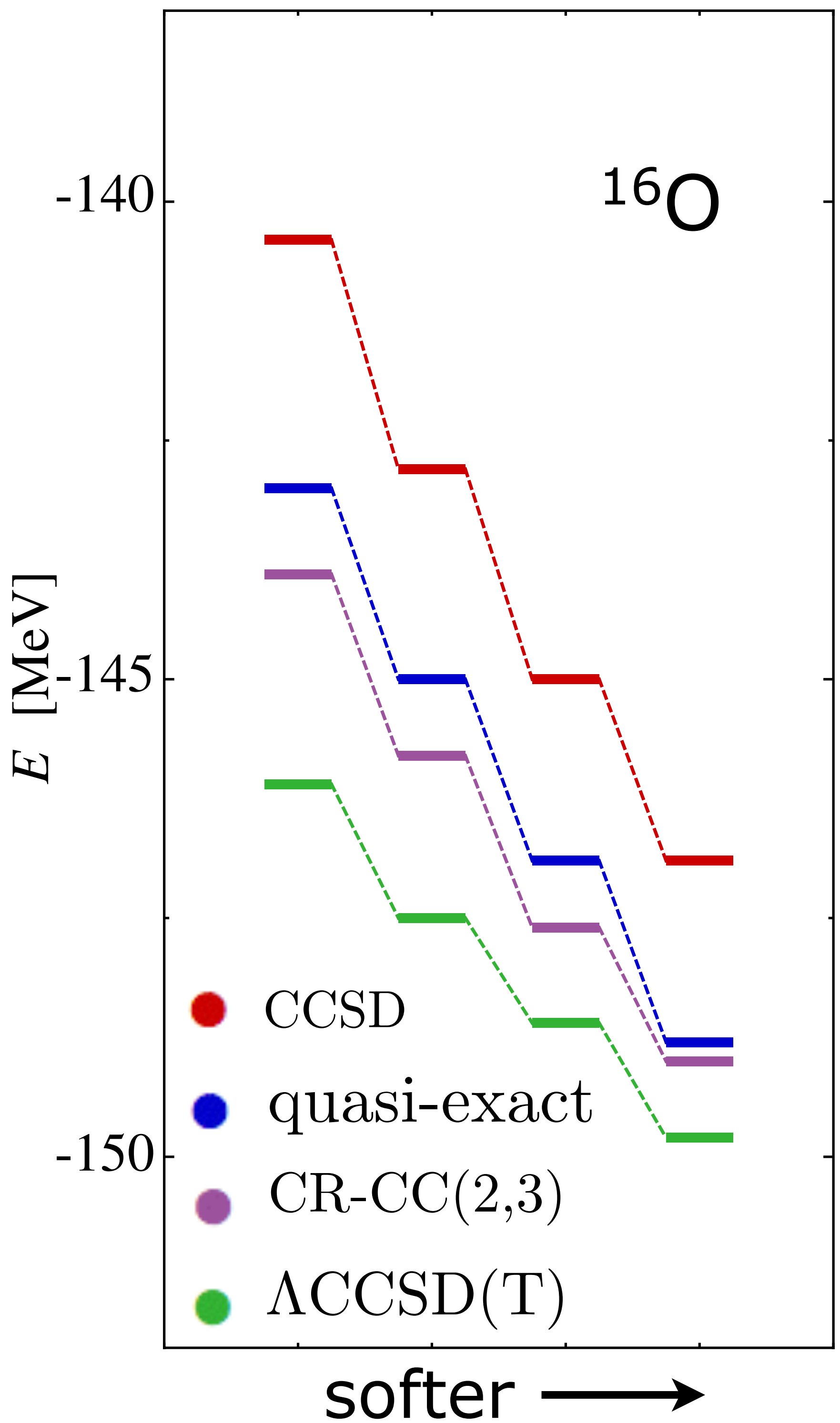
Coupled-Cluster Methods

chiral NN+3N interaction



CR-CC(2,3)

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

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- **CR-CC(2,3)** shows **excellent agreement** with quasi-exact diagonalizations

3N Interactions and NO Approximation

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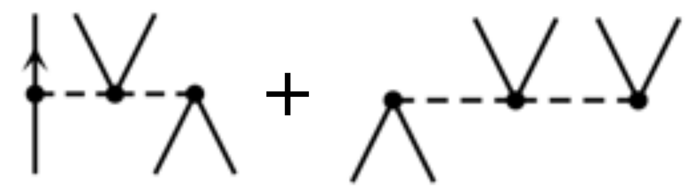
- **Full inclusion** of $\hat{V}_{3\mathrm{N}}$ challenging

$\hat{V}_{3\mathrm{N}} =$  $+ \cdots$

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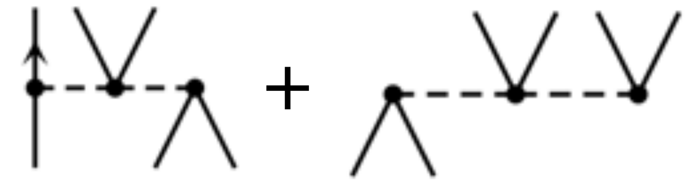
$\hat{V}_{3\mathrm{N}} =$  $+ \cdots$

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$$\hat{V}_{3\mathrm{N}} = \hat{W}^{0\mathrm{B}} + \hat{W}^{1\mathrm{B}} + \hat{W}^{2\mathrm{B}} + \hat{W}^{3\mathrm{B}} \quad \text{(via normal ordering)}$$

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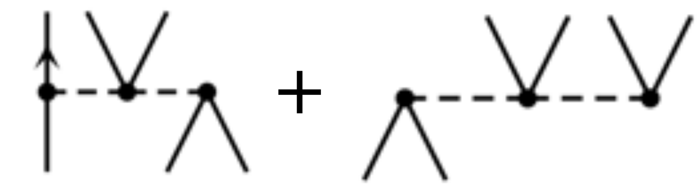
$\hat{V}_{3\mathrm{N}} =$  $+ \cdots$

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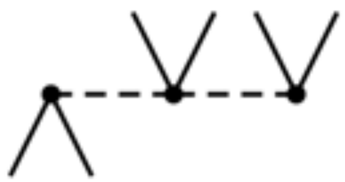
$\hat{V}_{3\mathrm{N}} =$  $+$  $+ \cdots$

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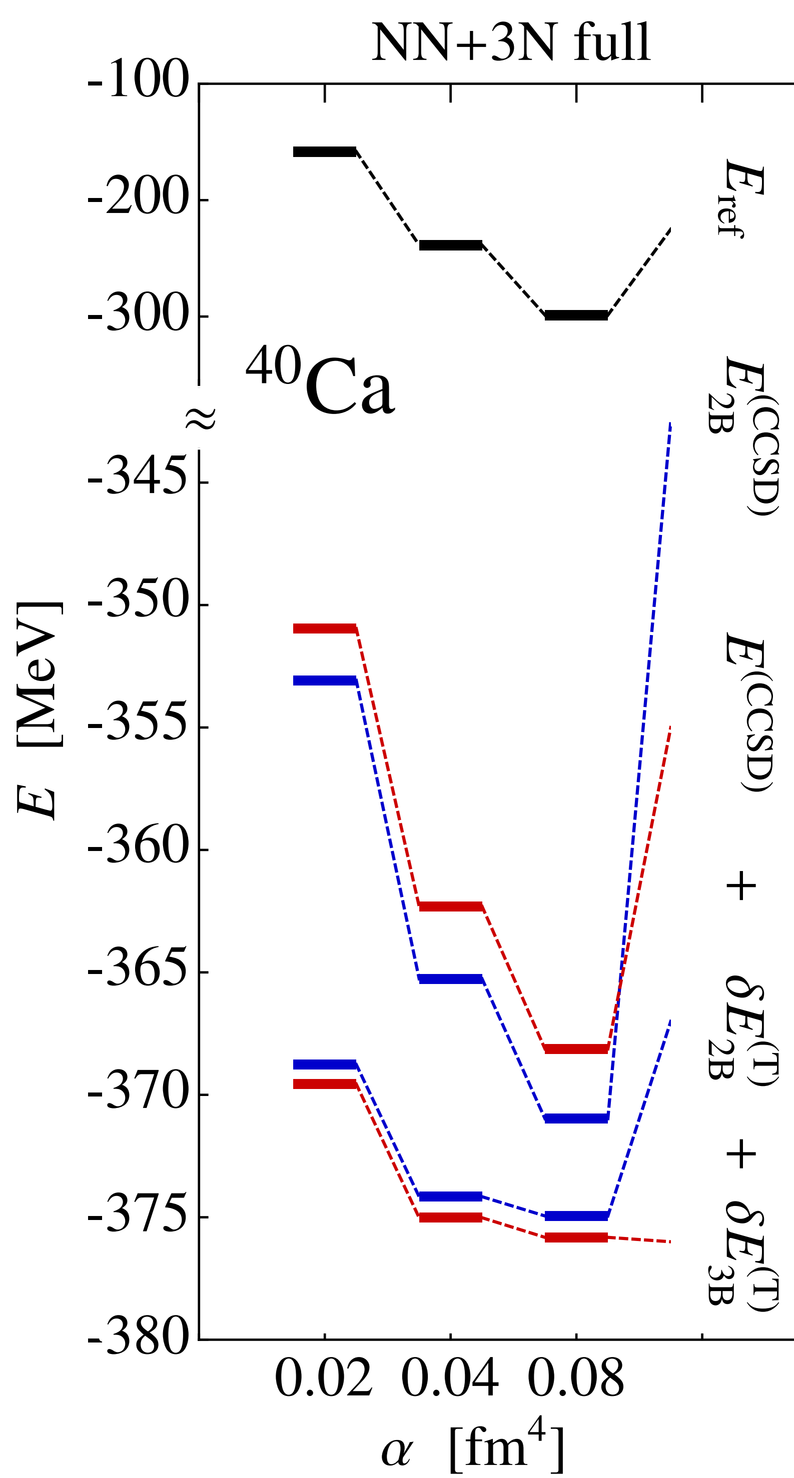
- Generalization of Coupled-Cluster theory to **3N Hamiltonians** elaborate, but possible

- Currently, Coupled-Cluster theory is the **only medium-mass *ab initio* method** capable of including full 3N interactions

Coupled Cluster with Full 3N Interactions



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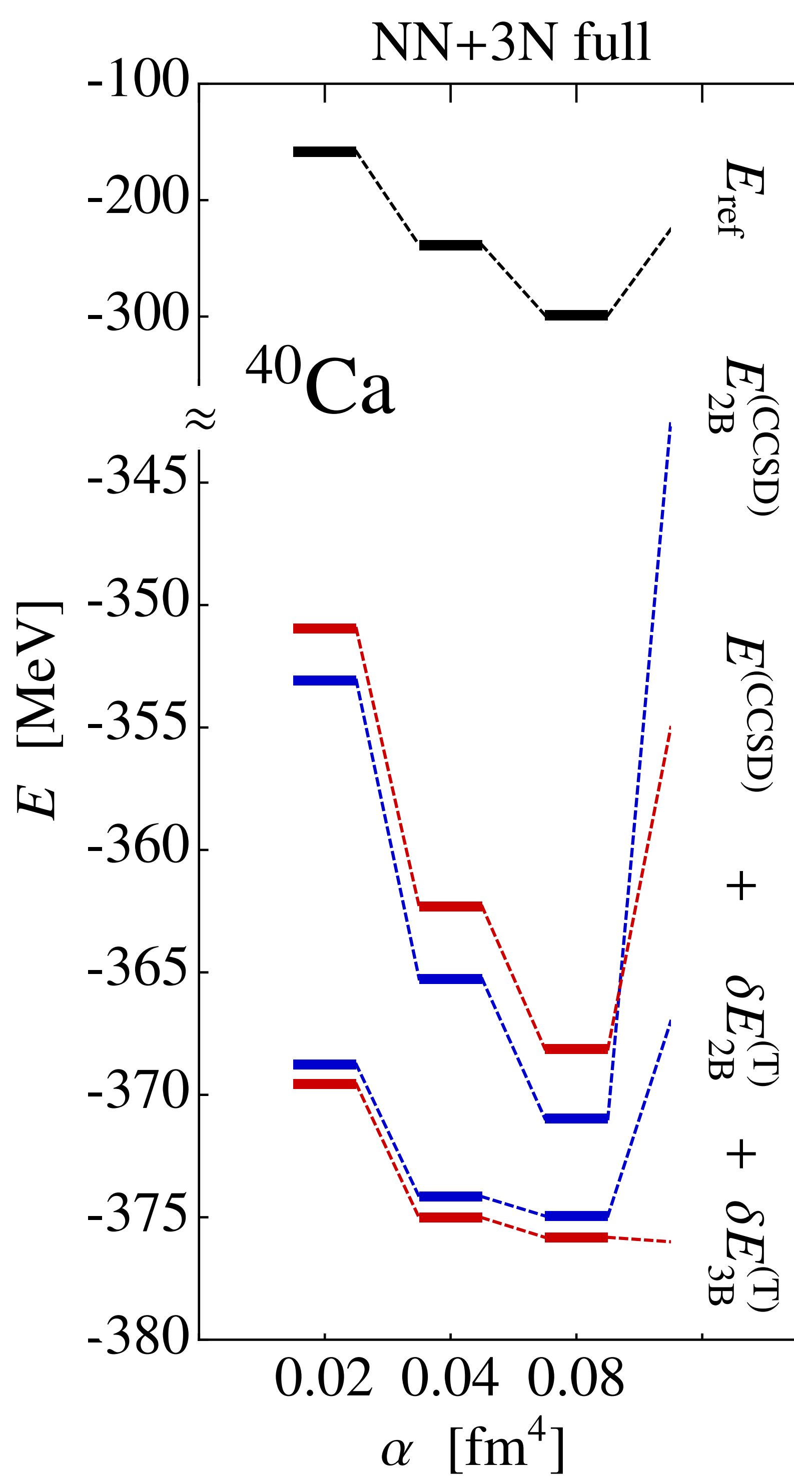

- Accuracy of normal-ordering approximation verified for **medium-mass nuclei** (Error < 1%)

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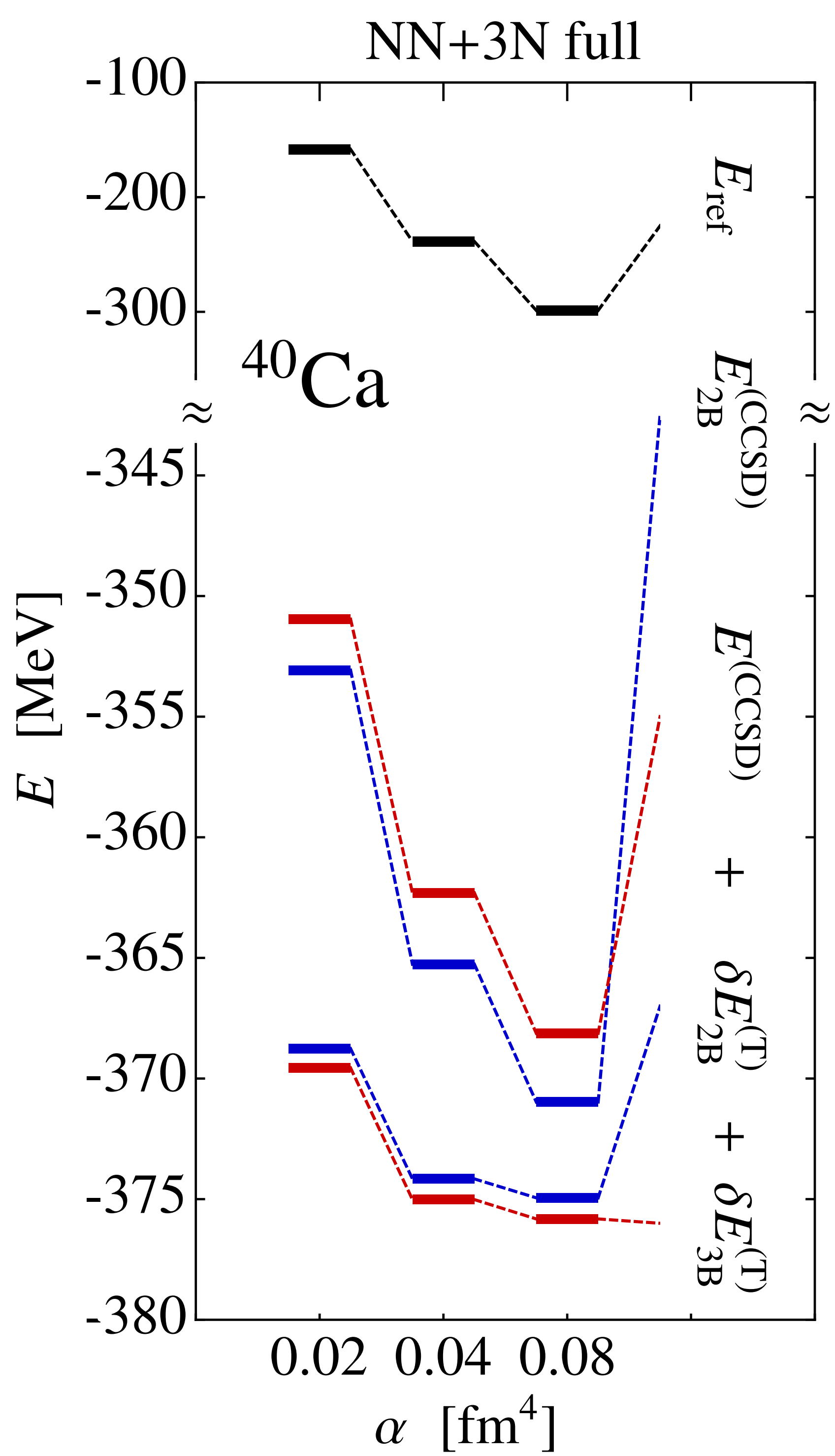

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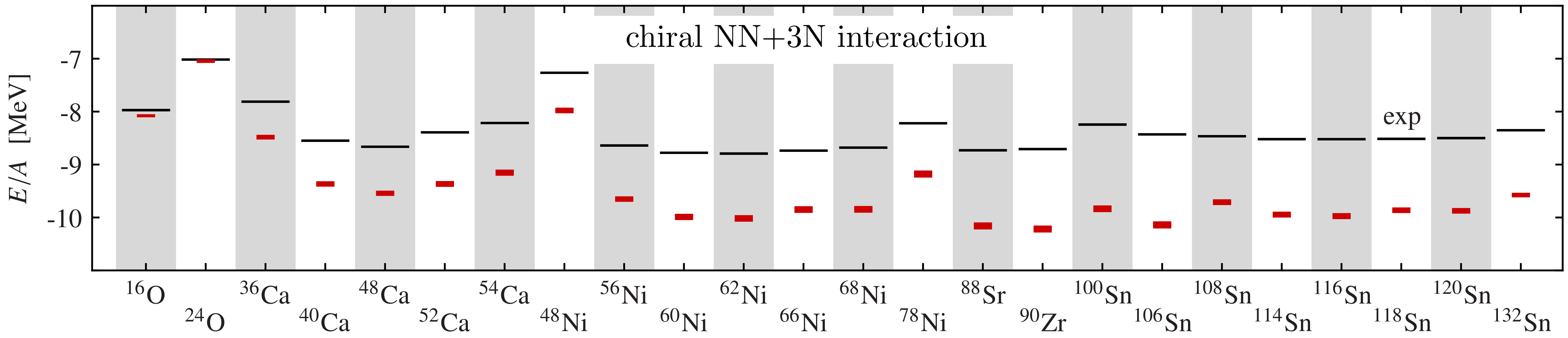
- Discarded 3N interaction **relevant** for **CCSD**, **irrelevant** for **triples correction**

Heavy Nuclei from Chiral Interactions



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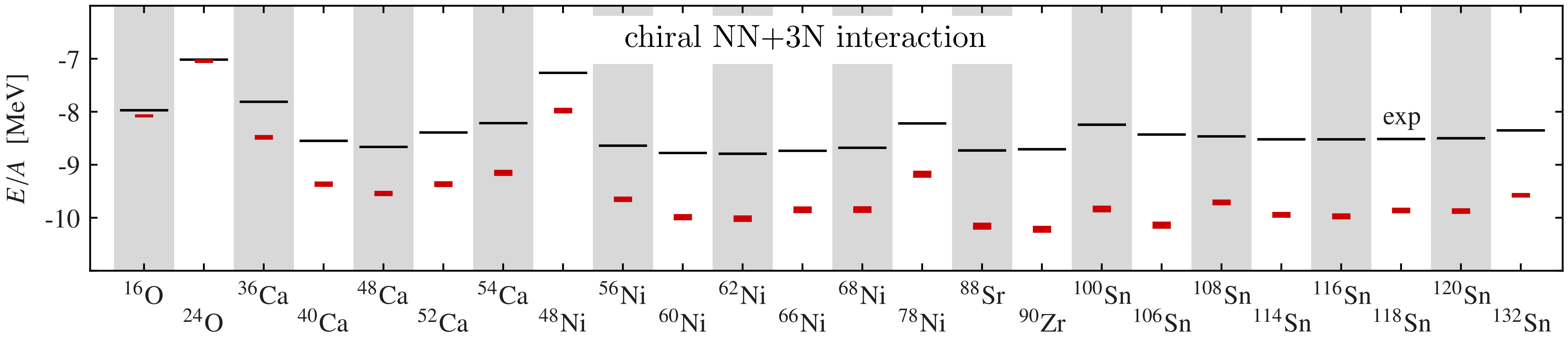

- **Many-body treatment**: Uncertainties 2-4%

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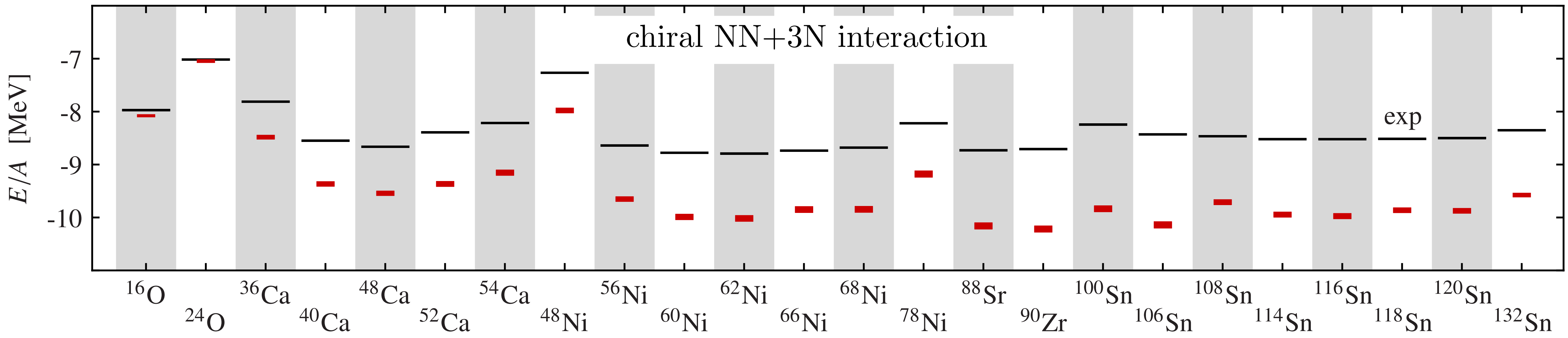

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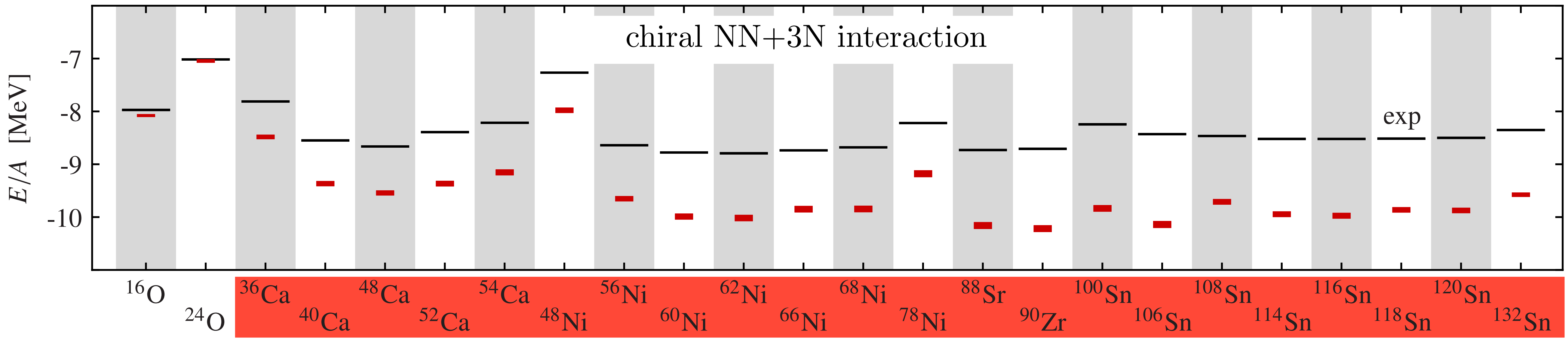

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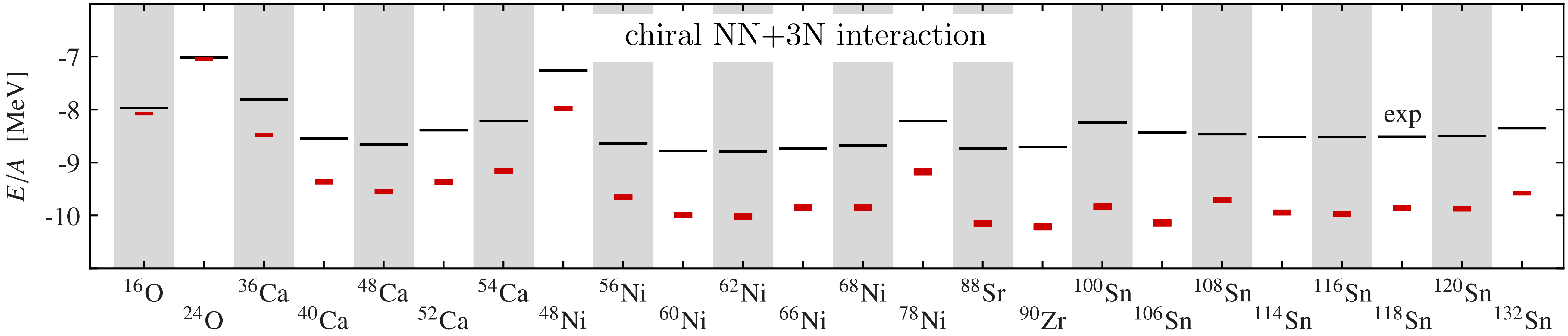

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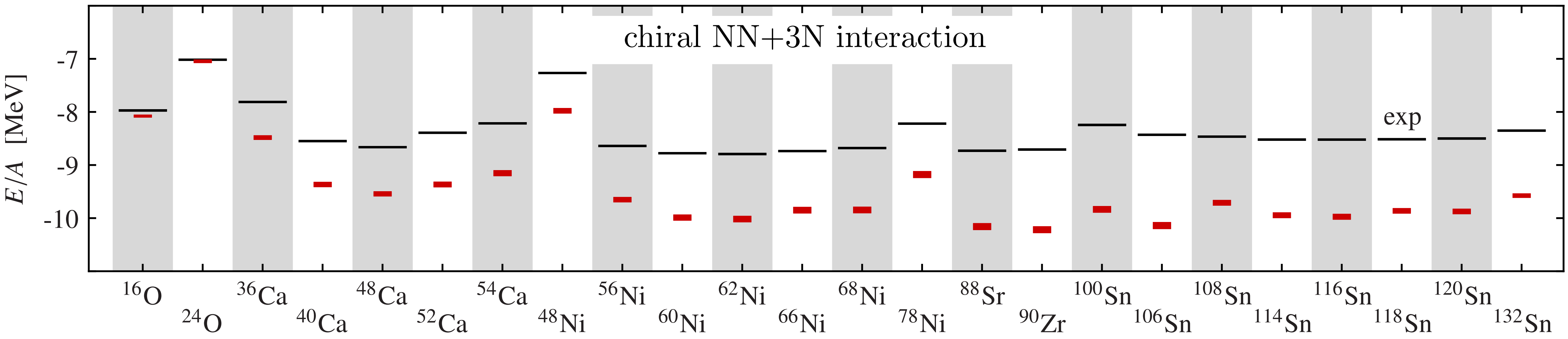

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  ✳ Next step: **Consistent 3N** interaction at N^{3}LO

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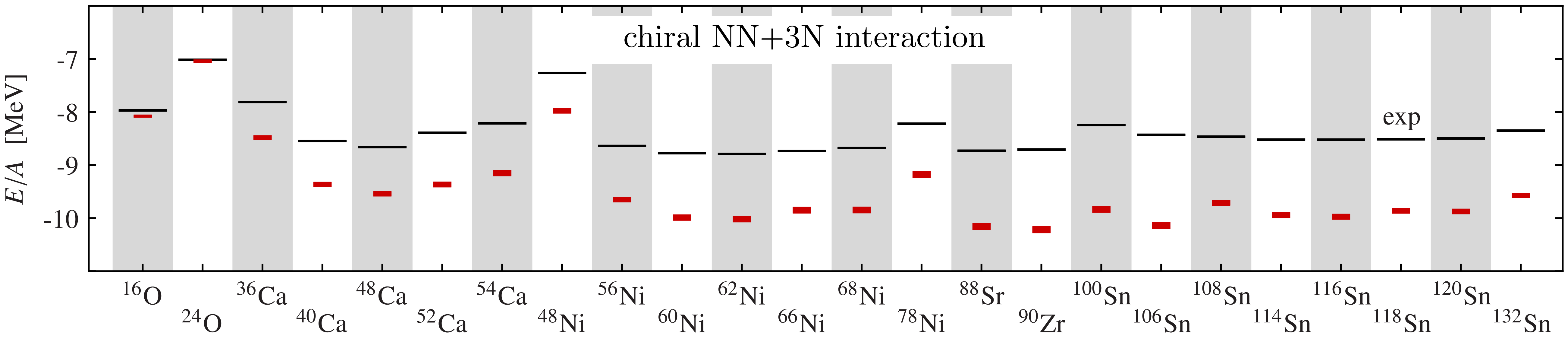

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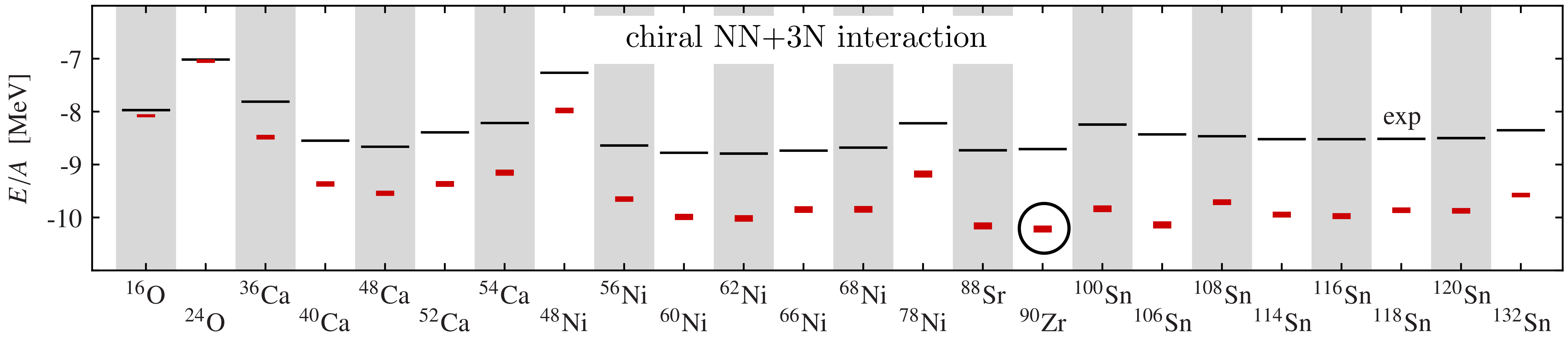

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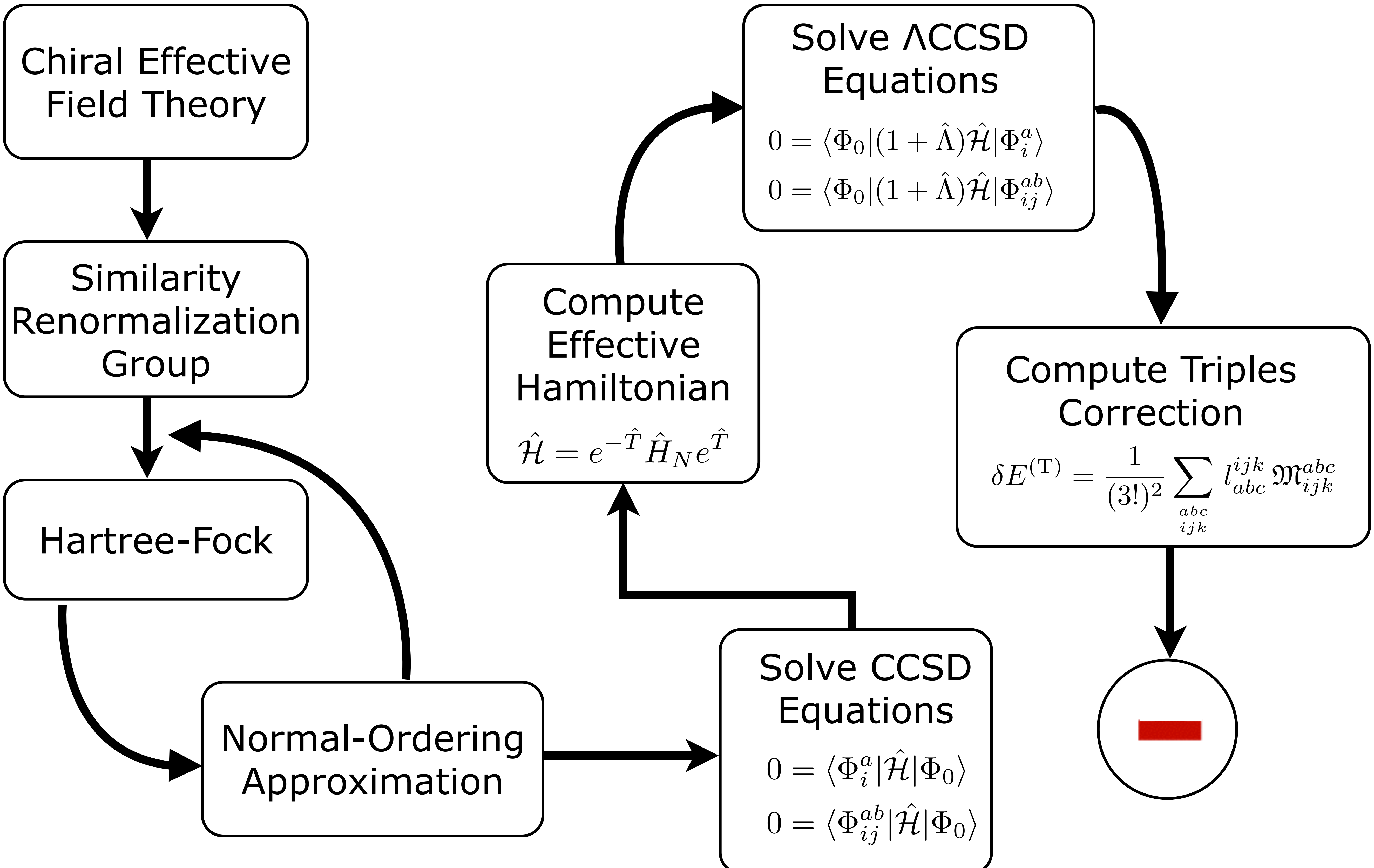
Computational Scheme

Chiral Effective Field Theory

−

Computational Scheme



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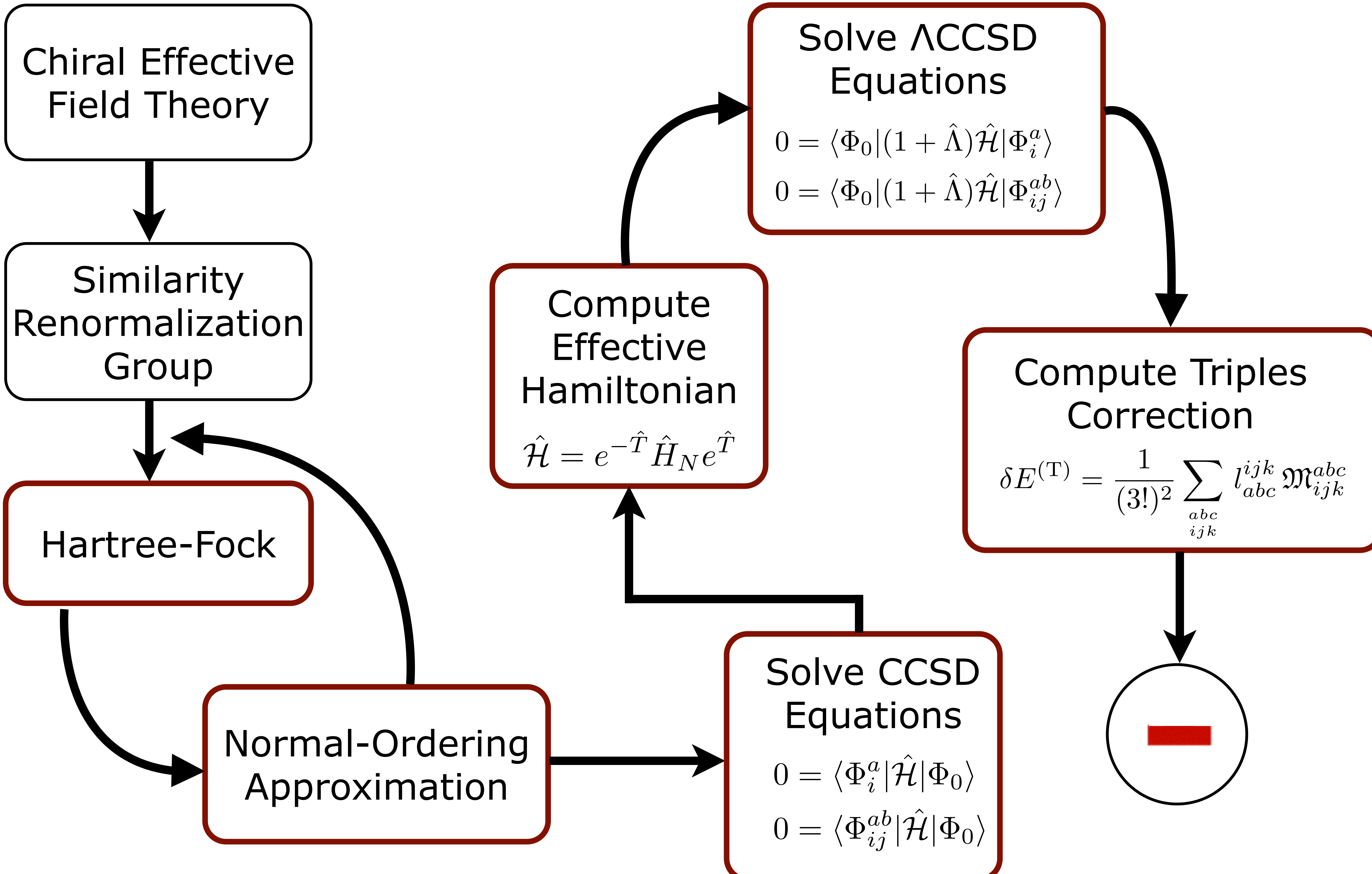
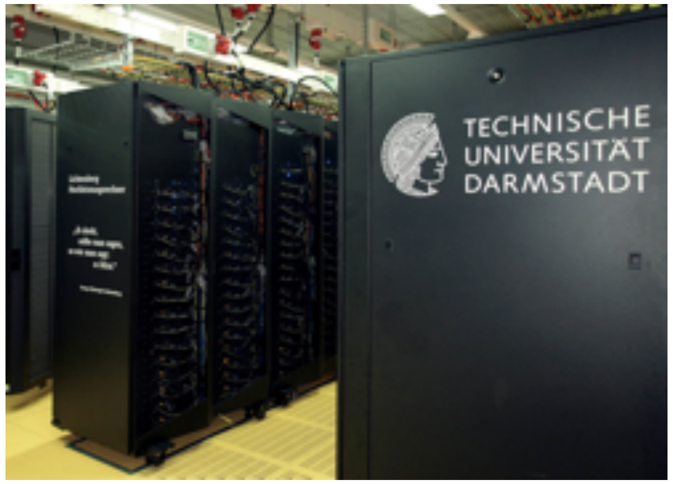


Computing Facilities



Lichtenberg Cluster
TU Darmstadt

Loewe-CSC
Goethe-Universität Frankfurt

Edison
National Energy Research
Scientific Computing Center

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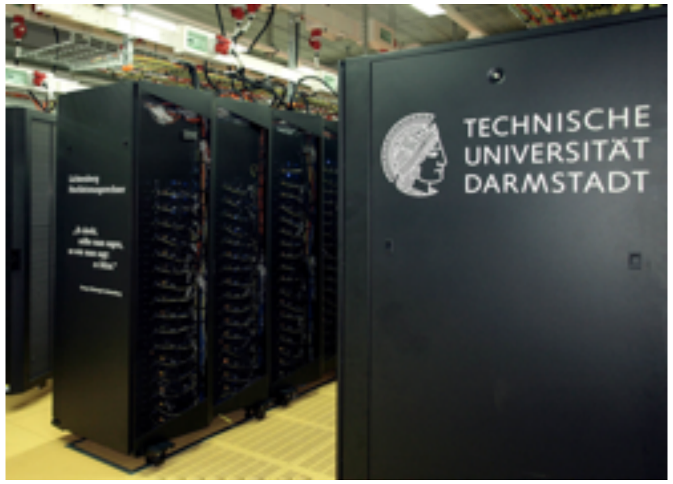

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Thanks!

Excited States

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- Generate excited states via **linear 1p1h and 2p2h excitations** on top of the **fully correlated** Coupled-Cluster ground state

$$|\Psi_\mu\rangle = \hat{\mathfrak{R}}_\mu \, |\Psi^{(\mathrm{CCSD})}\rangle$$

$$\hat{\mathfrak{R}}_\mu = (r_\mu)_0 + \sum_{ai} (r_\mu)_i^a \, \{\hat{a}_a^\dagger \hat{a}_i\} + \frac{1}{4} \sum_{abij} (r_\mu)_{ij}^{ab} \, \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\}$$

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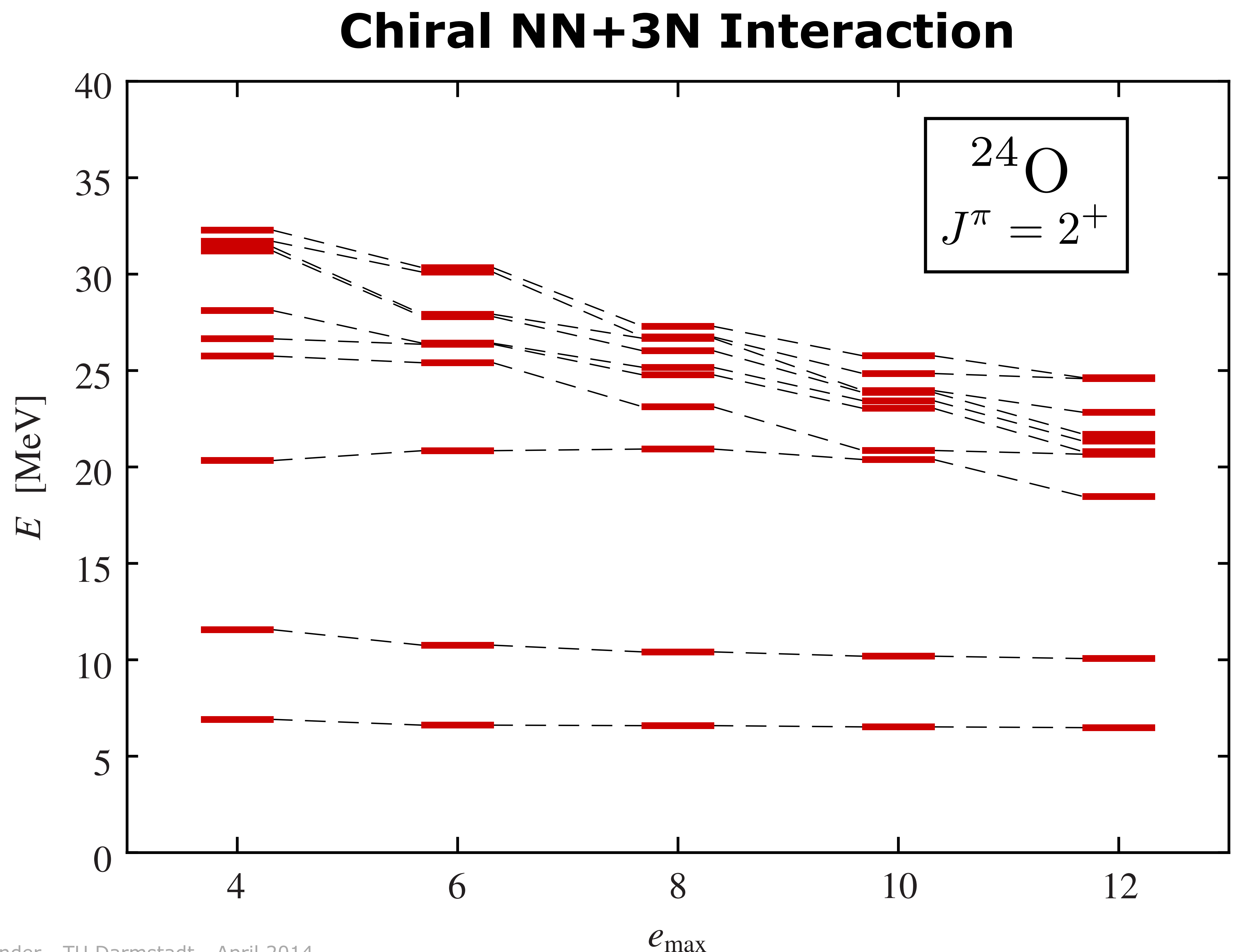
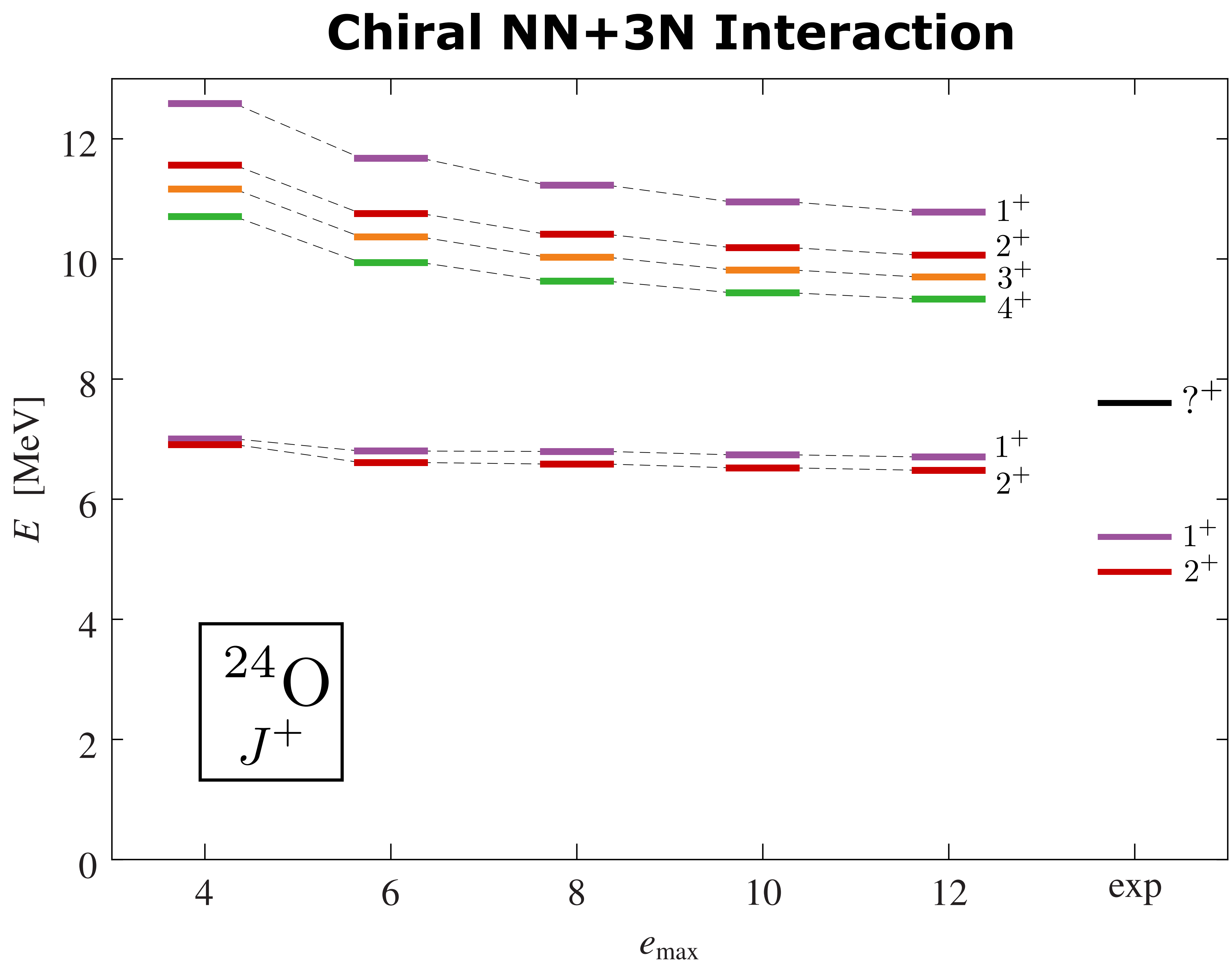
- Solve **non-Hermitean** eigenvalue problem

$$\left(\hat{\mathcal{H}}^{(\mathrm{CCSD})} \, \hat{\mathfrak{R}}_\mu \right)_c |\Phi_0\rangle = \omega_\mu \, \hat{\mathfrak{R}}_\mu \, |\Phi_0\rangle$$

^{24}O Spectrum from Coupled Cluster



^{24}O: Low-Lying Positive-Parity States



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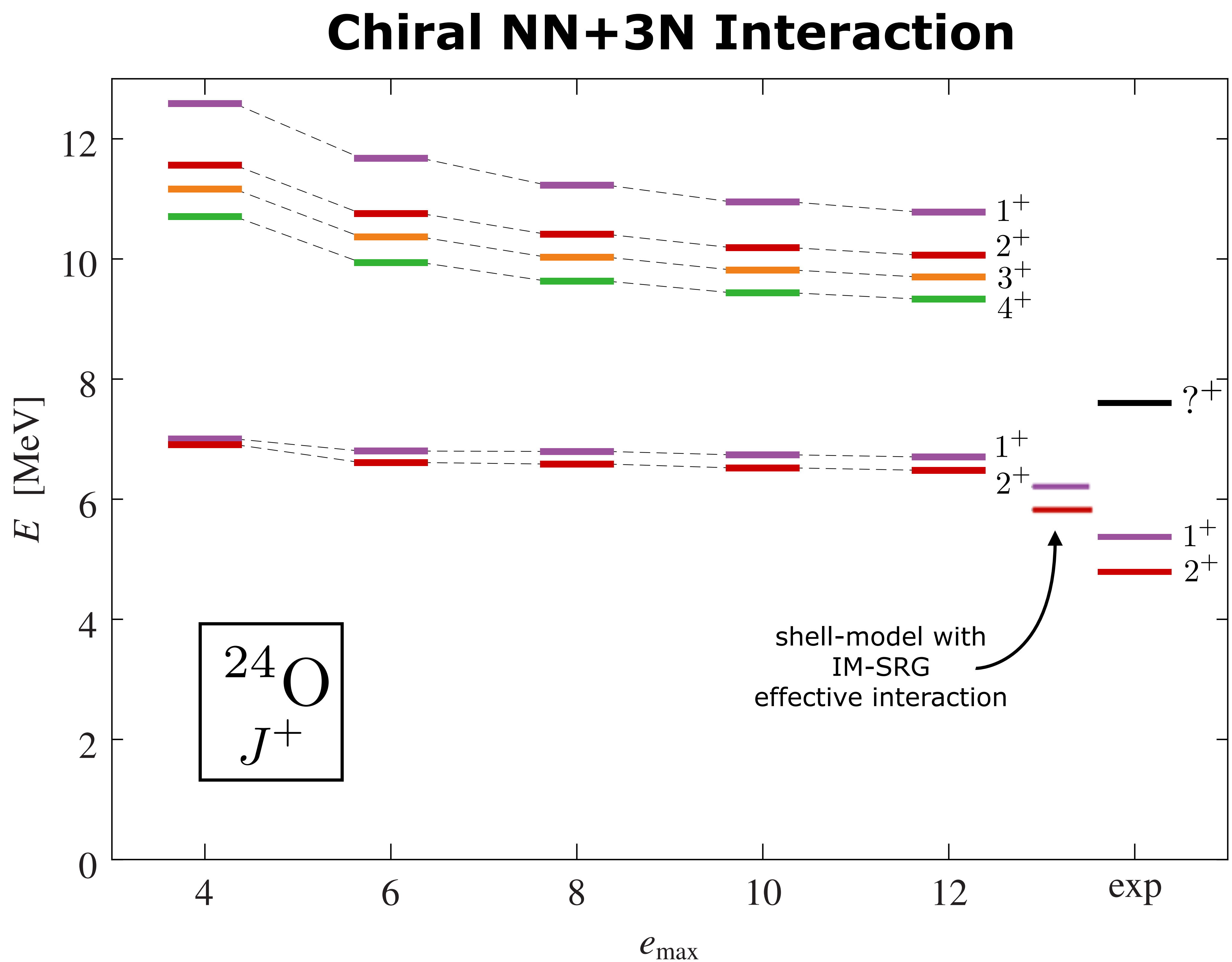

Publications

PRL 107, 072501 (2011) PHYSICAL REVIEW LETTERS week ending 12 AUGUST 2011

Similarity-Transformed Chiral $NN + 3N$ Interactions for the *Ab Initio* Description of ^{12}C and ^{16}O

Robert Roth,[1,*] Joachim Langhammer,[1] Angelo Calci,[1] Sven Binder,[1] and Petr Navrátil[2,3]

PRL 109, 052501 (2012) PHYSICAL REVIEW LETTERS week ending 3 AUGUST 2012

Medium-Mass Nuclei with Normal-Ordered Chiral $NN + 3N$ Interactions

Robert Roth,[1,*] Sven Binder,[1] Klaus Vobig,[1] Angelo Calci,[1] Joachim Langhammer,[1] and Petr Navrátil[2]

PHYSICAL REVIEW C 87, 021303(R) (2013)

***Ab initio* calculations of medium-mass nuclei with explicit chiral $3N$ interactions**

Sven Binder,[1,*] Joachim Langhammer,[1] Angelo Calci,[1] Petr Navrátil,[2] and Robert Roth[1]

PHYSICAL REVIEW C 87, 034307 (2013)

In-medium similarity renormalization group with chiral two- plus three-nucleon interactions

H. Hergert,[1,*] S. K. Bogner,[2] S. Binder,[3] A. Calci,[3] J. Langhammer,[3] R. Roth,[3] and A. Schwenk[3,4]

PRL 110, 242501 (2013) PHYSICAL REVIEW LETTERS week ending 14 JUNE 2013

***Ab Initio* Calculations of Even Oxygen Isotopes with Chiral Two-Plus-Three-Nucleon Interactions**

H. Hergert,[1,*] S. Binder,[2] A. Calci,[2] J. Langhammer,[2] and R. Roth[2]

PHYSICAL REVIEW C 88, 054319 (2013)

Extension of coupled-cluster theory with a noniterative treatment of connected triply excited clusters to three-body Hamiltonians

Sven Binder,[1,*] Piotr Piecuch,[2,†] Angelo Calci,[1,‡] Joachim Langhammer,[1,§] Petr Navrátil,[3,||] and Robert Roth[1,¶]

Evolved Chiral NN+3N Hamiltonians for Ab Initio Nuclear Structure Calculations

Robert Roth,[*] Angelo Calci,[†] Joachim Langhammer,[‡] and Sven Binder[§]

submitted to Phys. Rev. C

Nonperturbative shell-model interactions from the in-medium similarity renormalization group

S. K. Bogner,[1,*] H. Hergert,[2,†] J. D. Holt,[3,4,1,‡] A. Schwenk,[3,4,§] S. Binder,[4] A. Calci,[4] J. Langhammer,[4] and R. Roth[4]

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In-mediu… …ractions

PRL … …ding 2013

Thanks for your attention!

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