Recent advances using coupled-cluster theory under NUCLEI

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SciDAC Scientific Discovery through Advanced Computing

NUCLEI Nuclear Computational Low-Energy Initiative

Outline

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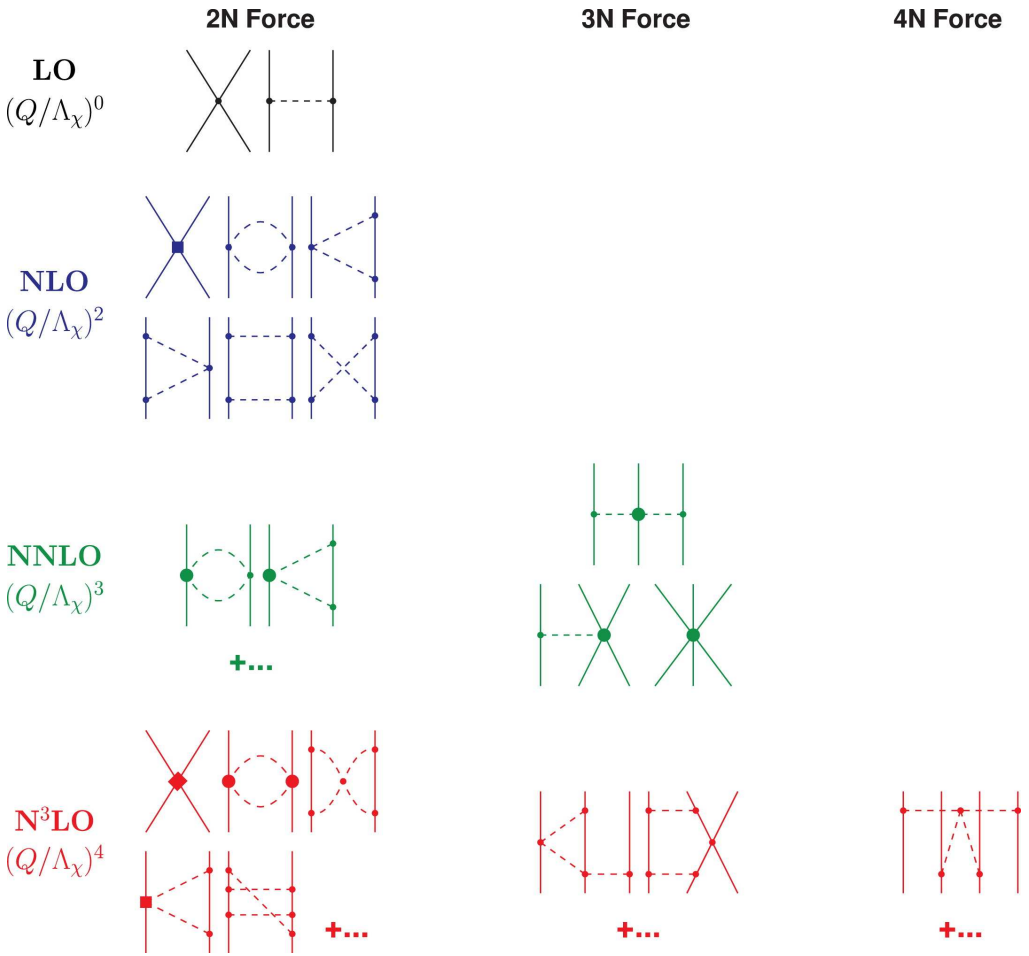
Chiral effective field theory

D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)



- Direct link to QCD.
- Perturbative expansion in momentum.
- Chiral symmetry is spontaneously and explicitly broken.
- The hierarchy of nuclear forces unfolds automatically.

Threebody forces: The way forward

The threebody force

- Chiral interaction at N^2LO.
- Jan Andreas Ekström (UiO, MSU).
- $N_{max} = 40+$ for triangular model space.
- Parallelized using MPI and scales to thousands of processes.

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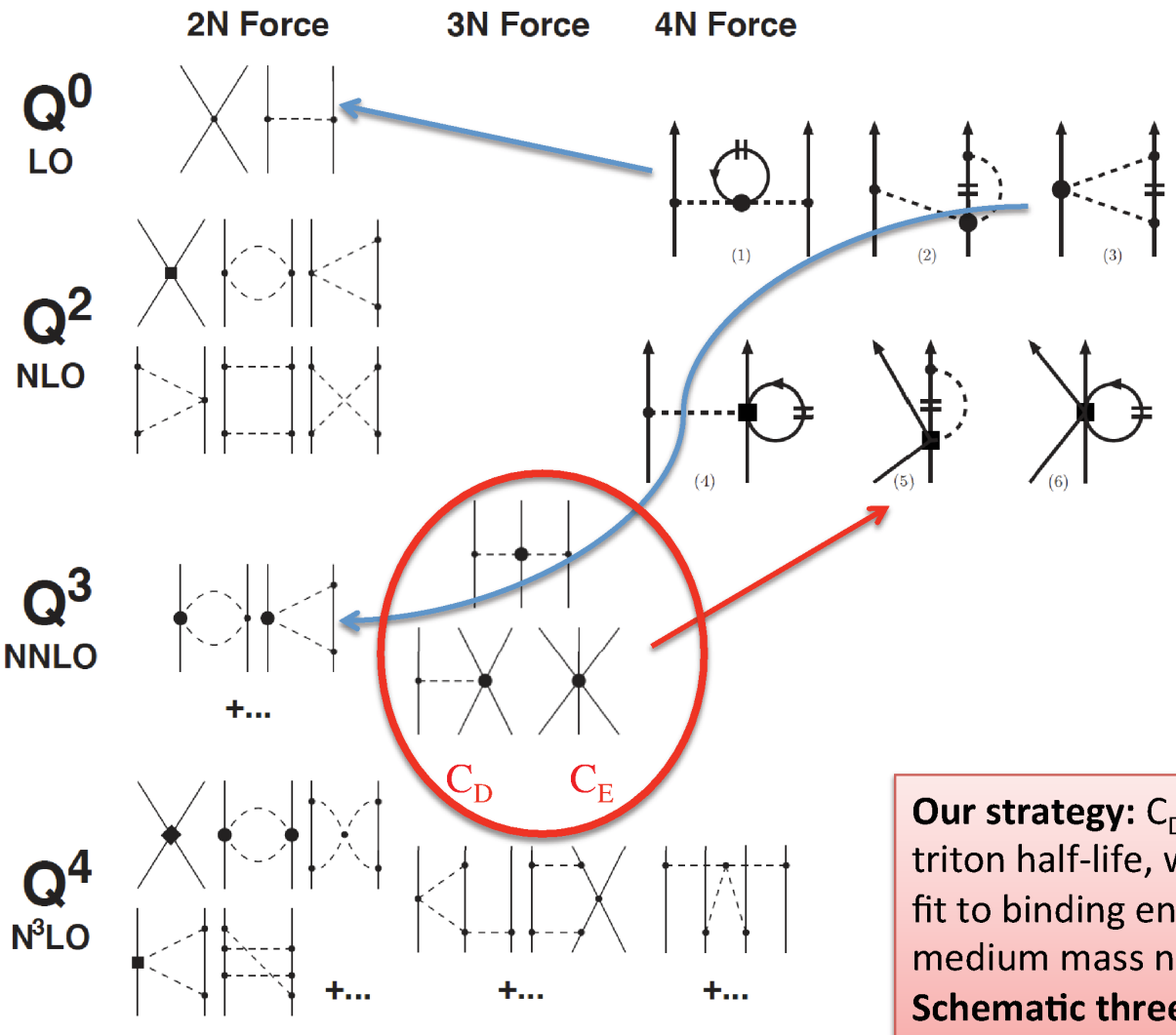
- Done with NNLO, working on N3LO.

Density dependent chiral threebody force



Integrating over the third leg in infinite nuclear matter and derive density dependent corrections to the nucleon-nucleon interaction.
J. W. Holt N. Kaiser and W. Weise. Phys.Rev.C 79, 054331 (2009)
K. Hebeler and A. Schwenk (2010)

Our strategy: C_D is given by fit to triton half-life, we fix C_E and k_F from fit to binding energy in selected medium mass nuclei:
Schematic three-nucleon forces

Threebody forces: The way forward

Threebody force in lab coordinates

- Computationally intensive – exponential scaling.
- Need atleast $N_{max} = 16$. Currently at $N_{max} = 14$
- Similarity transformation – Sum over triple matrix products.
- Two strategies
  1. Generate elements on the fly (Titan).
  2. Stored transformation coefficients (Beacon).

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- Work in progress.

Threebody forces: The way forward

Hartree-Fock with threebody forces

- Iteration with an extra three-body diagram.
- Transform matrix elements to Hartree-Fock basis.
- Similarity transformation coded as a triple matrix product.
- Can be done independantly for each block of conserved quantum numbers.
- Will put you in a square model space, even if you started from a triangular model space.

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- Done.

Normal-ordered Hamiltonian

$$\hat{\mathrm{H}} = E_0 + \hat{\mathrm{F}}_N + \hat{\mathrm{V}}_N + \hat{\mathrm{G}}_N$$

$$E_0 = \sum_i \langle i|\hat{\mathrm{t}}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\hat{\mathrm{v}}|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|\hat{\mathrm{v}}_3|ijk\rangle$$

$$\hat{\mathrm{F}}_N = \sum_{pq}\left(\langle p|\hat{\mathrm{t}}|q\rangle + \sum_i\langle pi|\hat{\mathrm{v}}|qi\rangle + \frac{1}{2}\sum_{ij}\langle ijp|\hat{\mathrm{v}}_3|ijq\rangle\right)\left\{a_p^\dagger a_q\right\}$$

$$\hat{\mathrm{V}}_N = \frac{1}{4}\sum_{pqrs}\left(\langle pq|\hat{\mathrm{v}}|rs\rangle + \sum_i\langle ipq|\hat{\mathrm{v}}_3|irs\rangle\right)\left\{a_p^\dagger a_q^\dagger a_s a_r\right\}$$

$$\hat{\mathrm{G}}_N = \frac{1}{36}\sum_{\substack{pqr\\stu}}\langle pqr|\hat{\mathrm{v}}_3|stu\rangle\left\{a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s\right\}$$

Threebody forces: The way forward

Coupled-cluster calculation for a closed core

- Huge storage requirements.
- An additional ≈ 900 diagrams for CCSDT.
- Computationally very intensive.
- Current implementation in m-scheme at CCSD level.
- Residual threebody elements needed for bare interaction.

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- Not done!.

Threebody forces: The way forward

Equation-of-motion

- Coupled-cluster creates a many-body effective interaction.
- Optimized for effective threebody operators that are built from twobody operators.
- If necessary, explicit threebody diagrams will be recoded.

Threebody forces: The way forward

Expectation values and transition probabilities

- No need for changes.

Preparing for Titan/Beacon

Coupled-cluster

- Large set of coupled non-linear equations.
- Solved iteratively by performing products of scalar tensor operators.
- Ideally programmed as matrix matrix products.
- Operators are j-coupled, but different diagrams require different coupling orders.
- Transformation between different coupling orders are also matrix operations.

Equation-of-motion

- Non-hermitian sparse eigenvalue problem.
- Solved iteratively by performing products of general spherical tensor operators.

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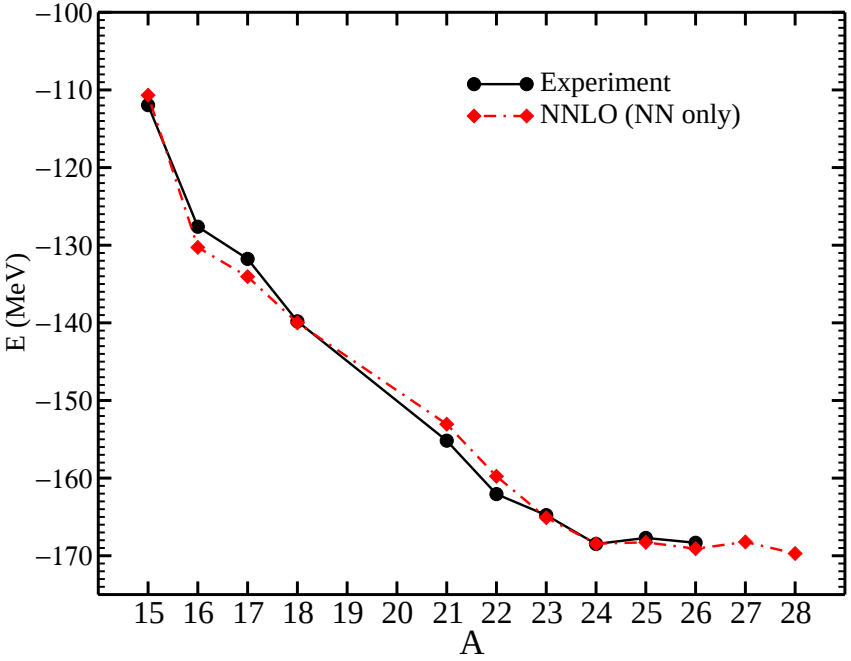
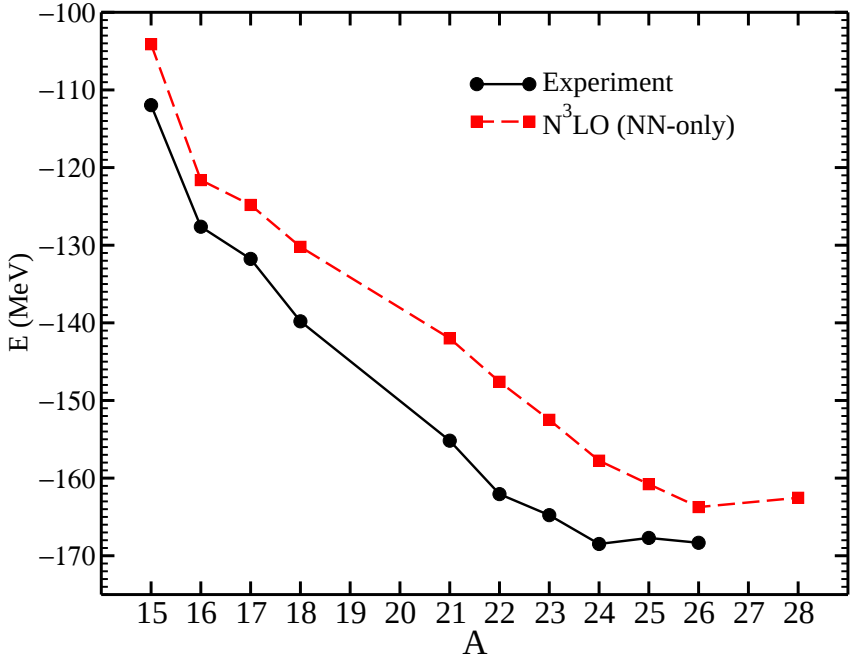
Strategy: Representing everything as matrix operations.

Outline

Oxygen binding energy





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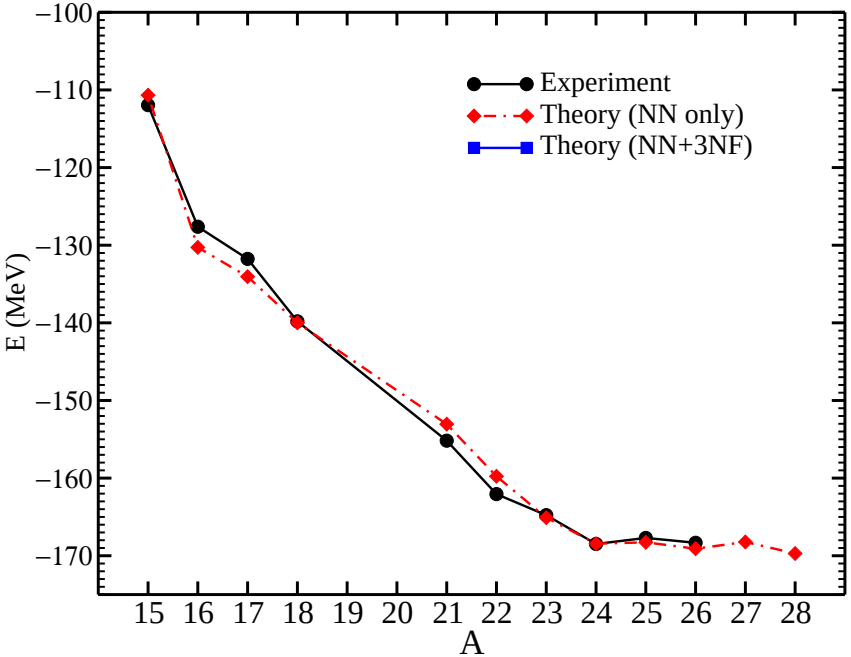
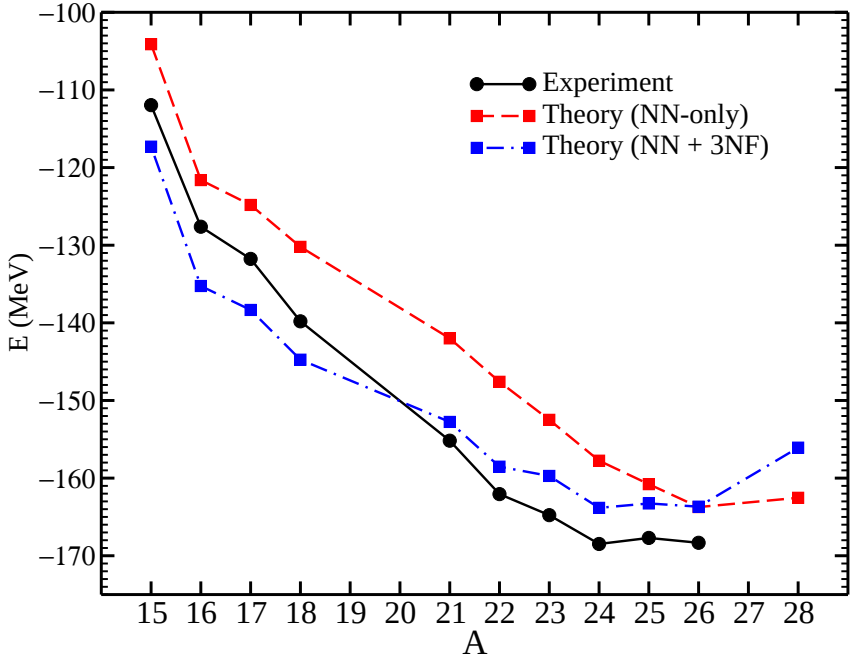
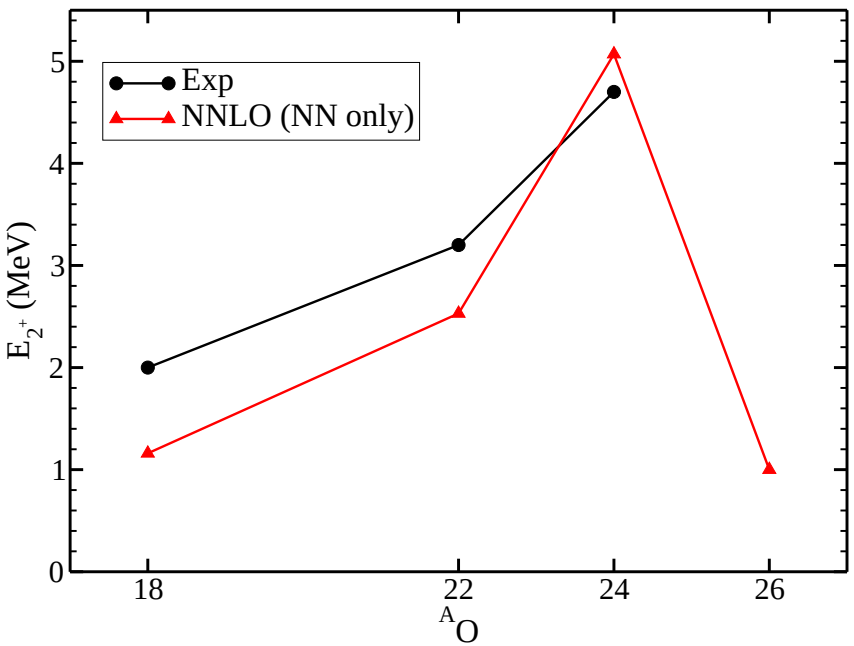
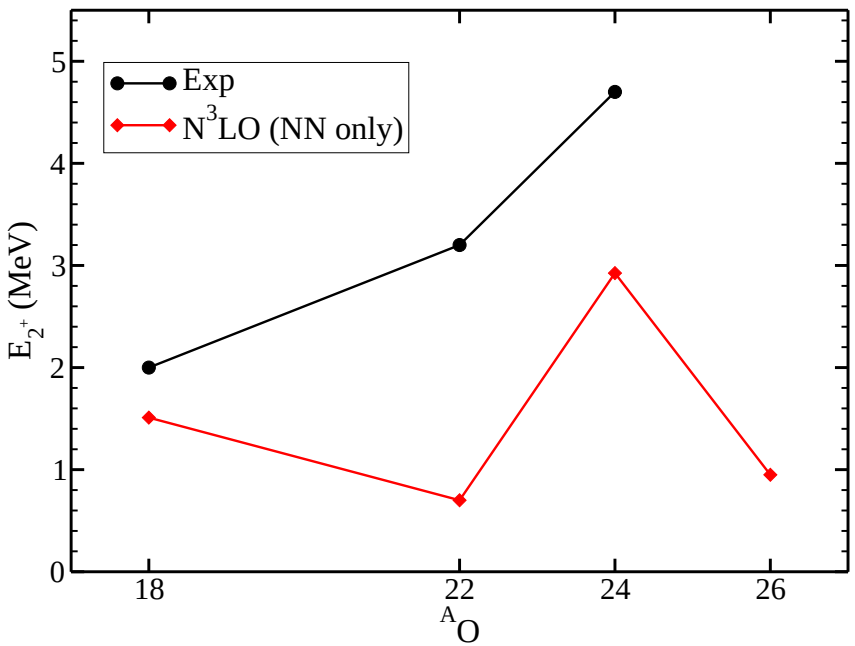




$J^\pi = 2^+$ systematics in oxygen isotopes

Preliminary





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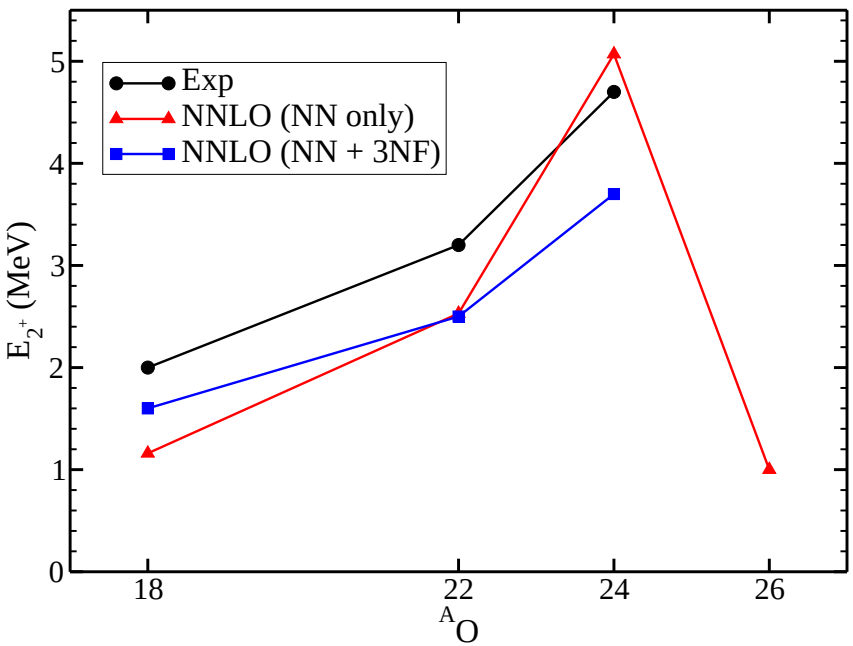

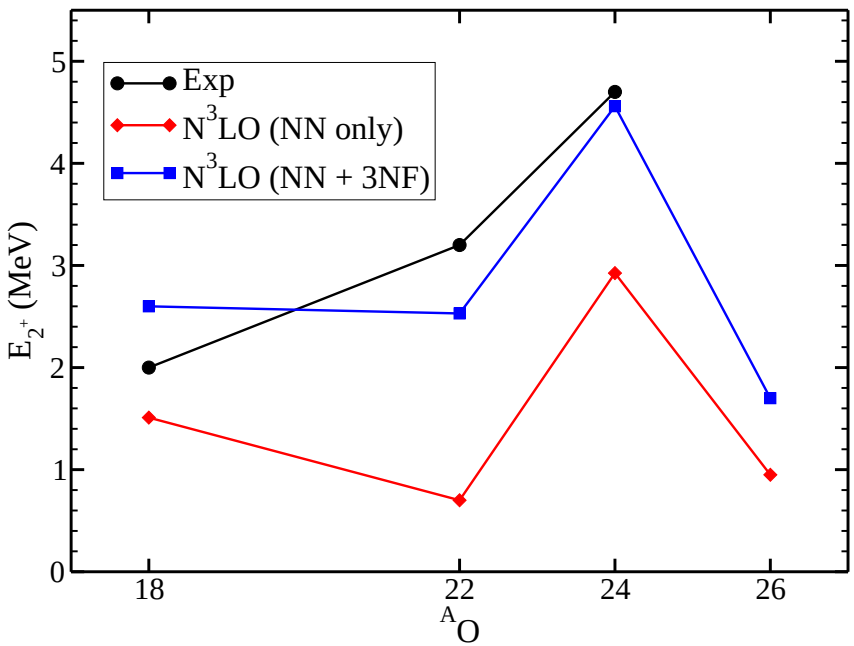

Calcium isotopes with NNLO (Optimized)

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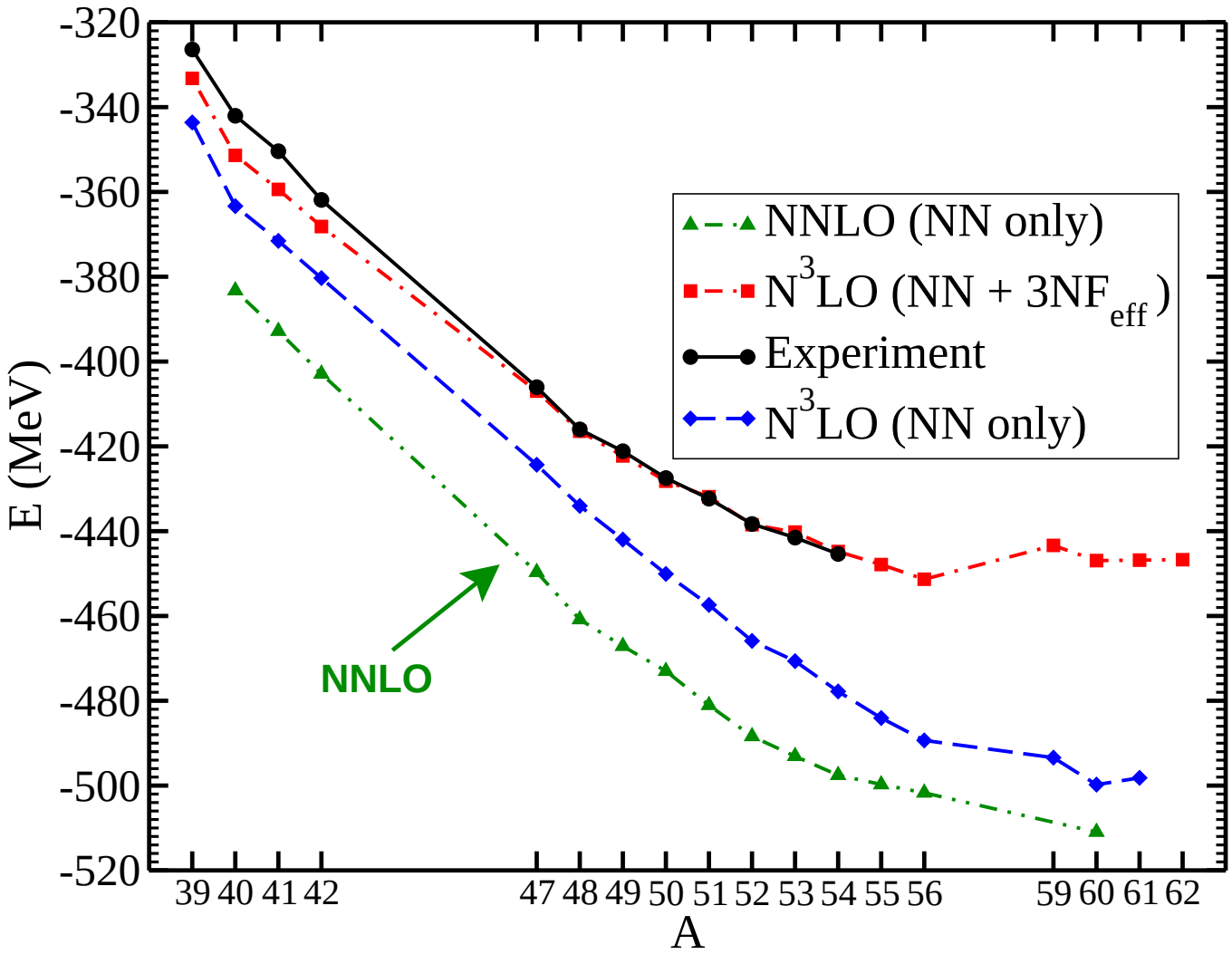

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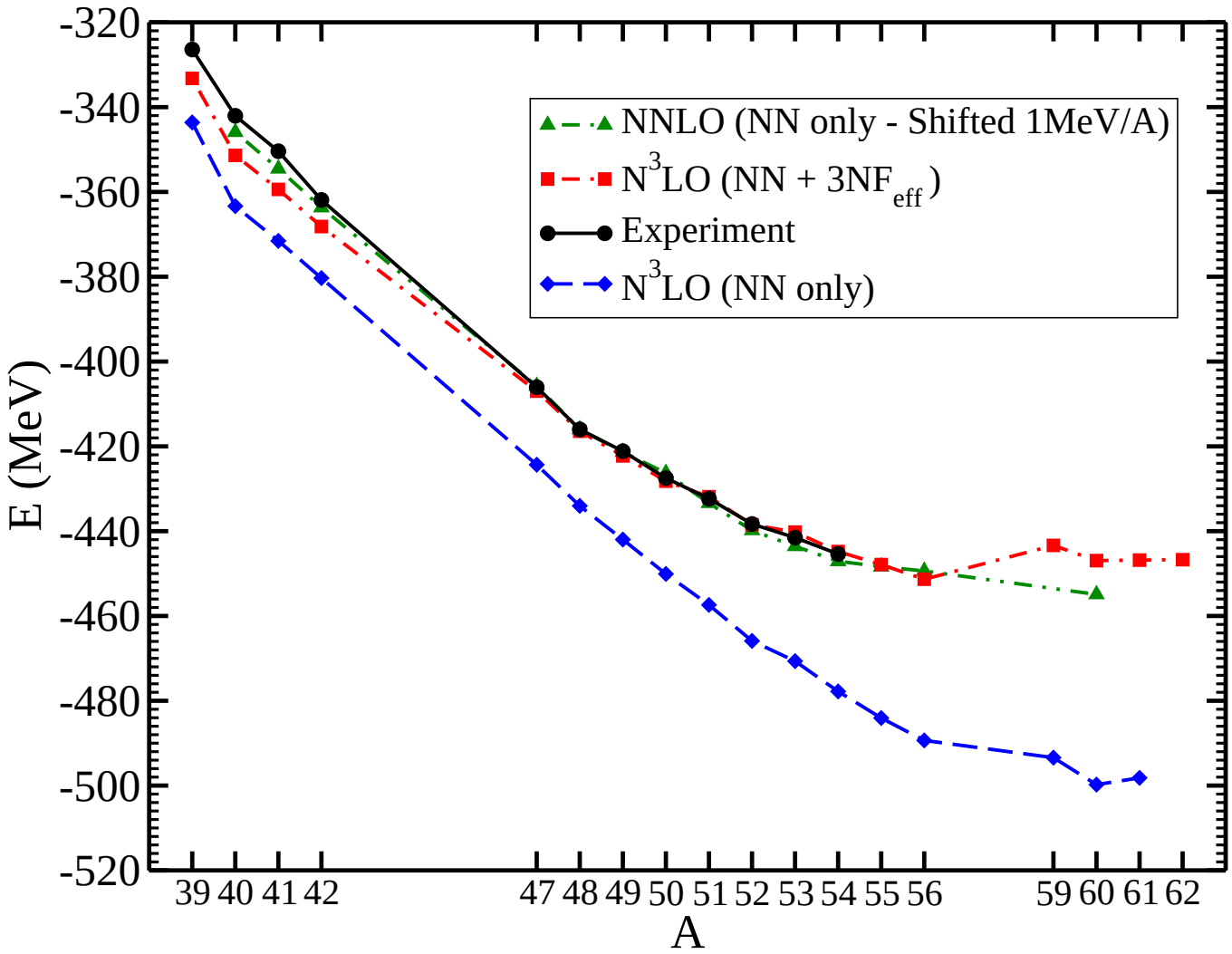

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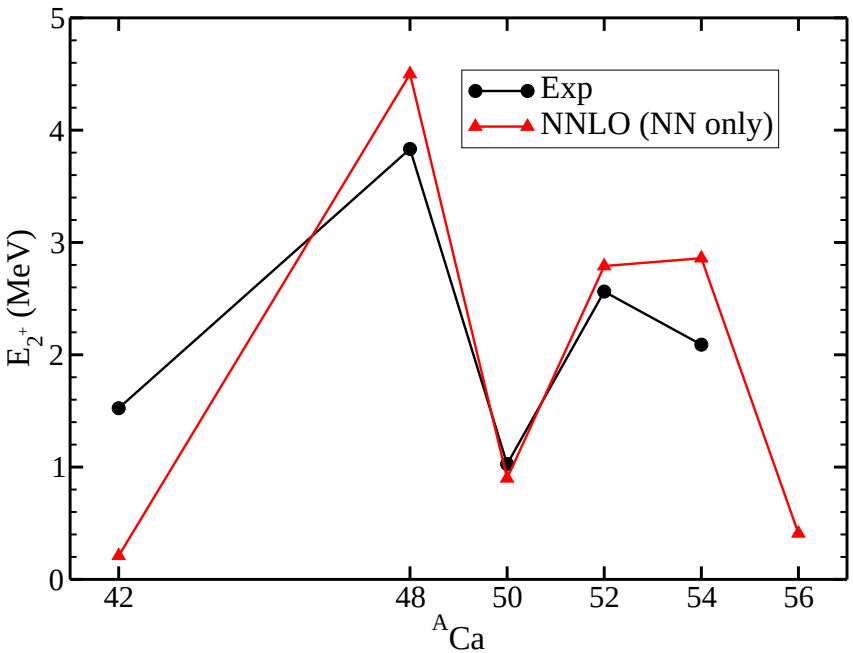

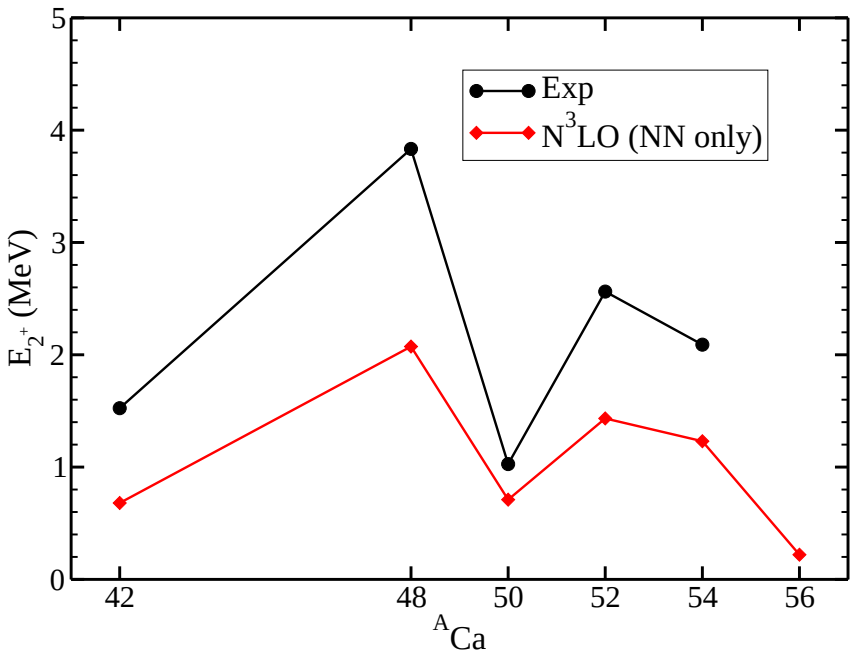

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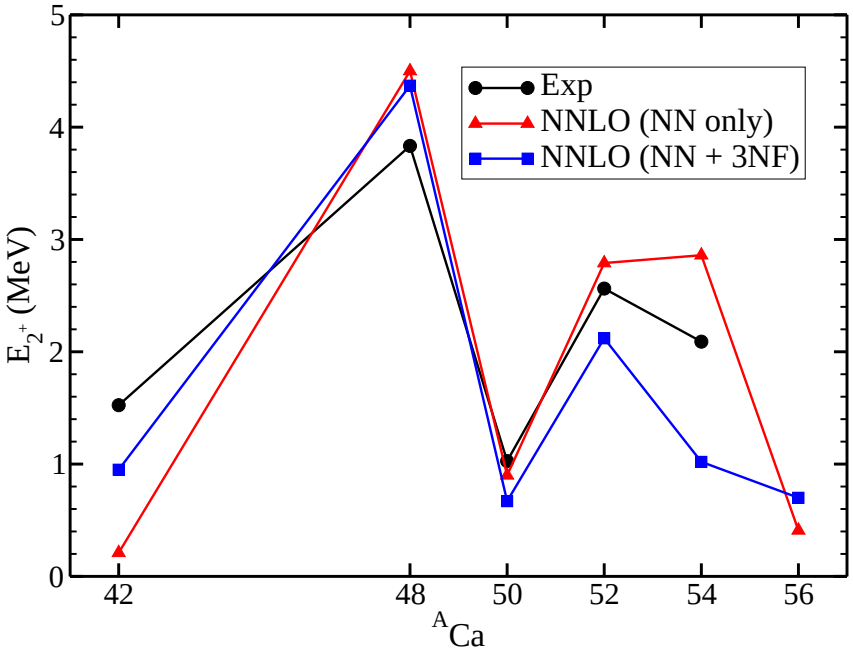

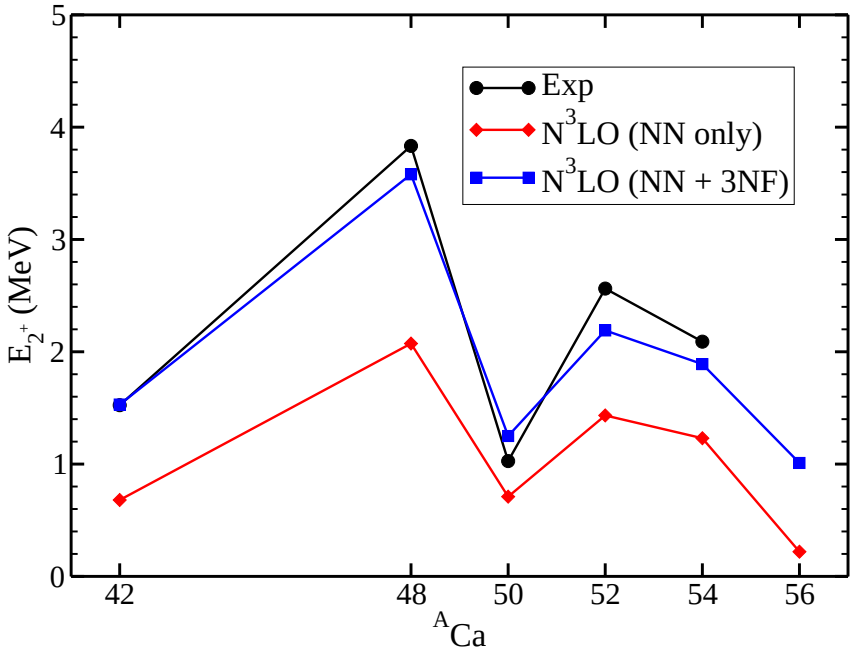

Questions?

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