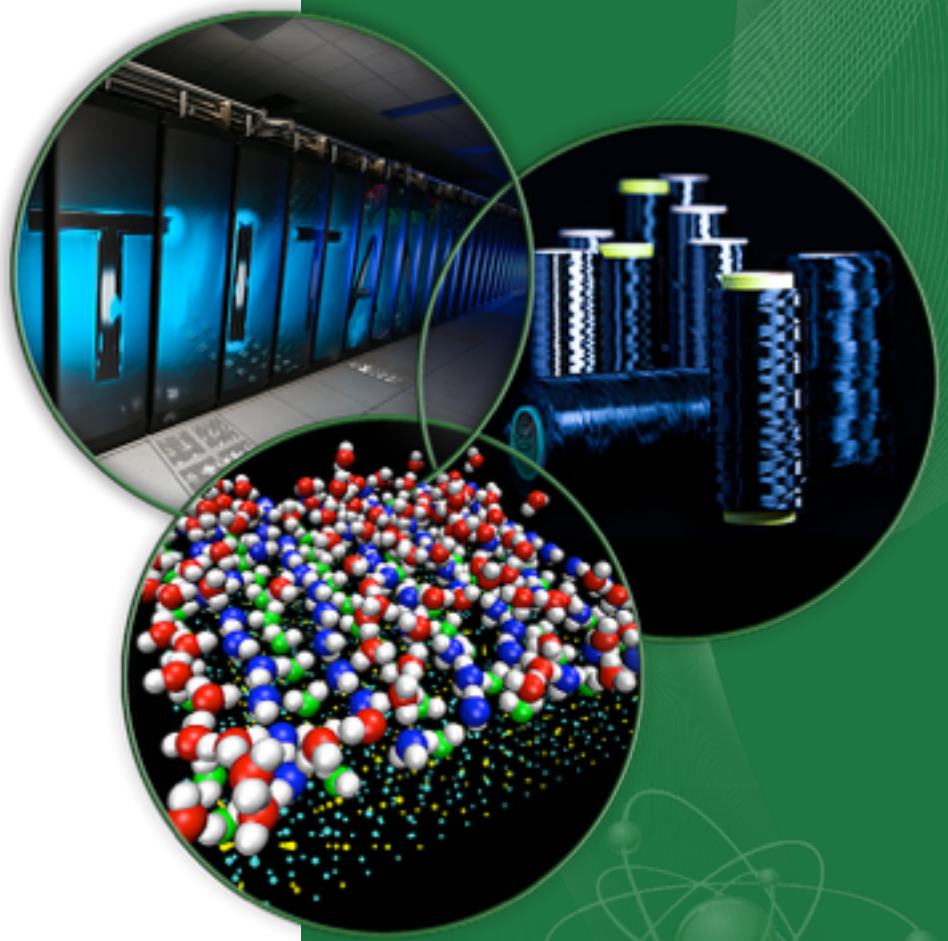
CCEI in Multiple Shells



Micah Schuster

Gustav Jansen

Gaute Hagen

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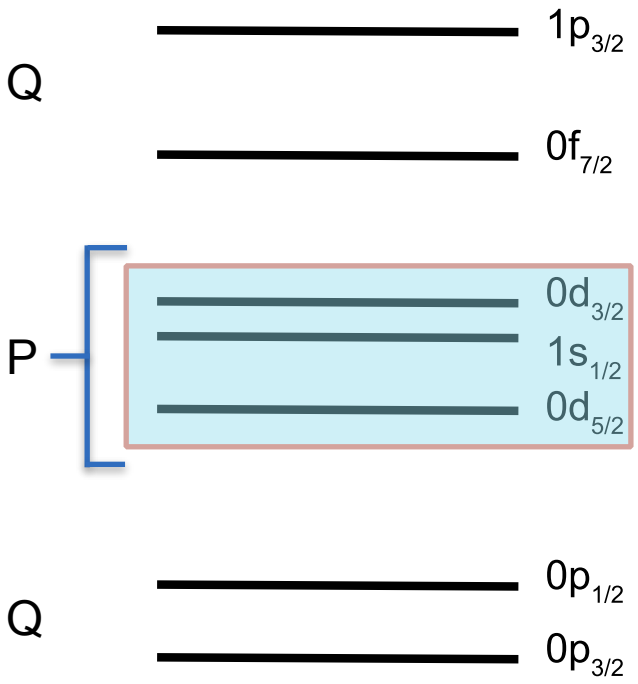
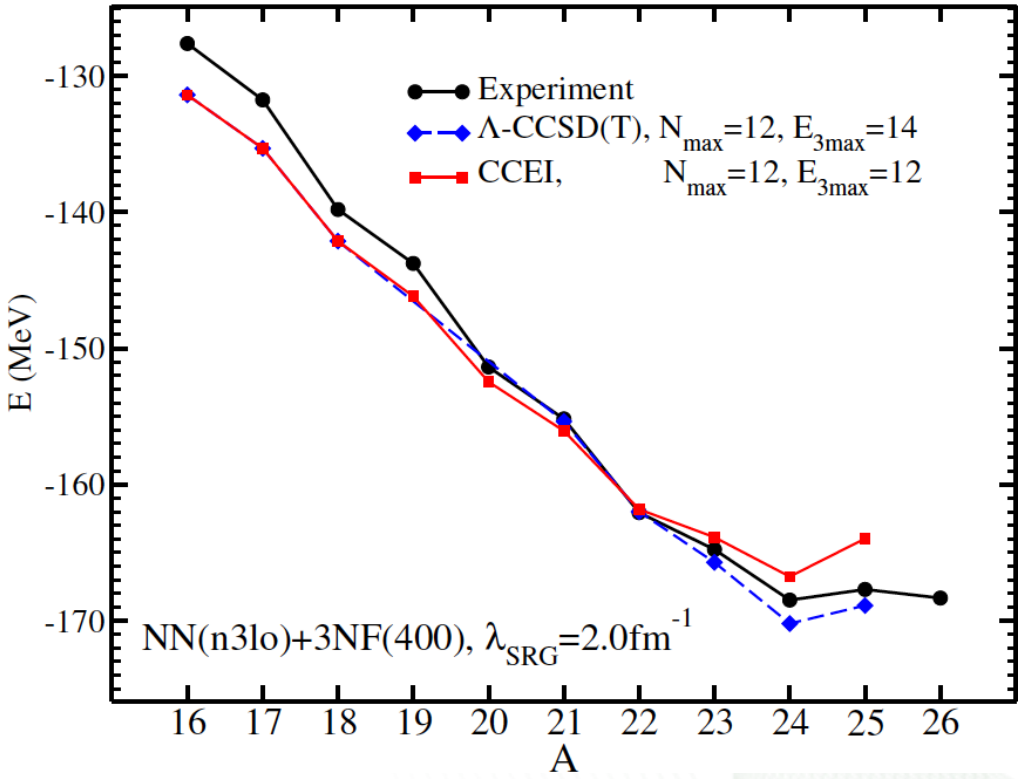
Coupled Cluster Effective Interaction

G. R. Jansen, J. Engel, G. Hagen, P. Navrátil, A. Signoracci, Phys. Rev. Lett. **113**, 142502 (2014).

- Start with chiral NN+3N.
- Solve for A, A+1 and A+2 using CC.
- Project A+1 and A+2 CC wave functions onto the sd-shell model space using Okubo-Lee-Suzuki.



Comparison between experiment, CCEI and "exact" coupled-cluster calculations with the inclusion of perturbative triples (Λ-CCSD(T)).



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A Look at Mass Dependence

- Multiple Ways to Compute CCEI:
  - A-dependent:

$$H_{\mathrm{CCEI}}^{\mathrm{eff}} = H_0^{A,A_c} + H_1^{A,A_c+1} + H_2^{A,A_c+2}$$

Λ-CCSD(T) EOM-CC-PA EOM-CC-2PA

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Λ-CCSD(T) EOM-CC-

G. R. Jansen, J. Engel, G. Hagan, P. Navrátil, A. Signoracci

Leads to one effective interaction per target nucleus.

Very time consuming!

A Look at Mass Dependence

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  - Fixed A:

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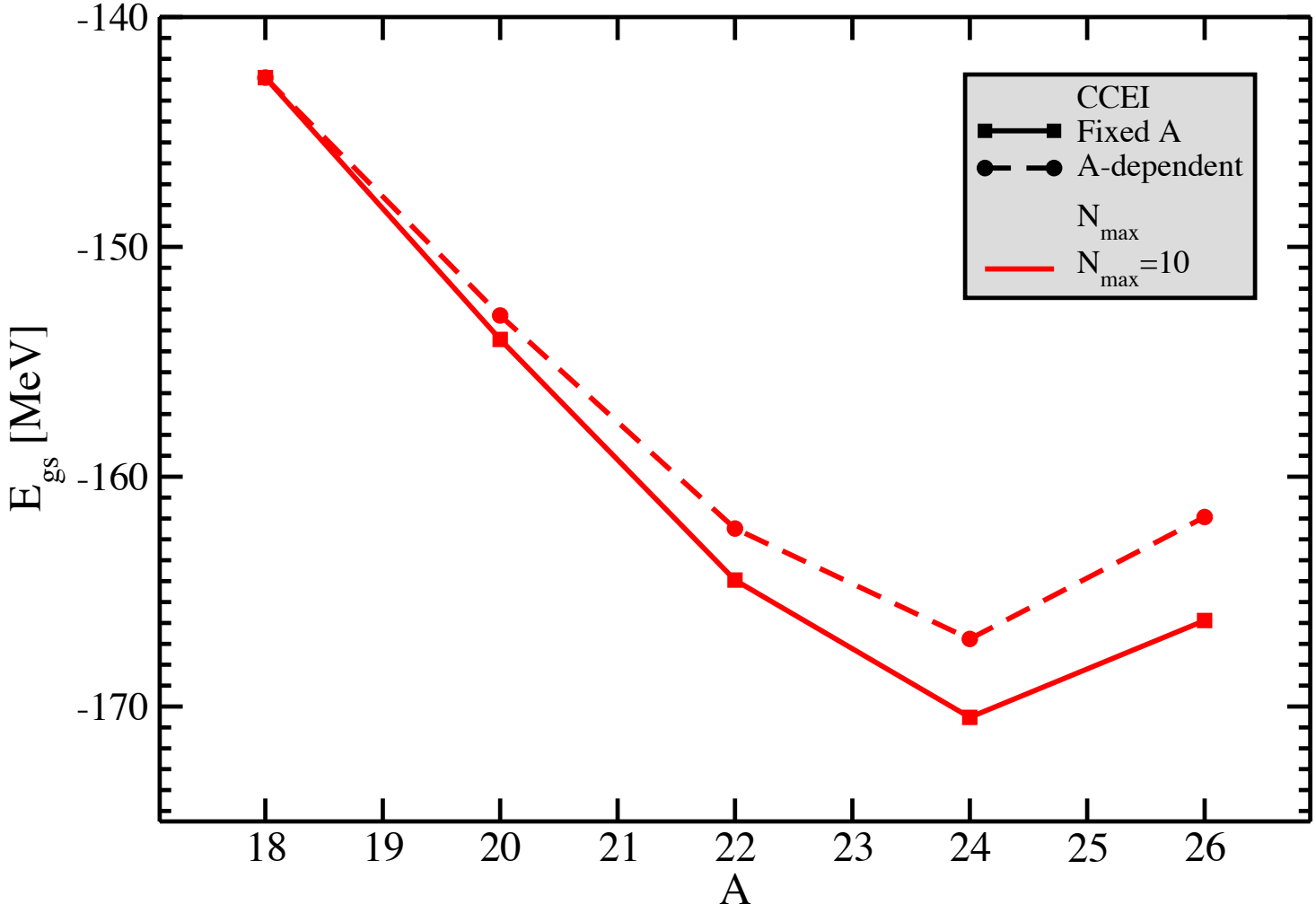

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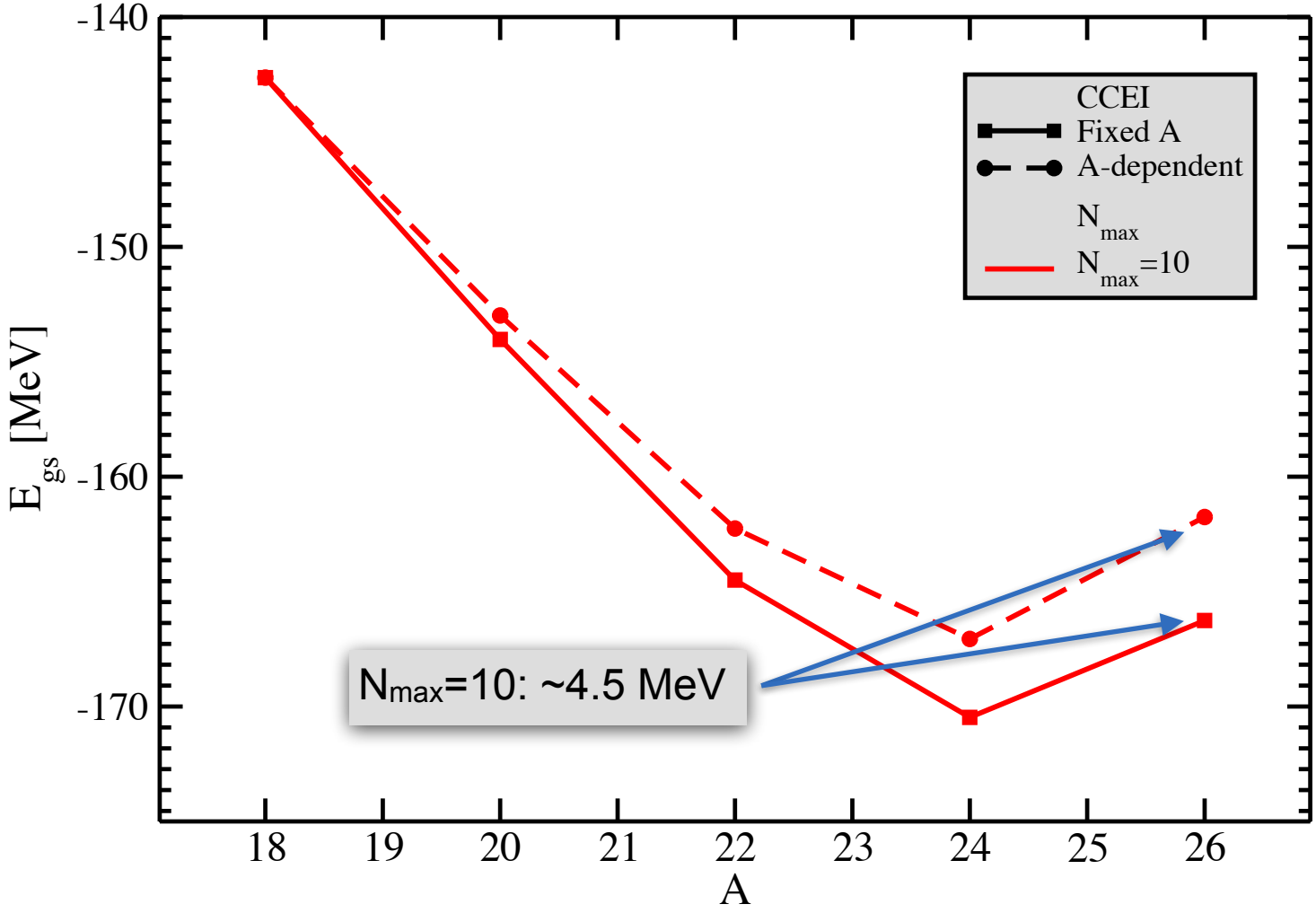

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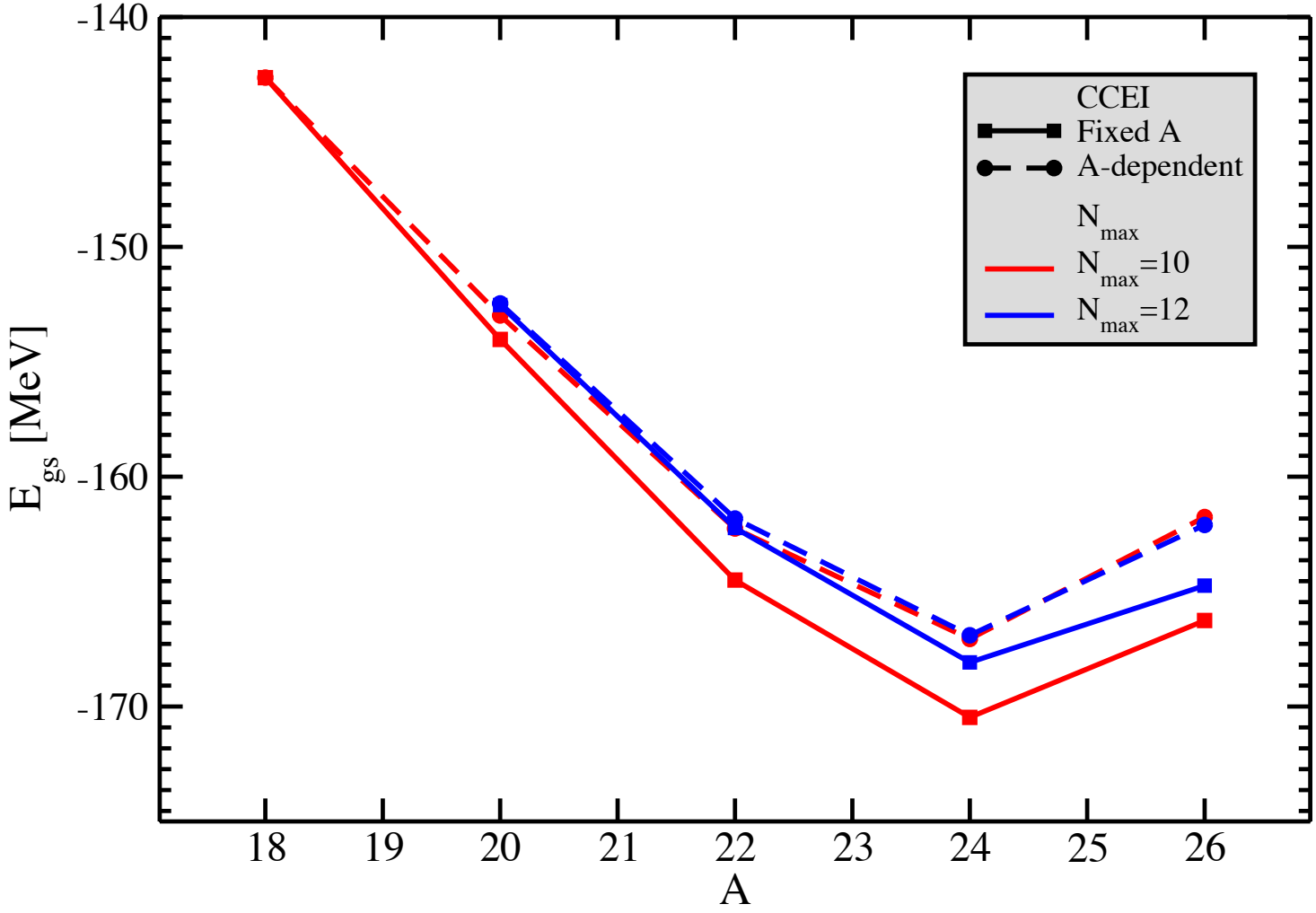

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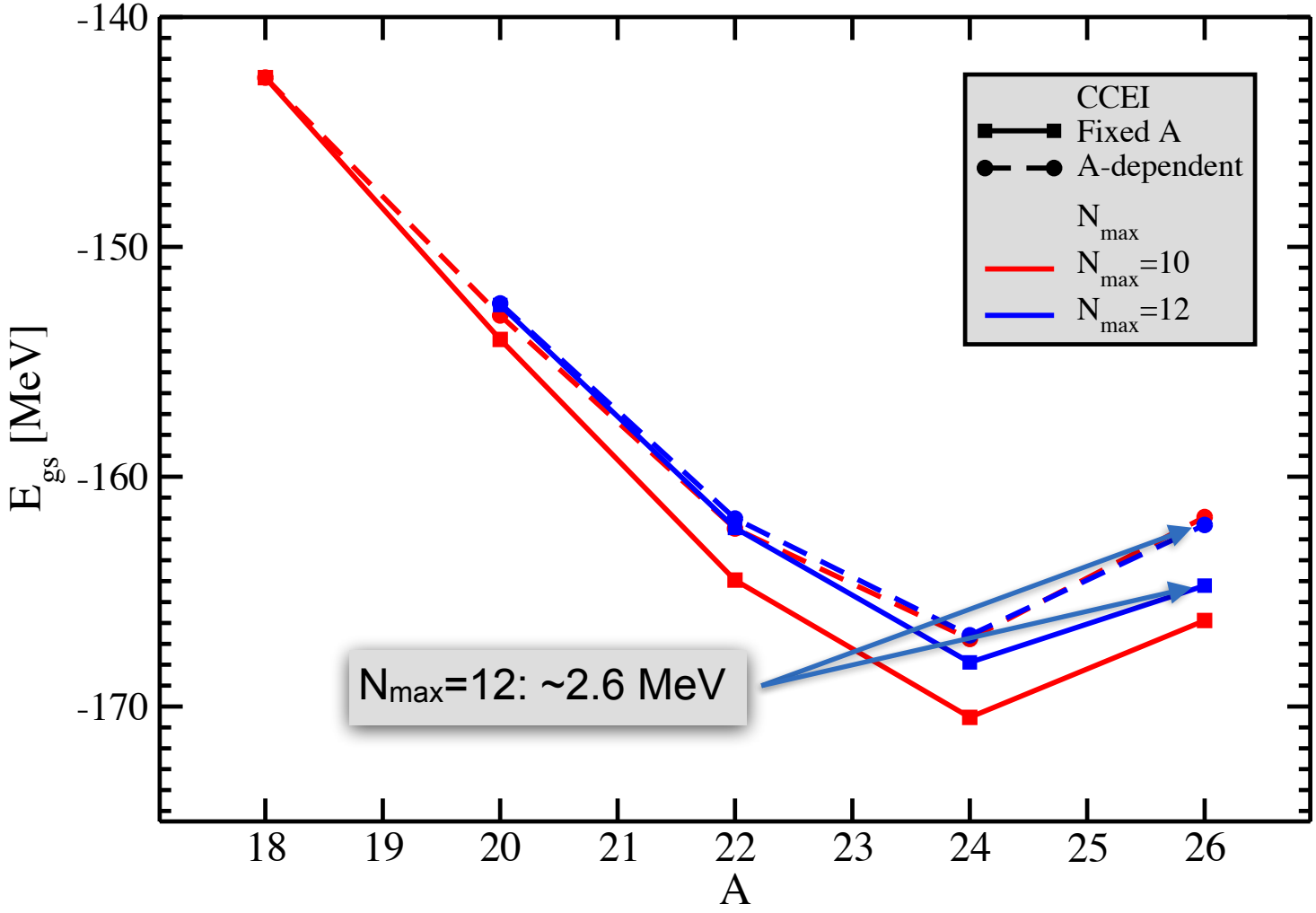

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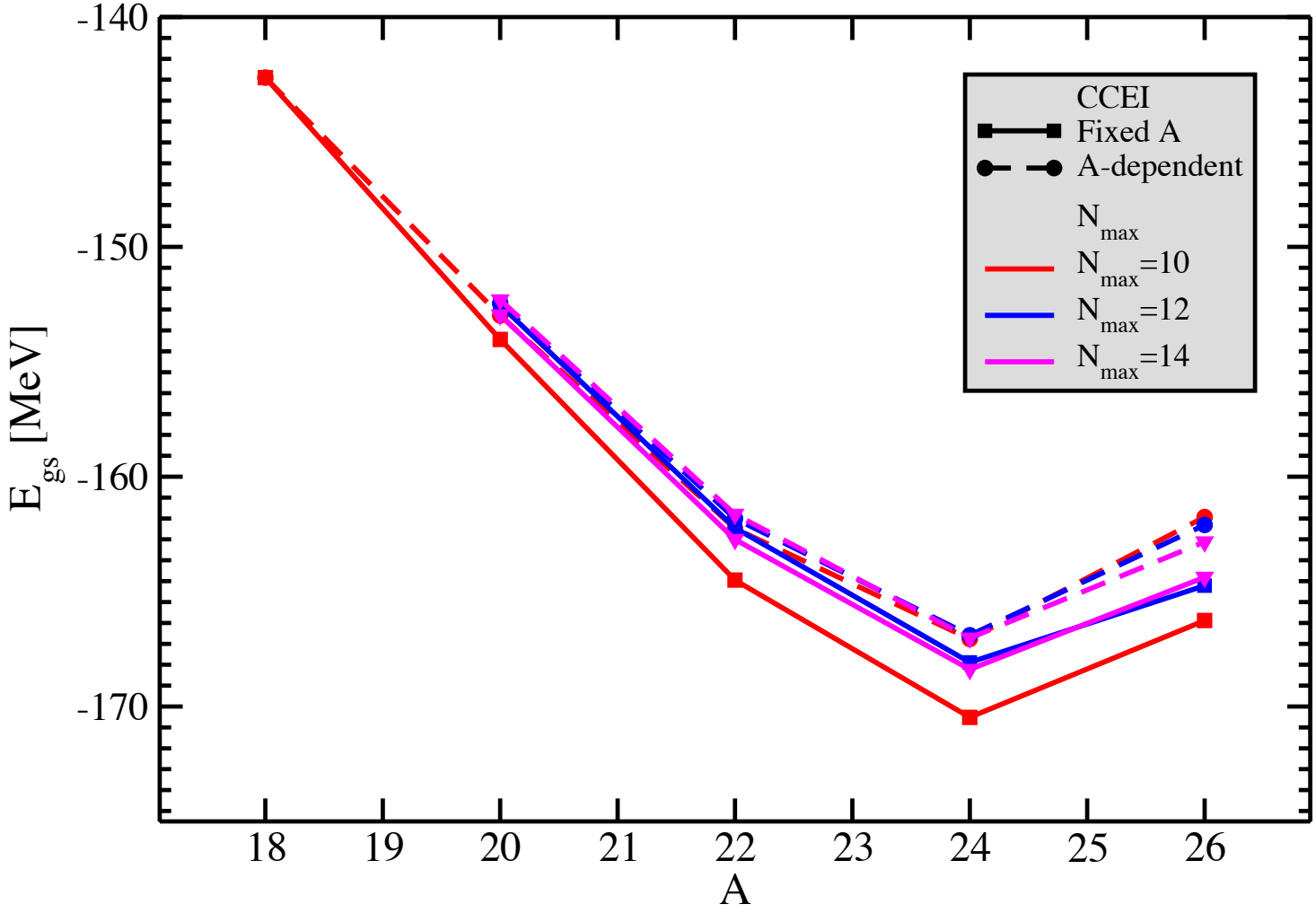

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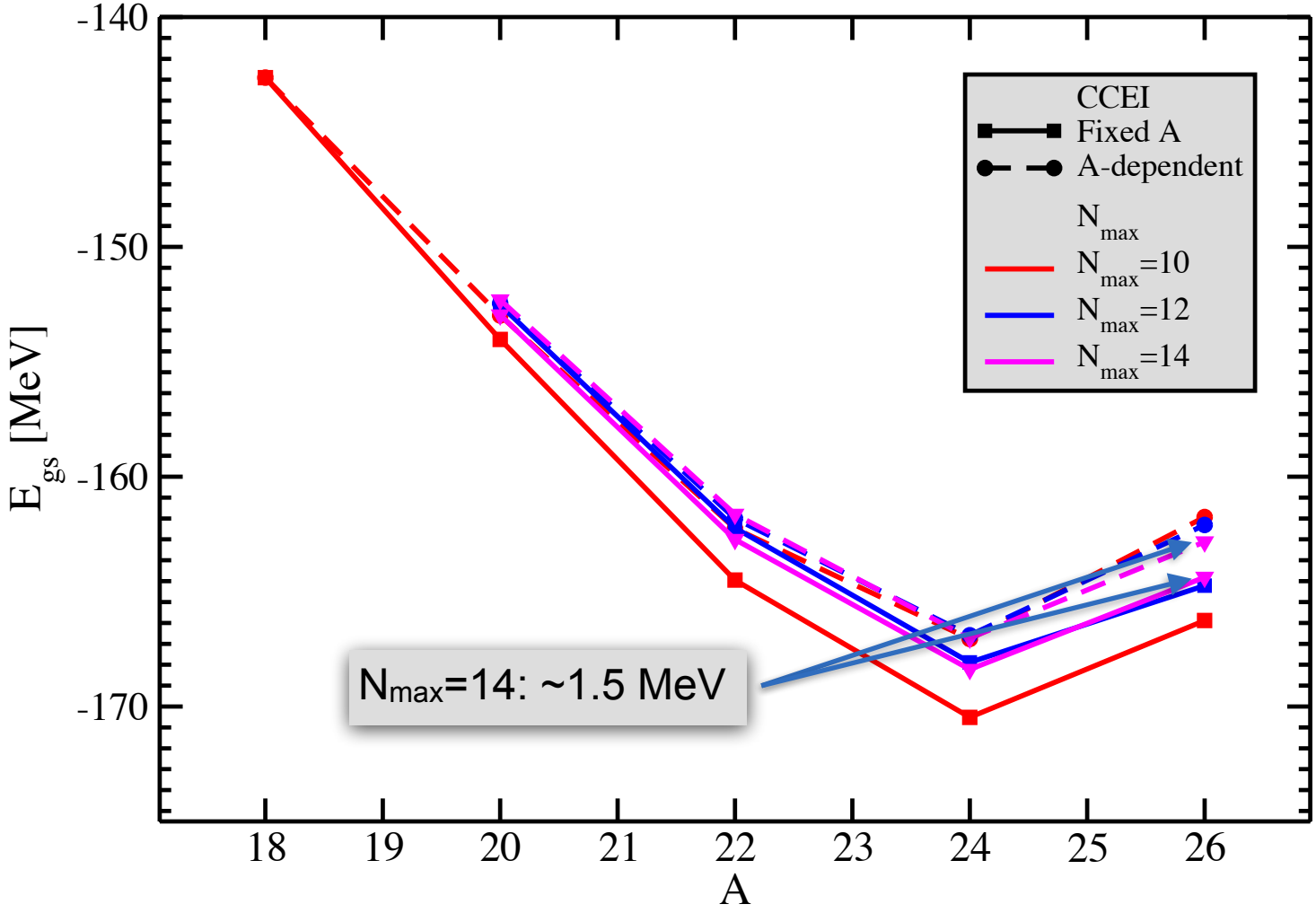

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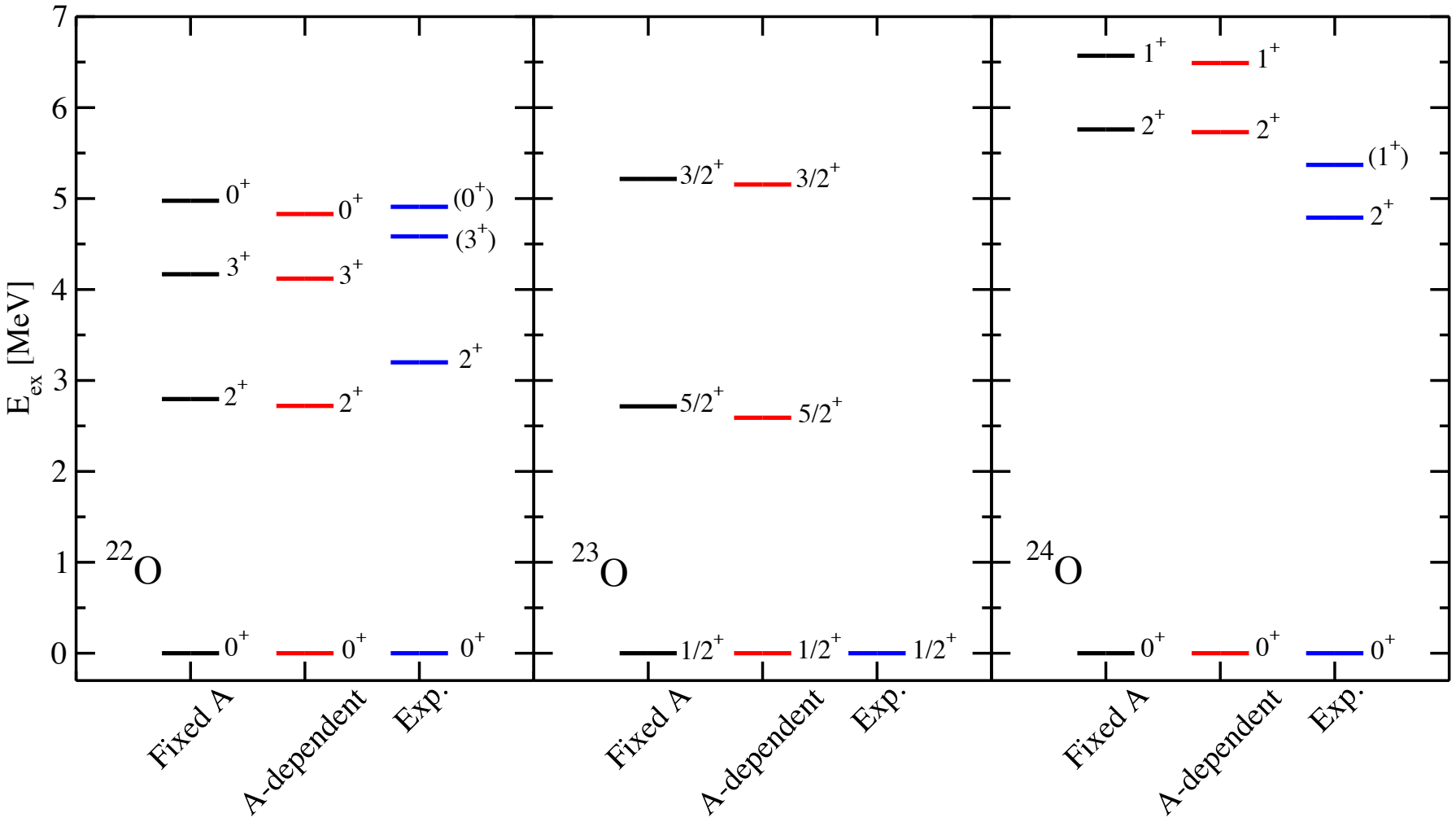

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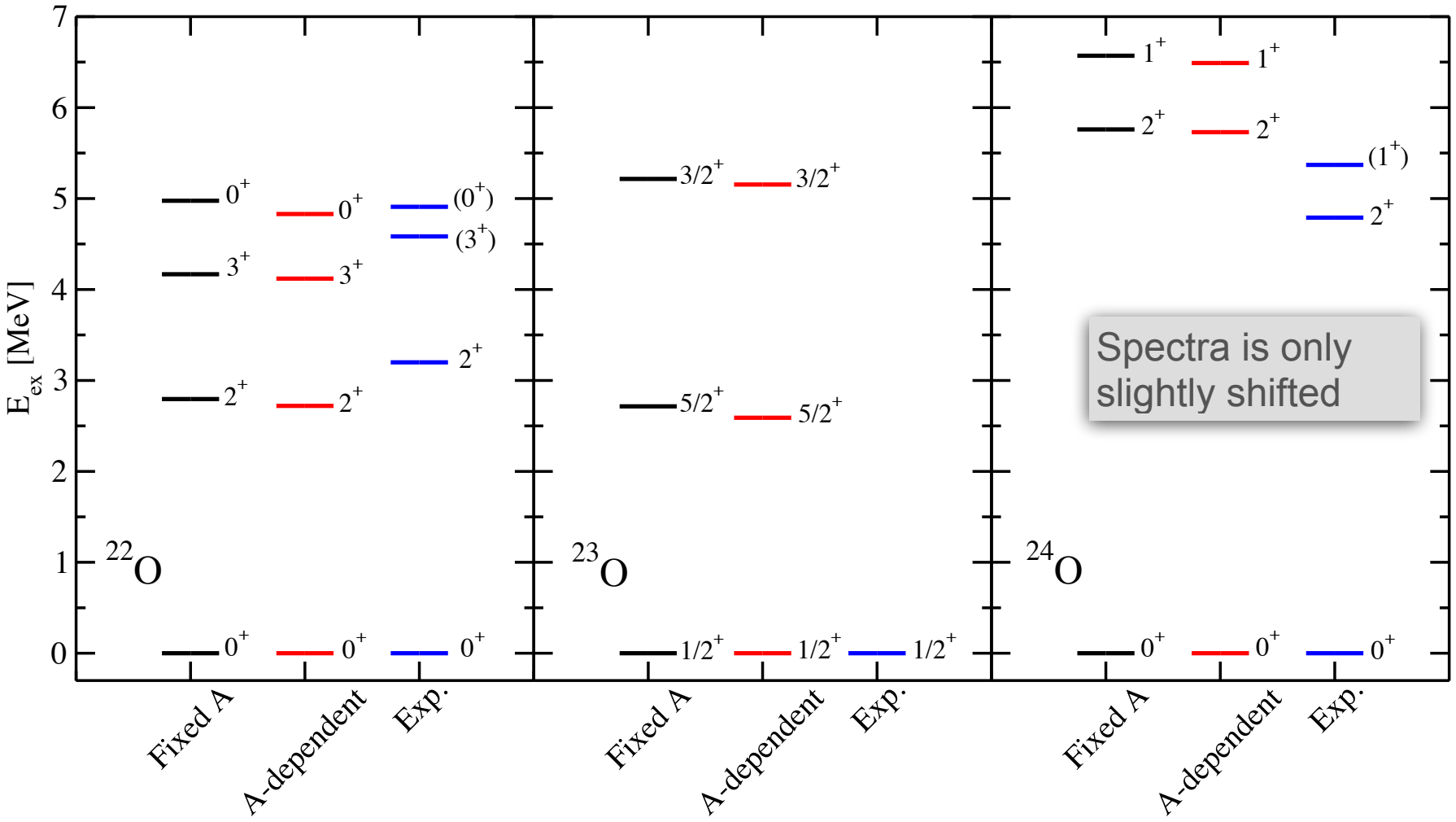

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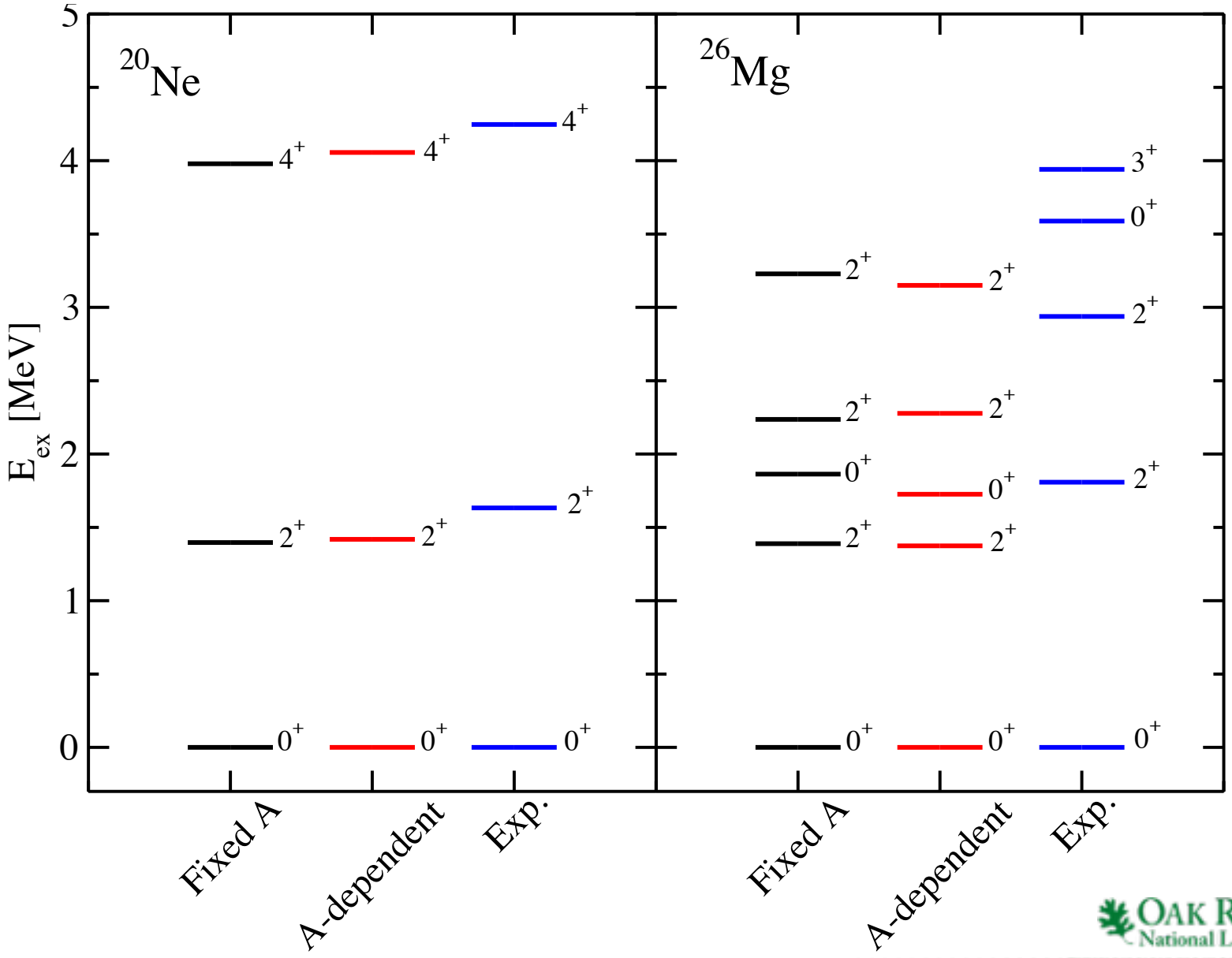

CCEI for Deformed Nuclei

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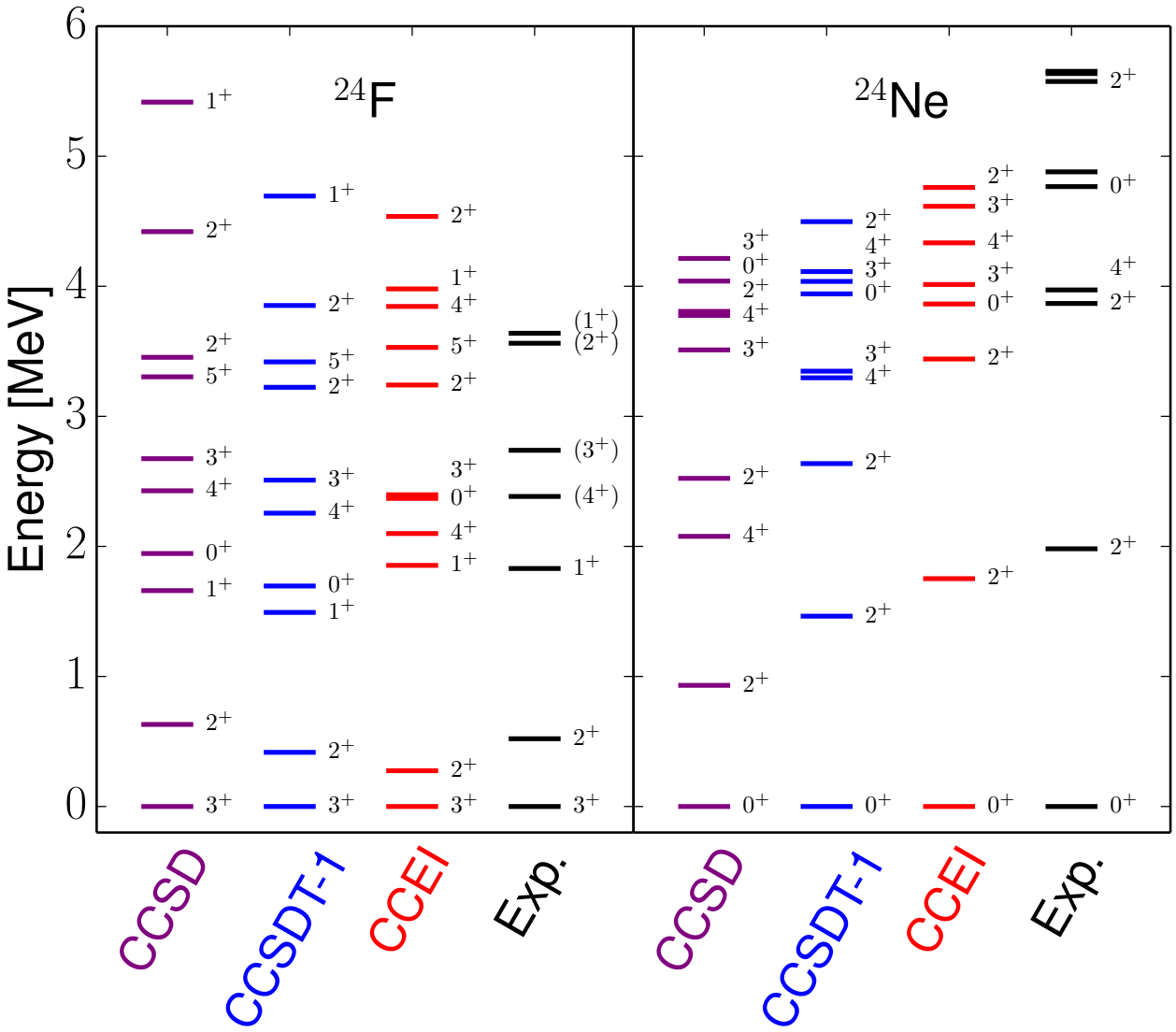

- Good agreement between EOM-CCSD, EOM-CCSDT-1 and CCEI in ^{24}F.

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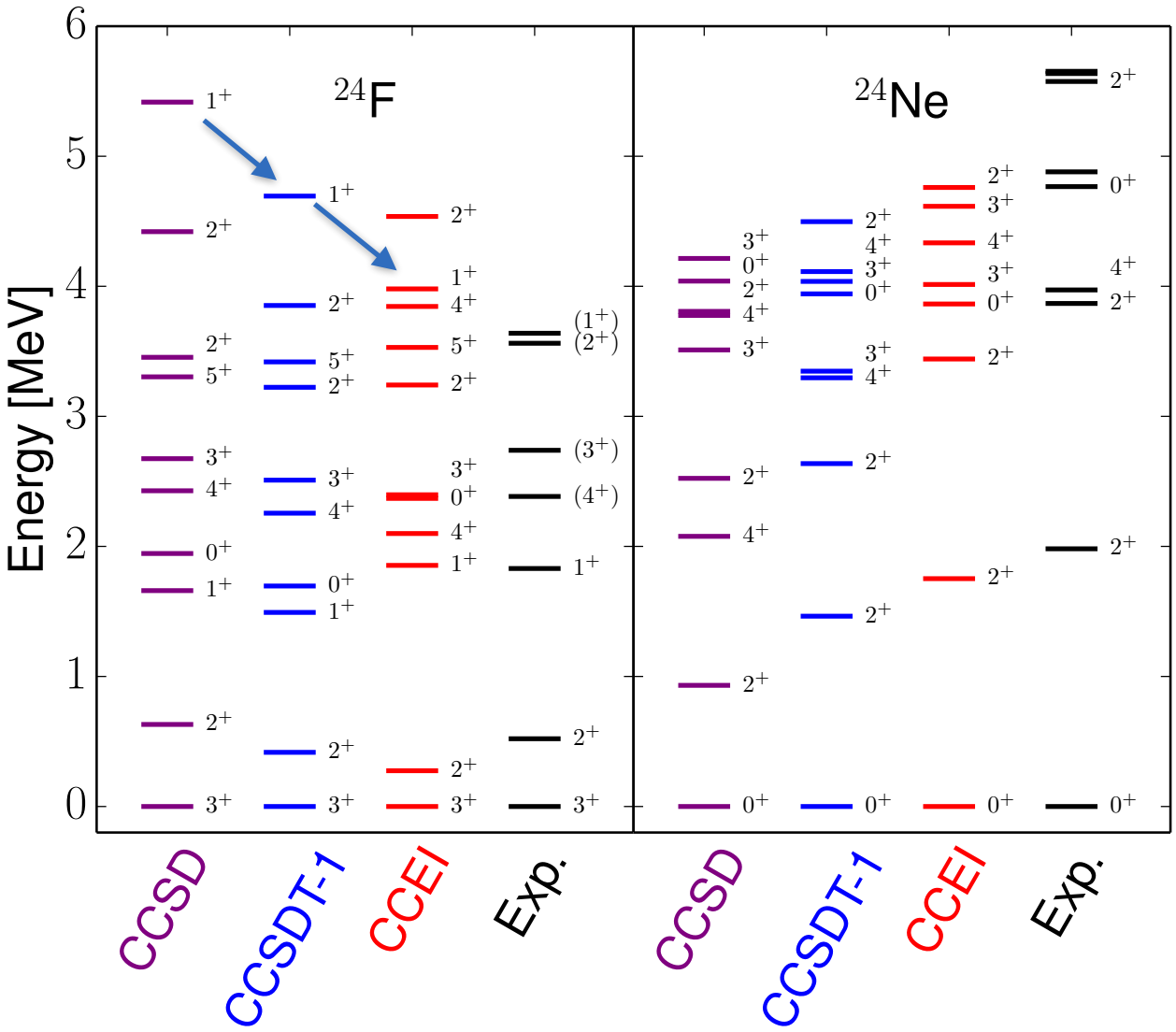

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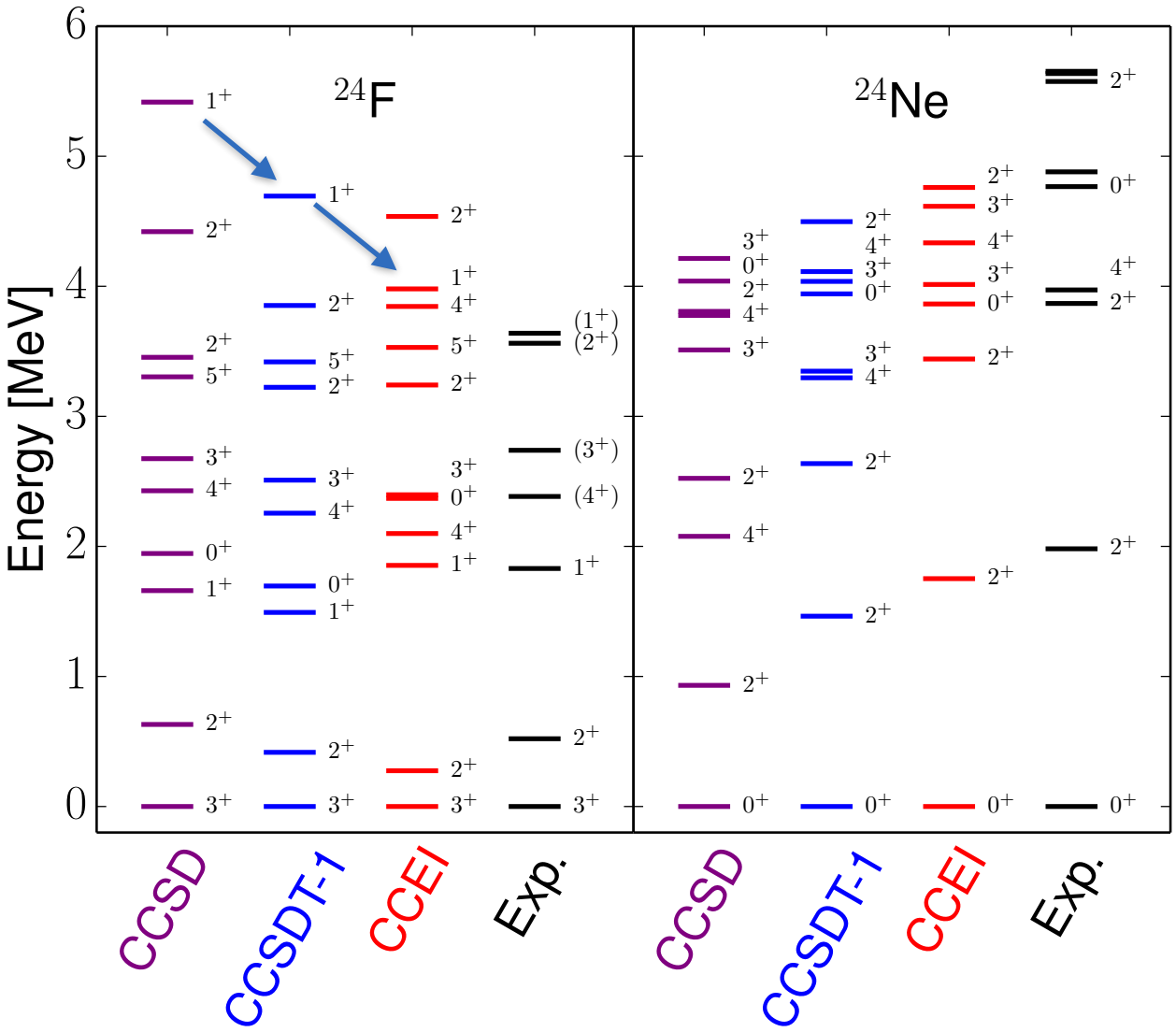

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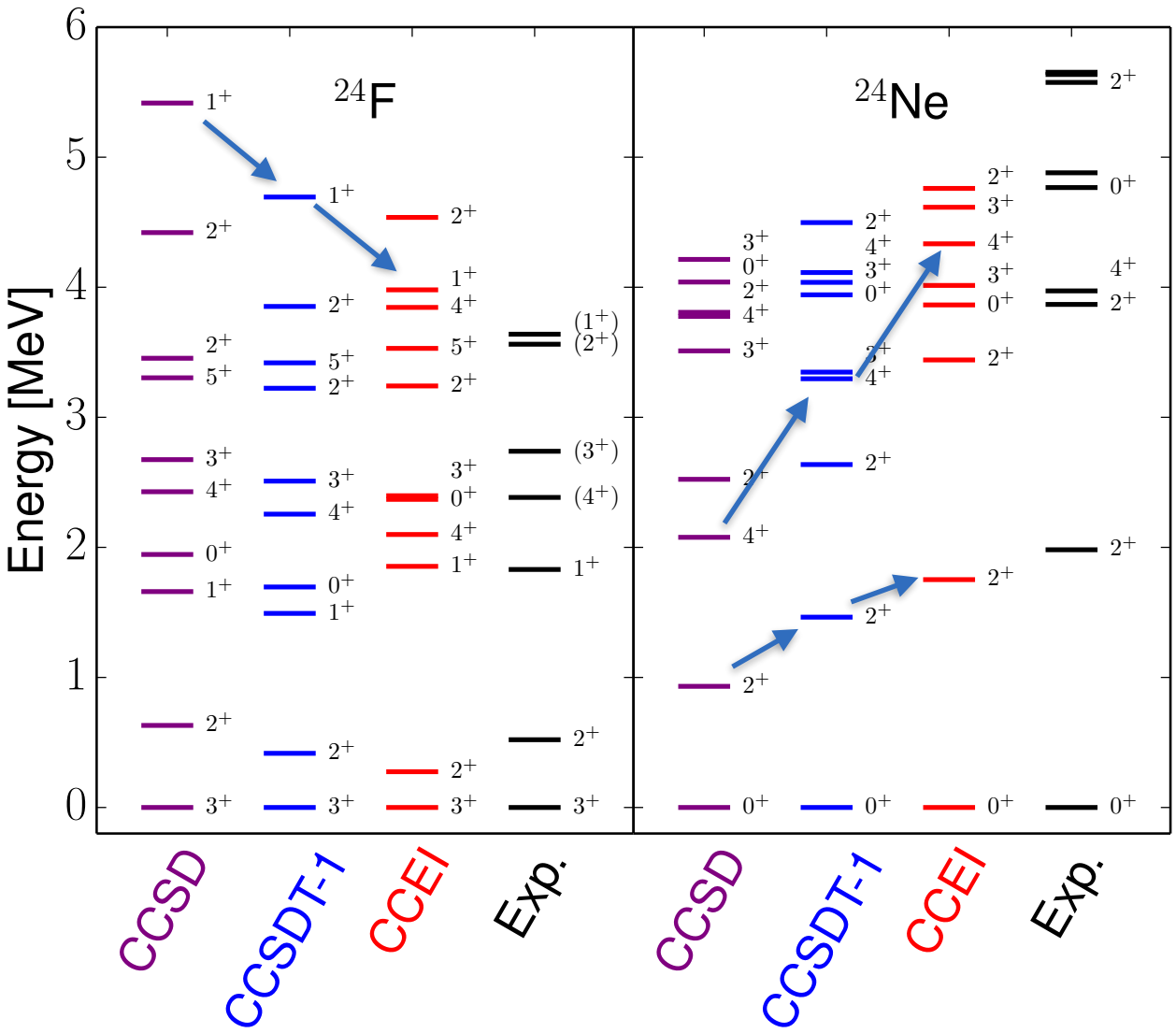

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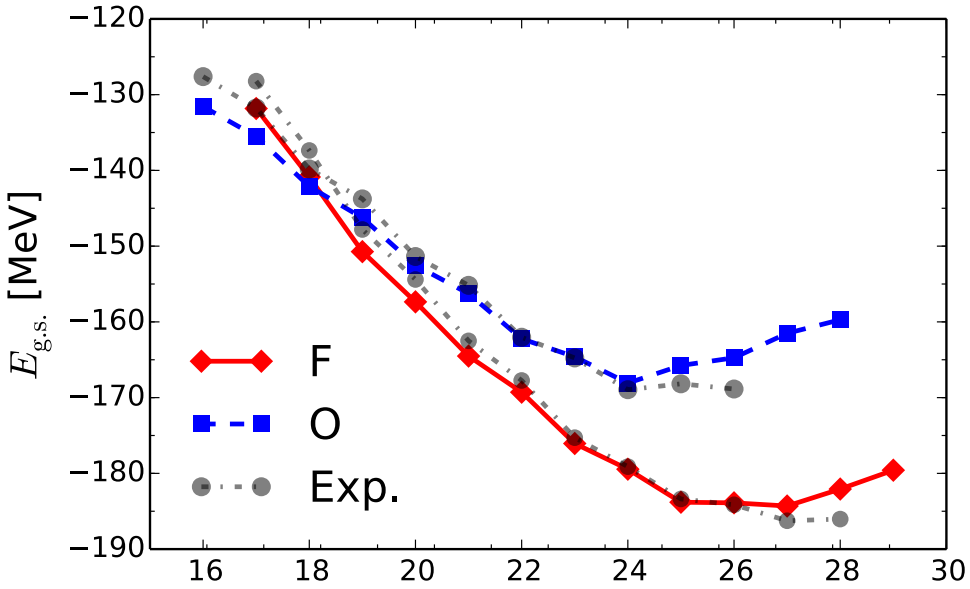
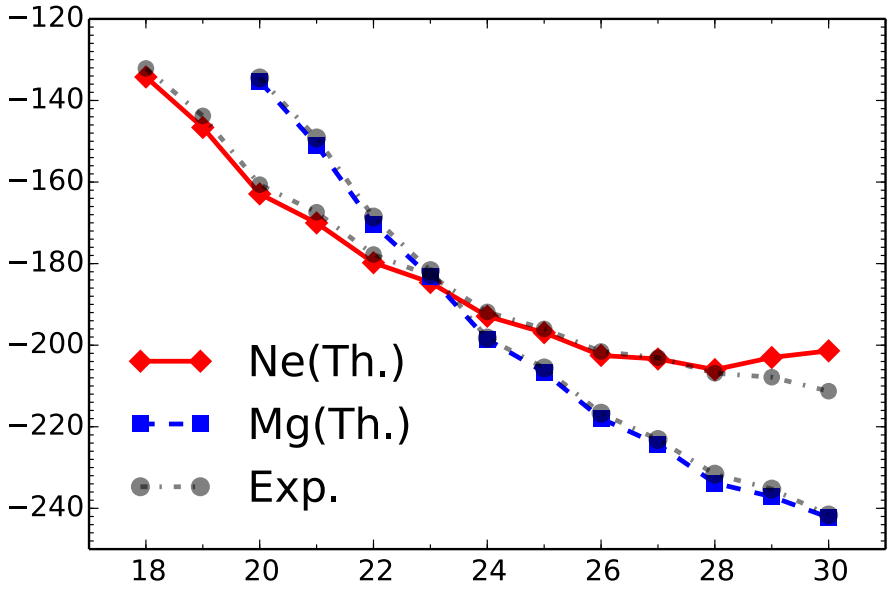
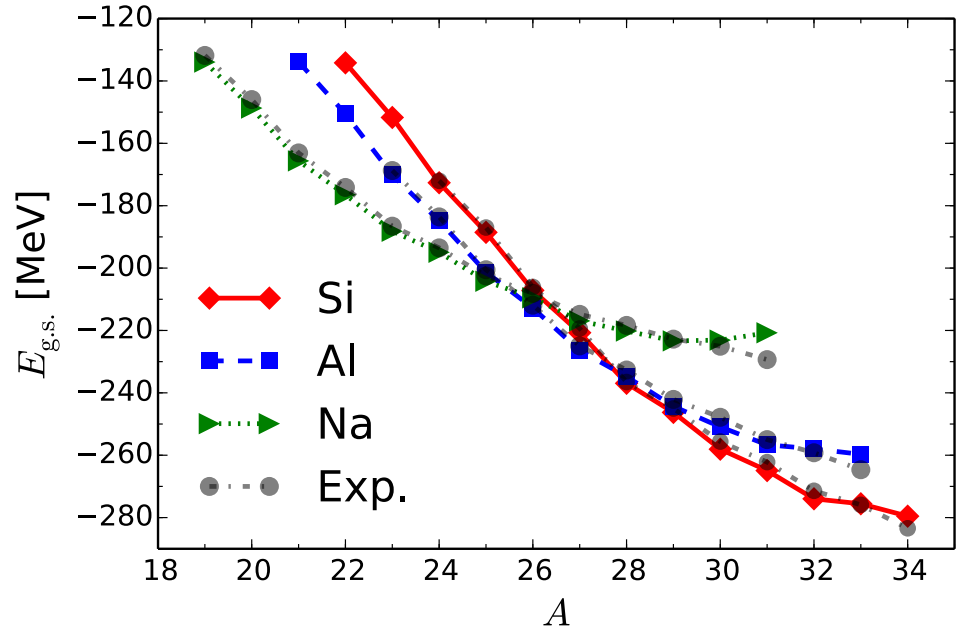
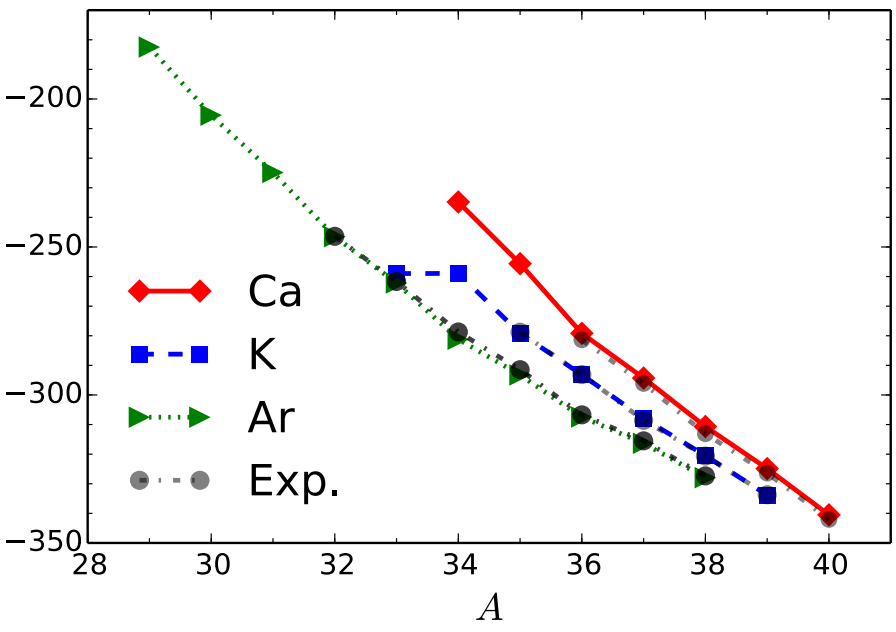
- Good agreement between EOM-CCSDT1 and CCEI in 24Ne.
- Larger role of 3p-3h excitations and, in general, improves agreement with CCEI.

CCEI for Deformed Nuclei









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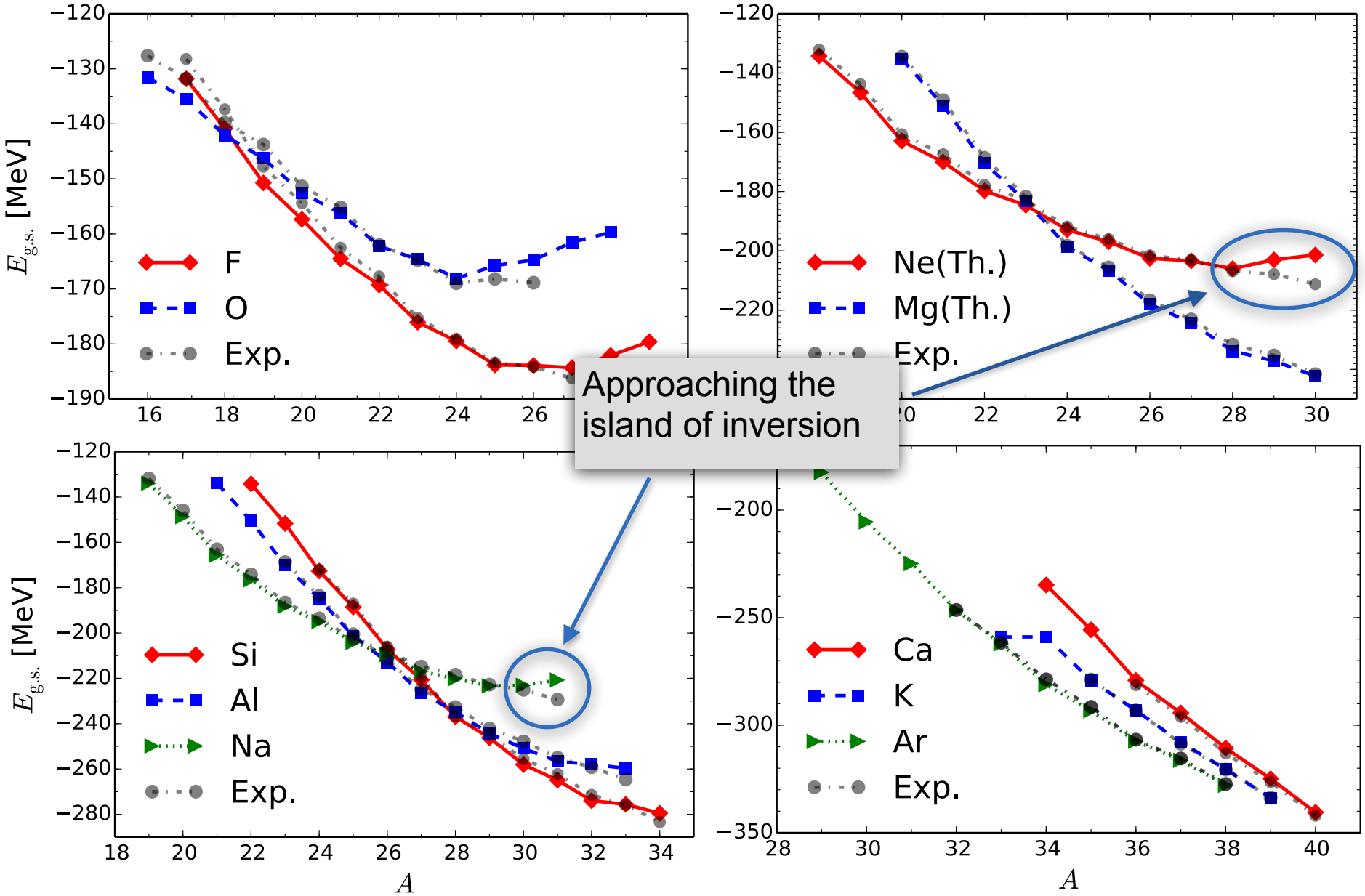

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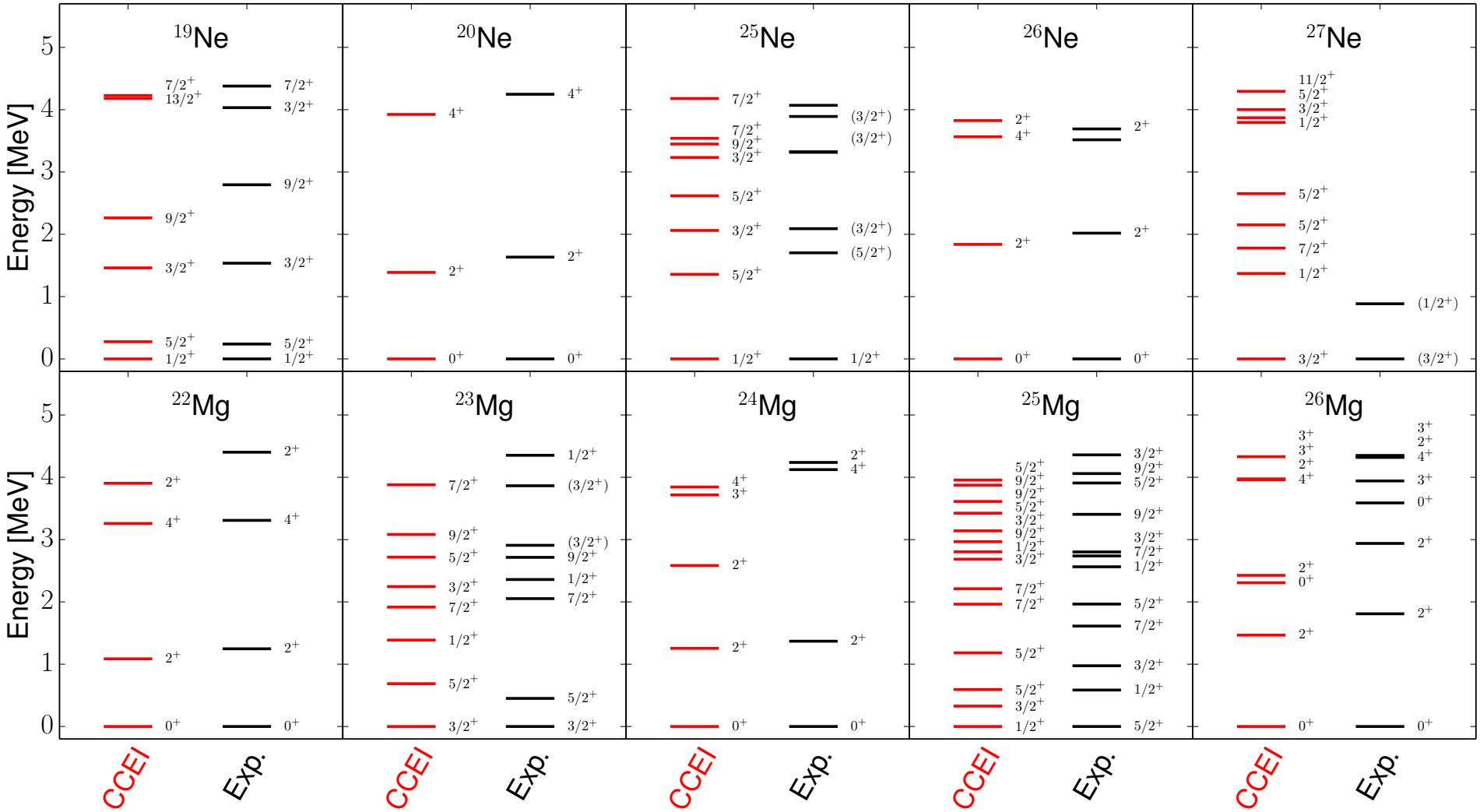
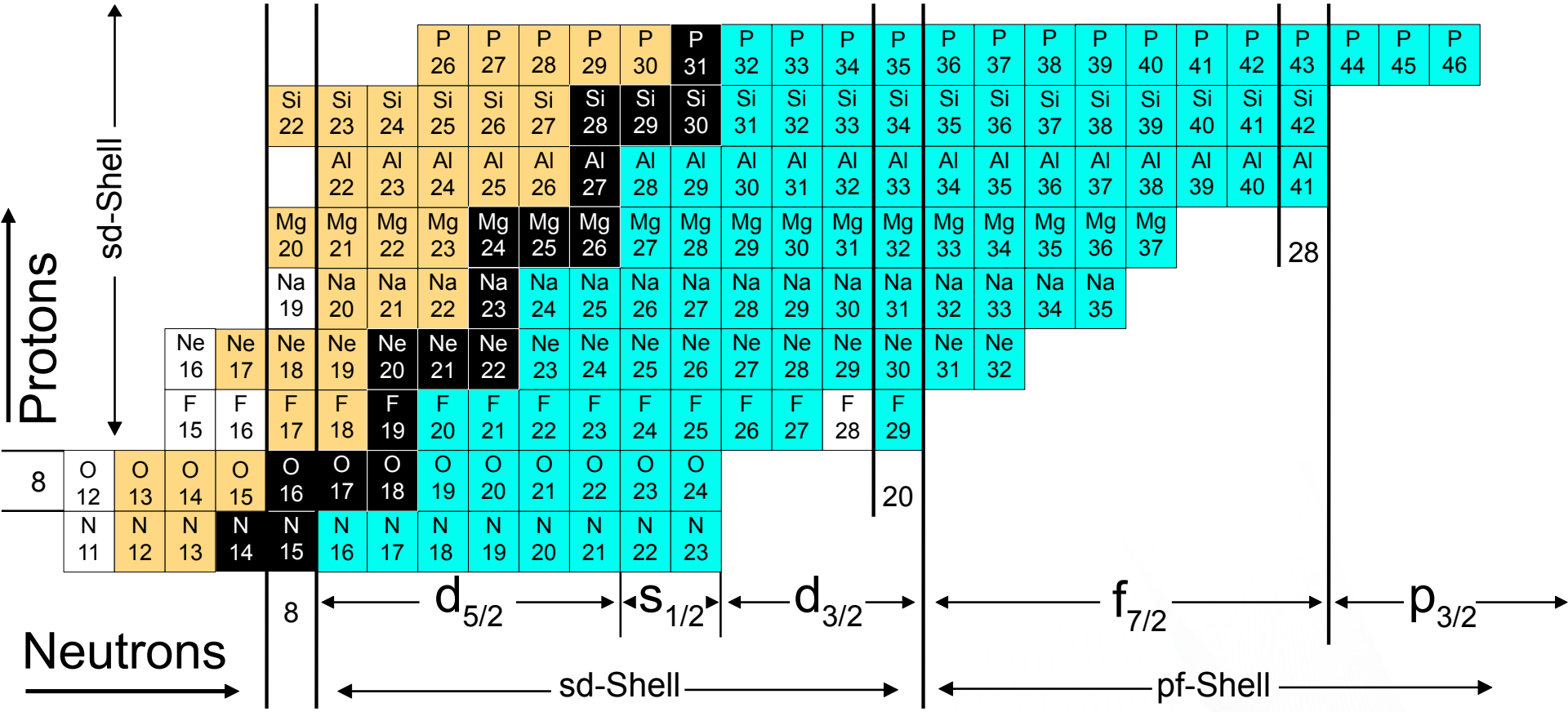


Toward the Island of Inversion



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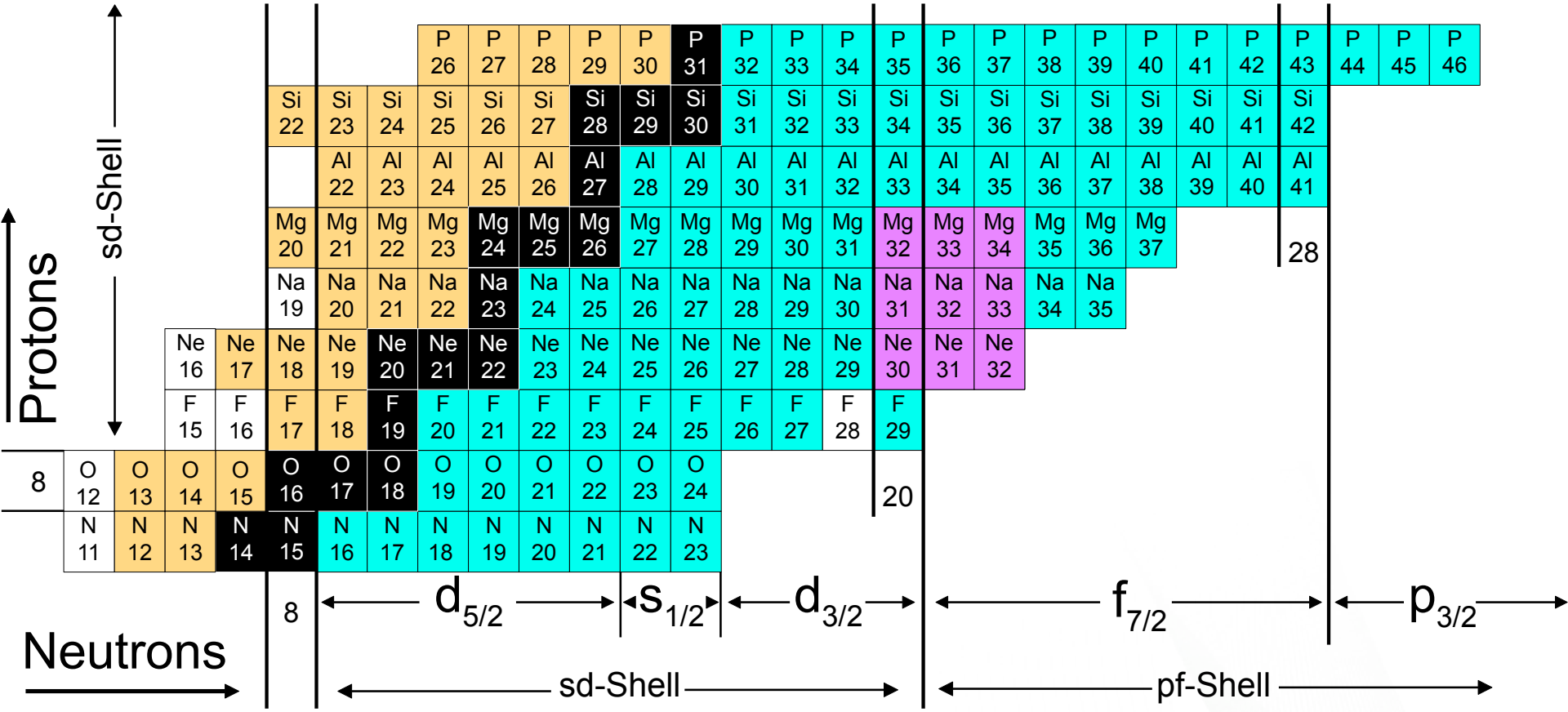

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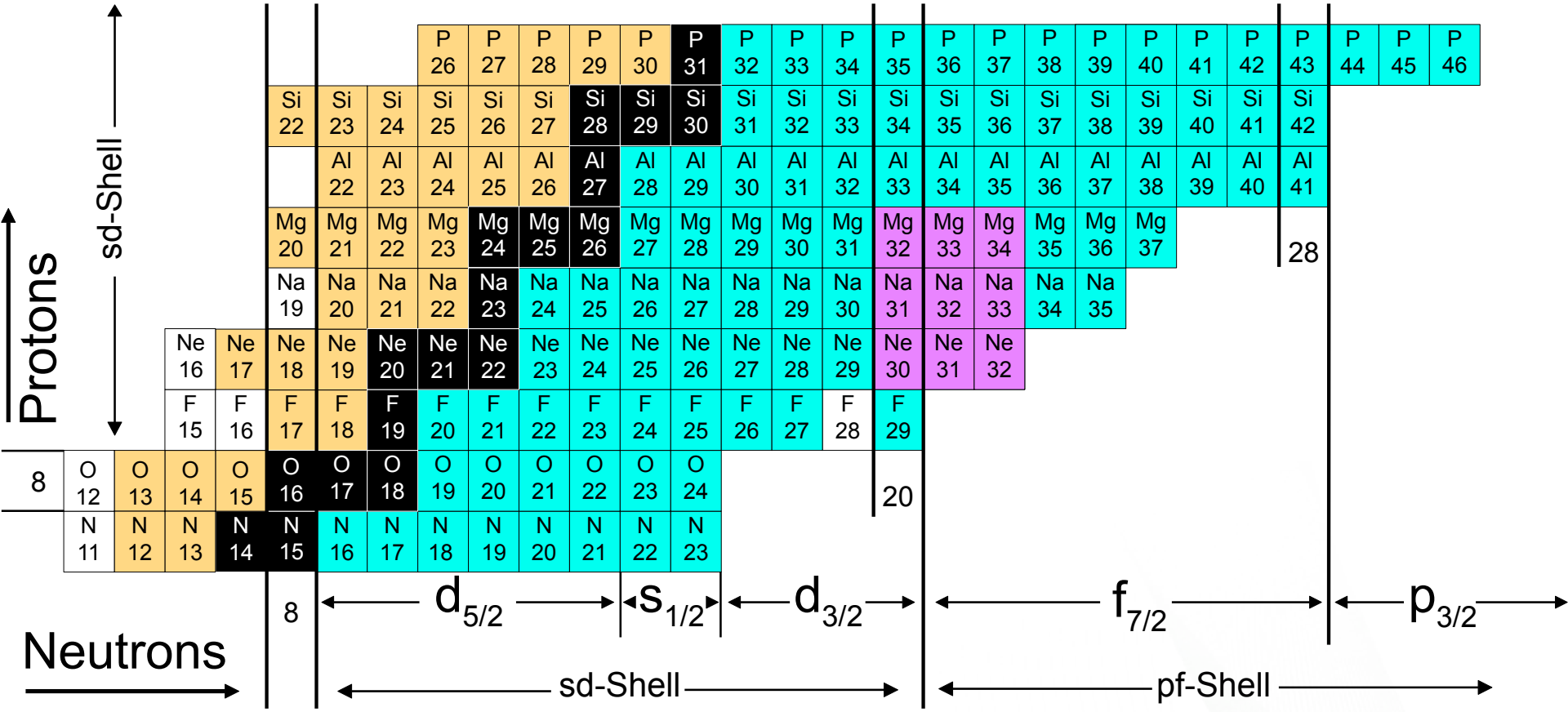

How do we use the CCEI machinery to get to this region?

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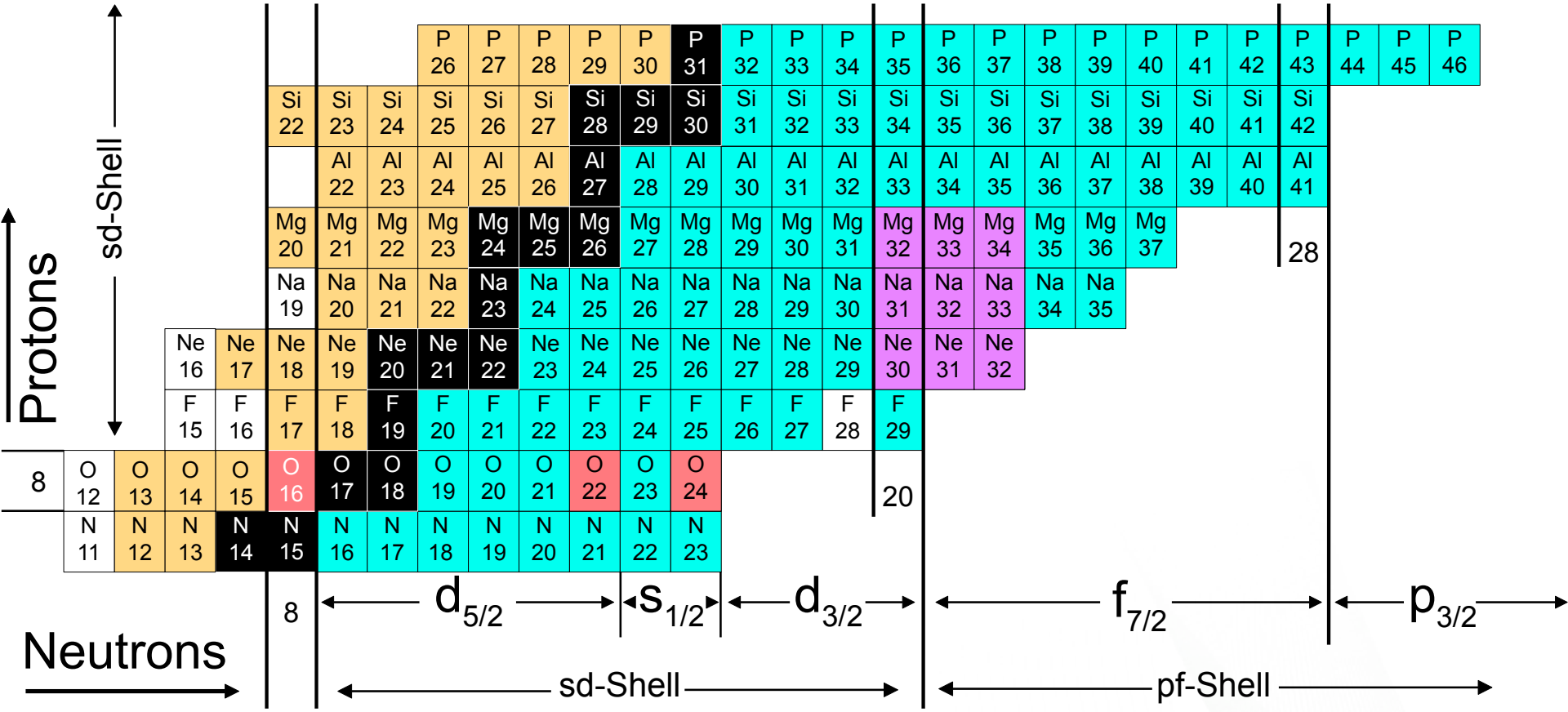

How do we use the CCEI machinery to get to this region?

Select a Core: ^{16}O, ^{22}O, ^{24}O

^{24}O Core CCEI

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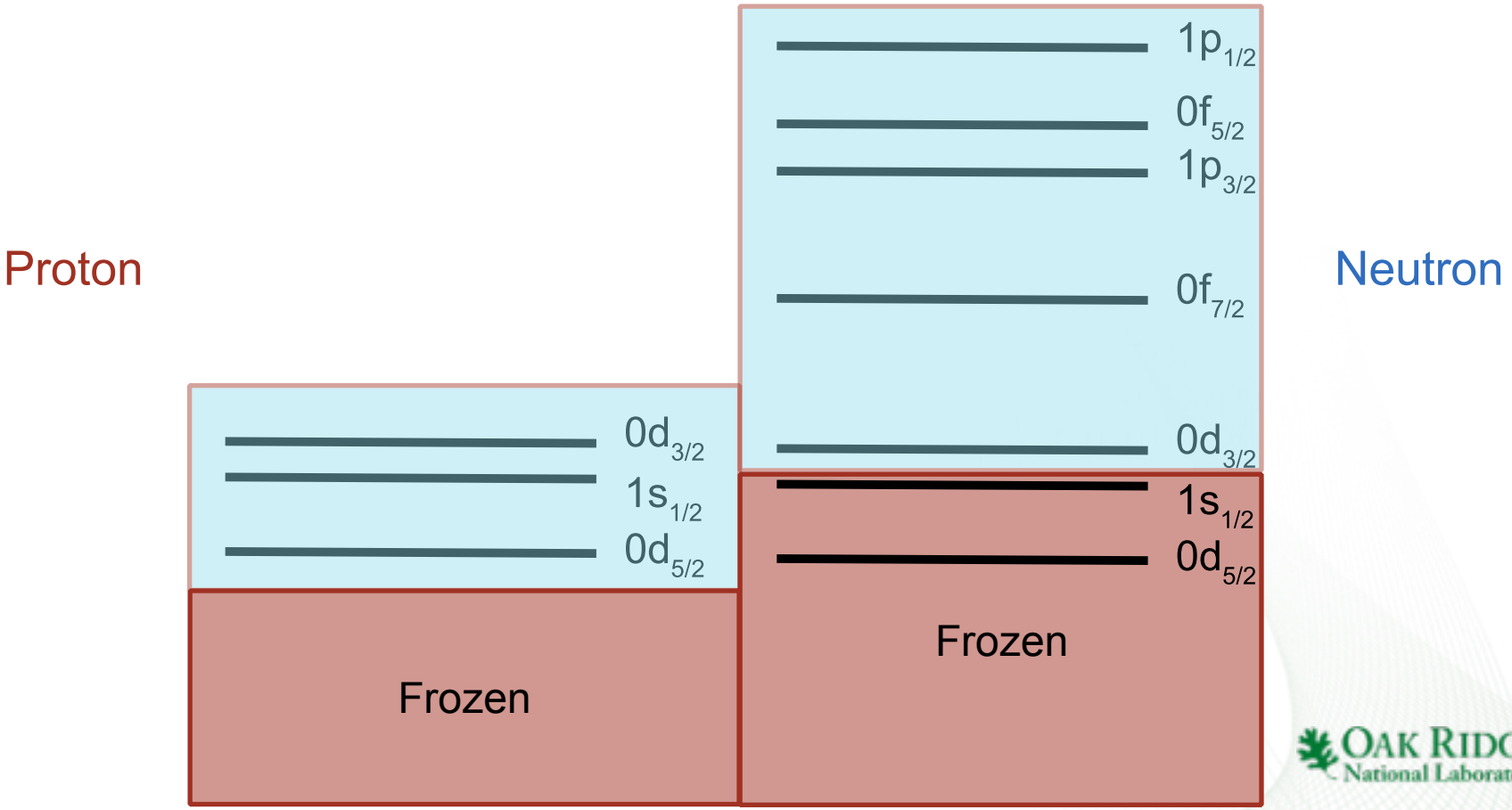

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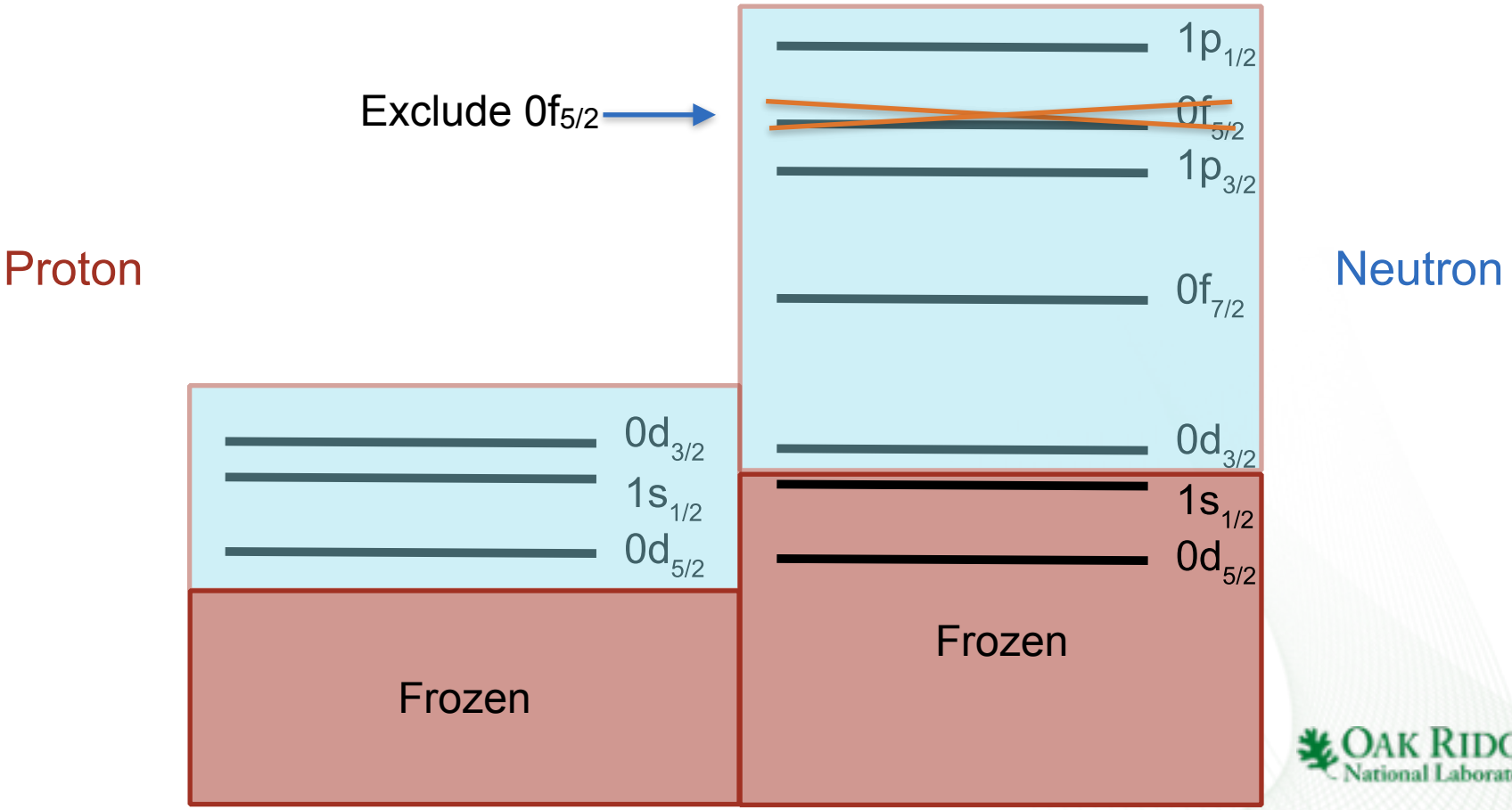
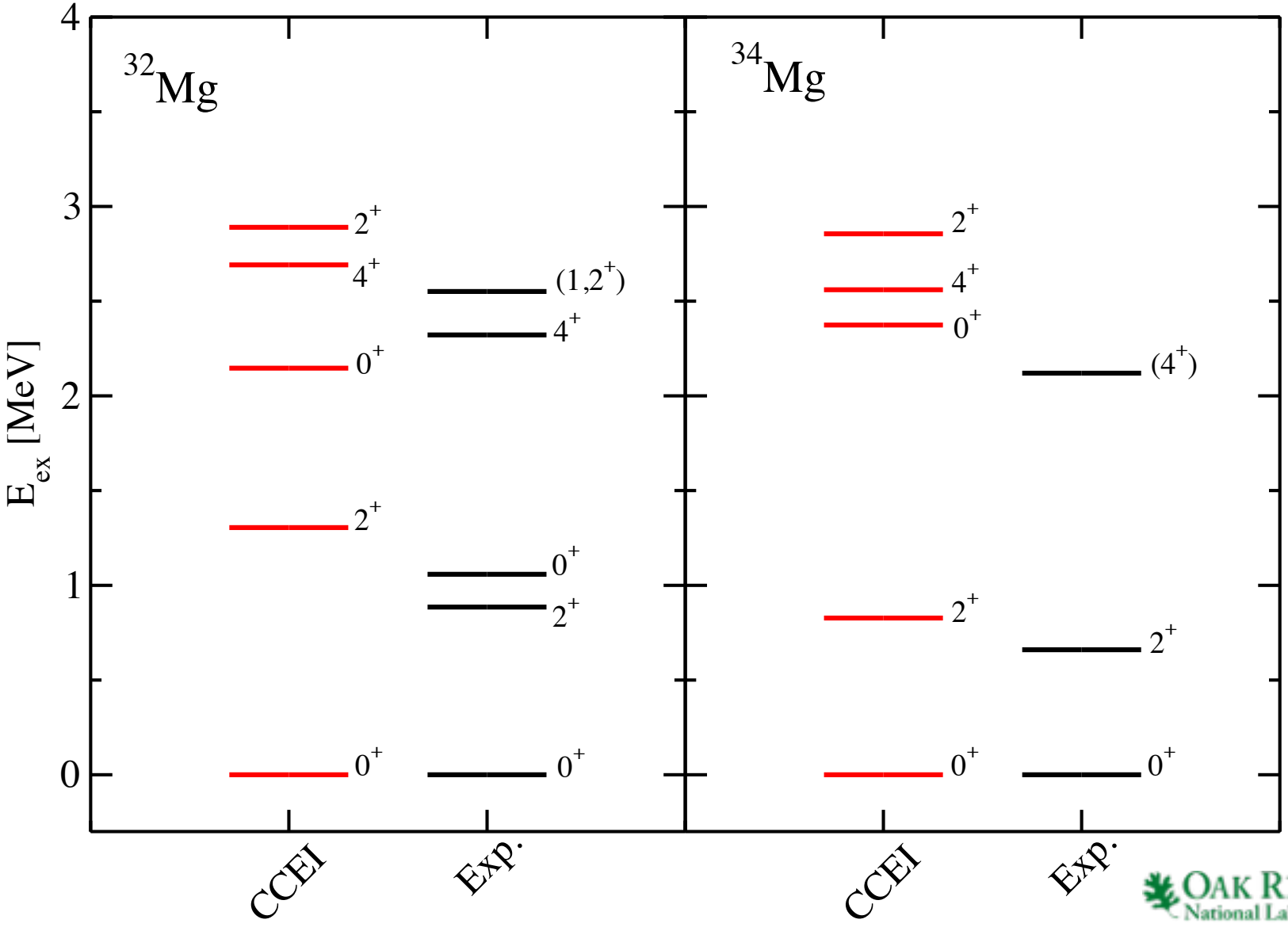


Preliminary sd-pf CCEI Results



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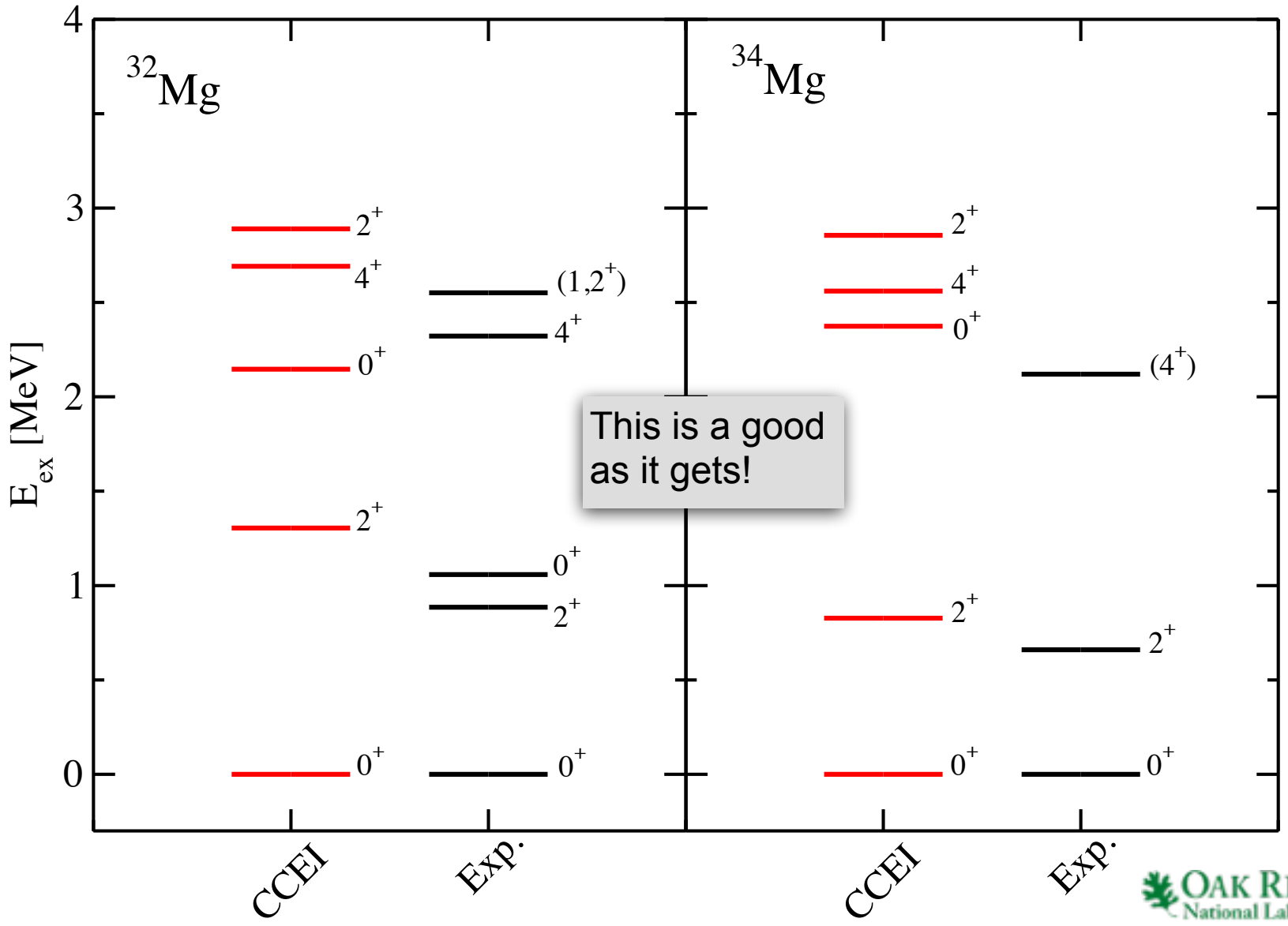

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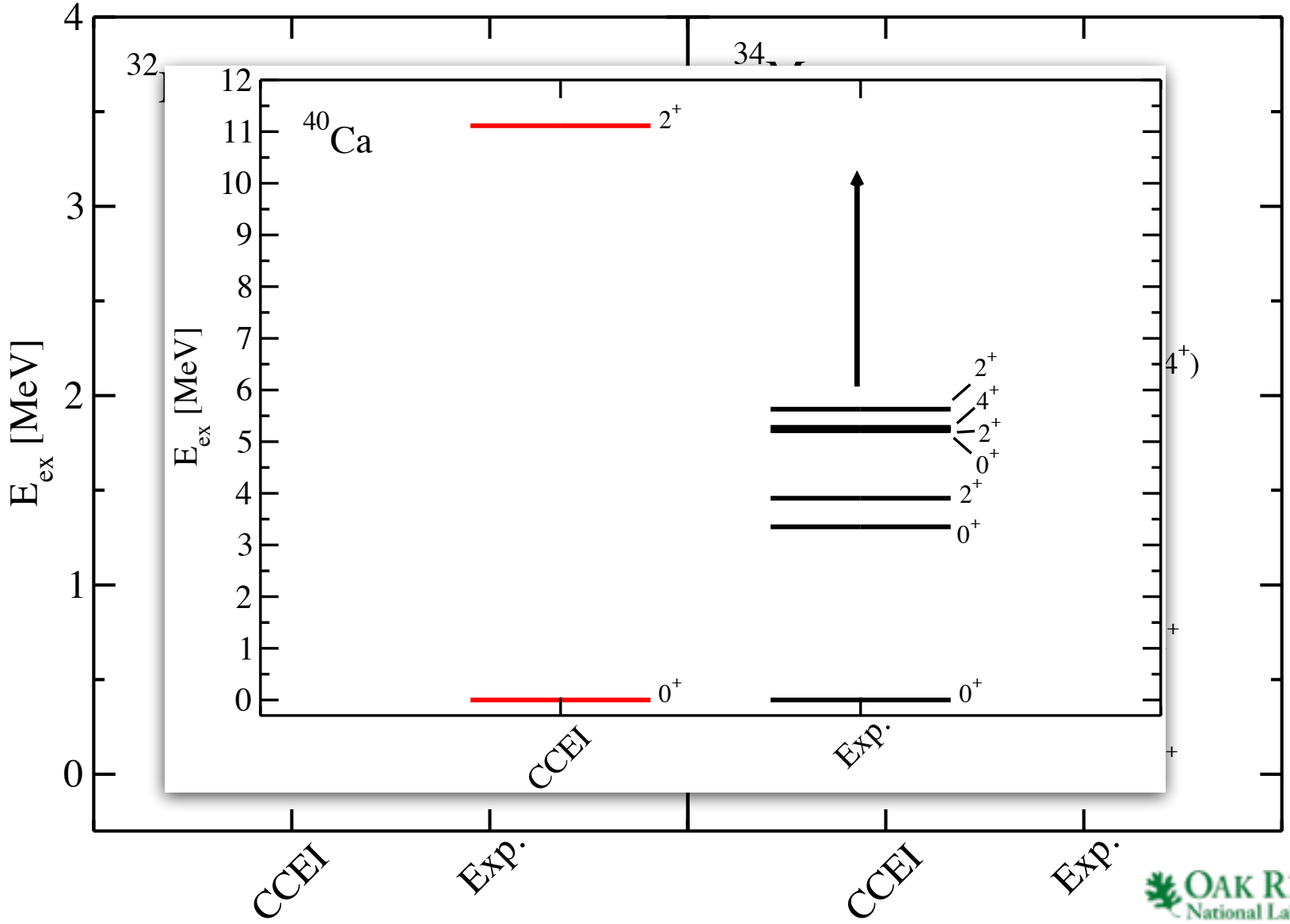

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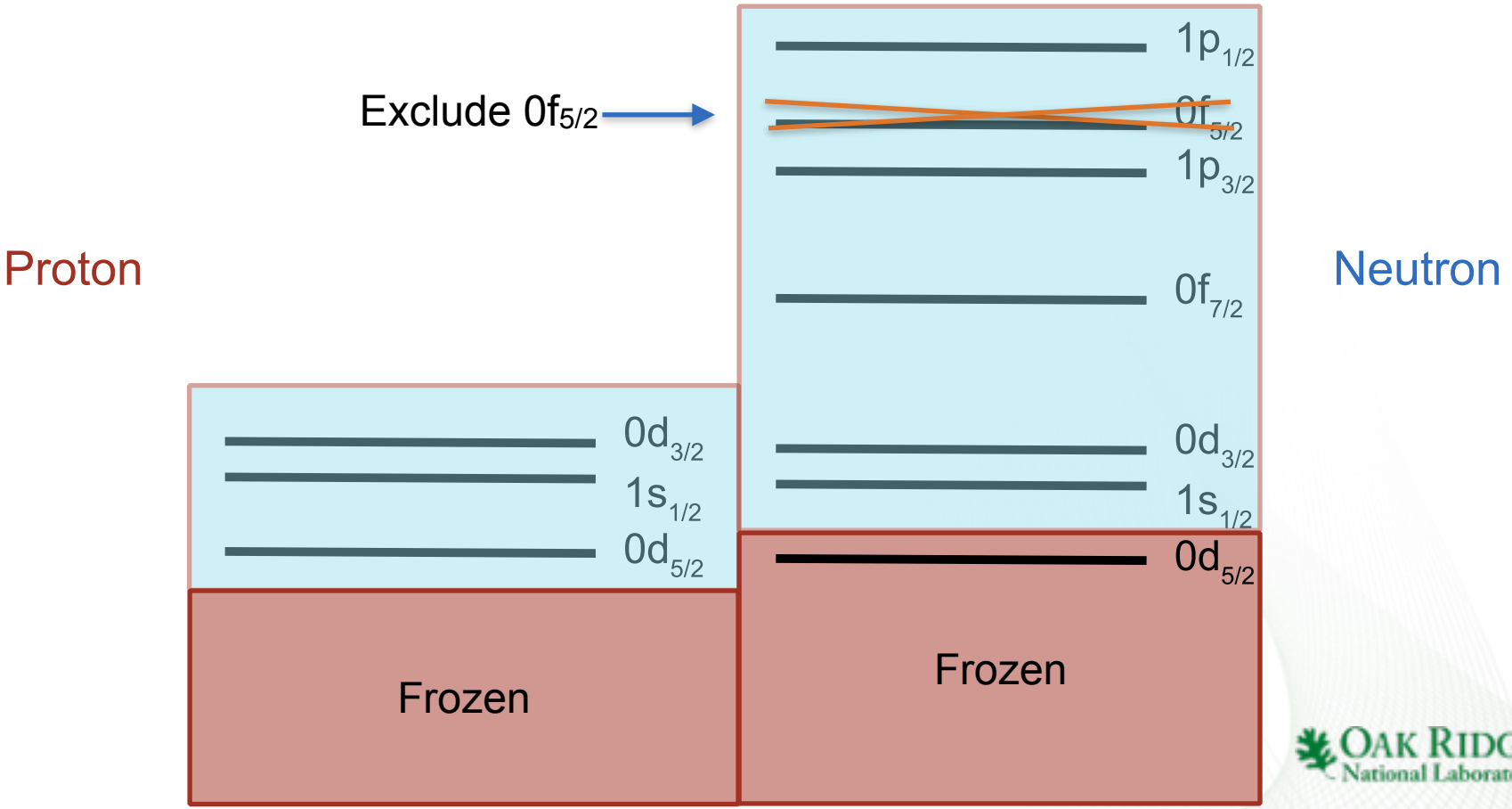

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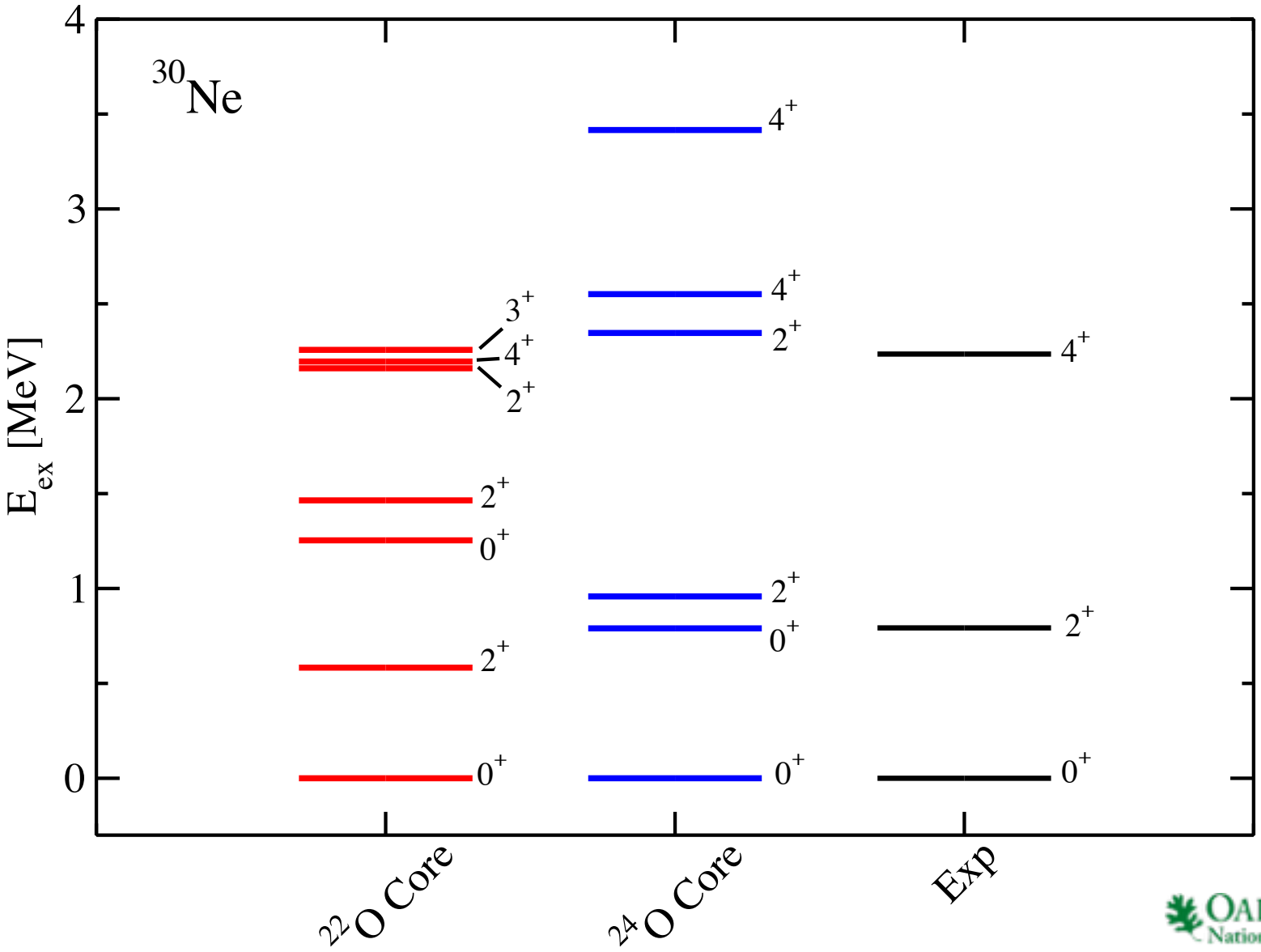

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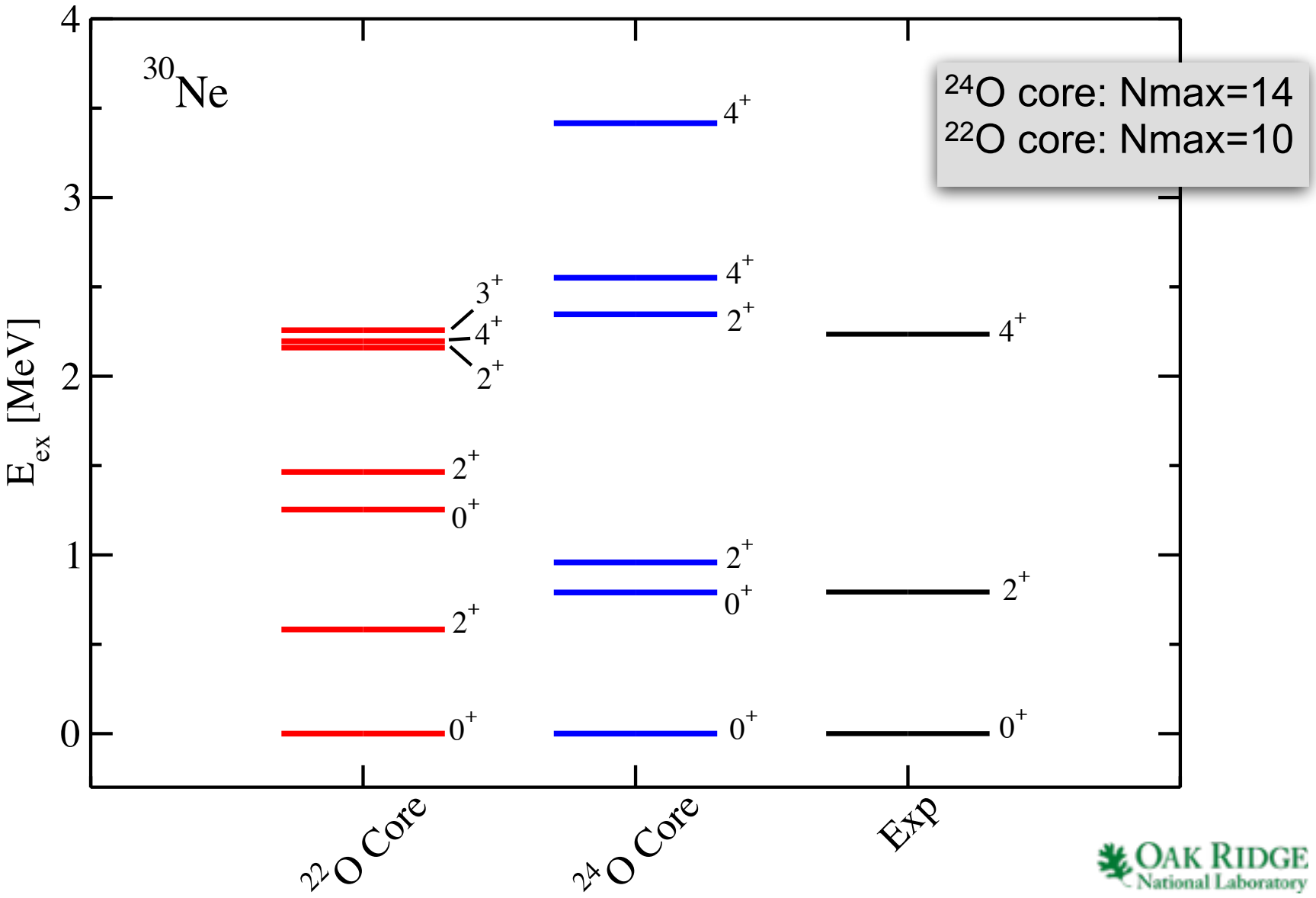

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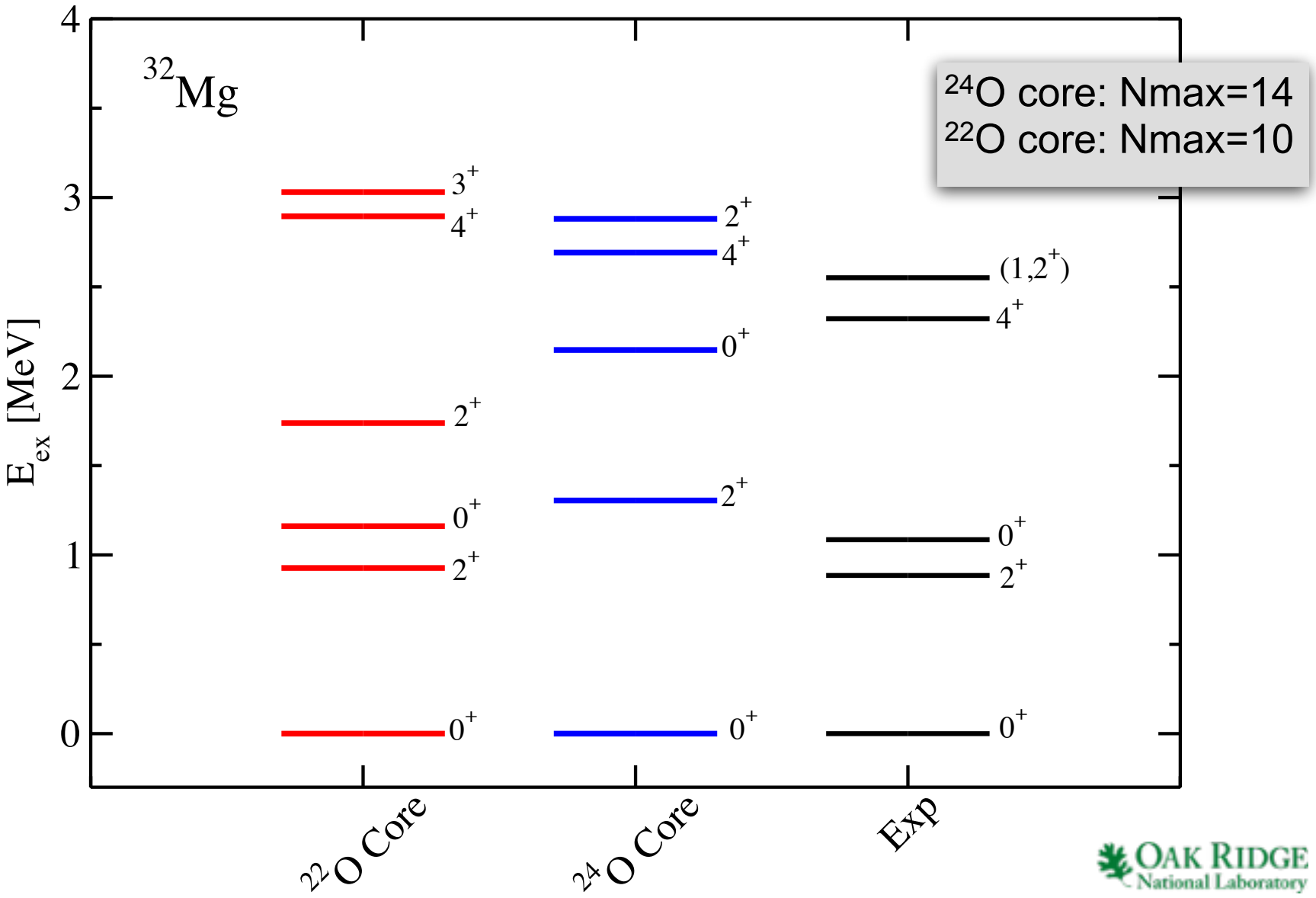

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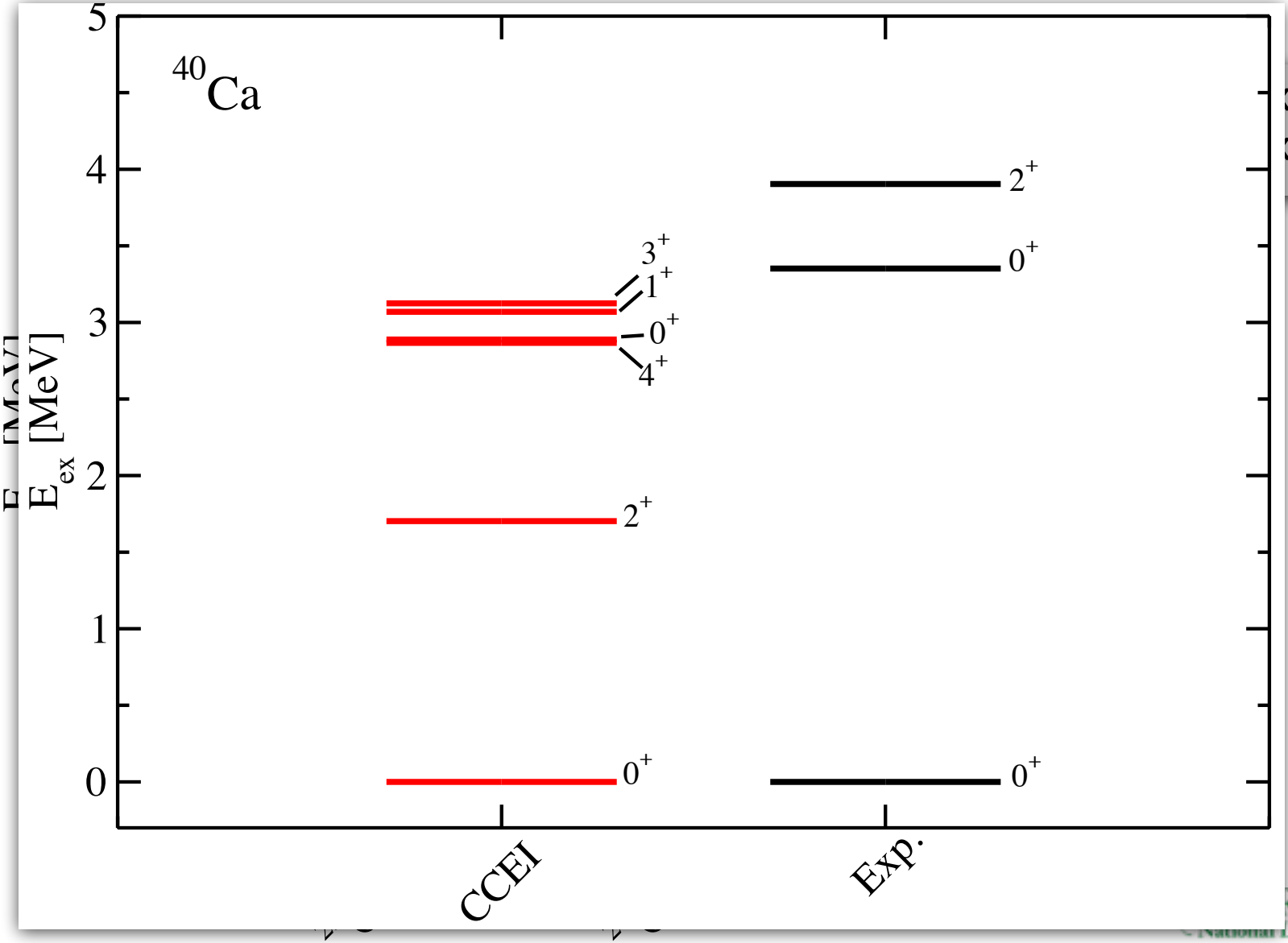


=14
=10

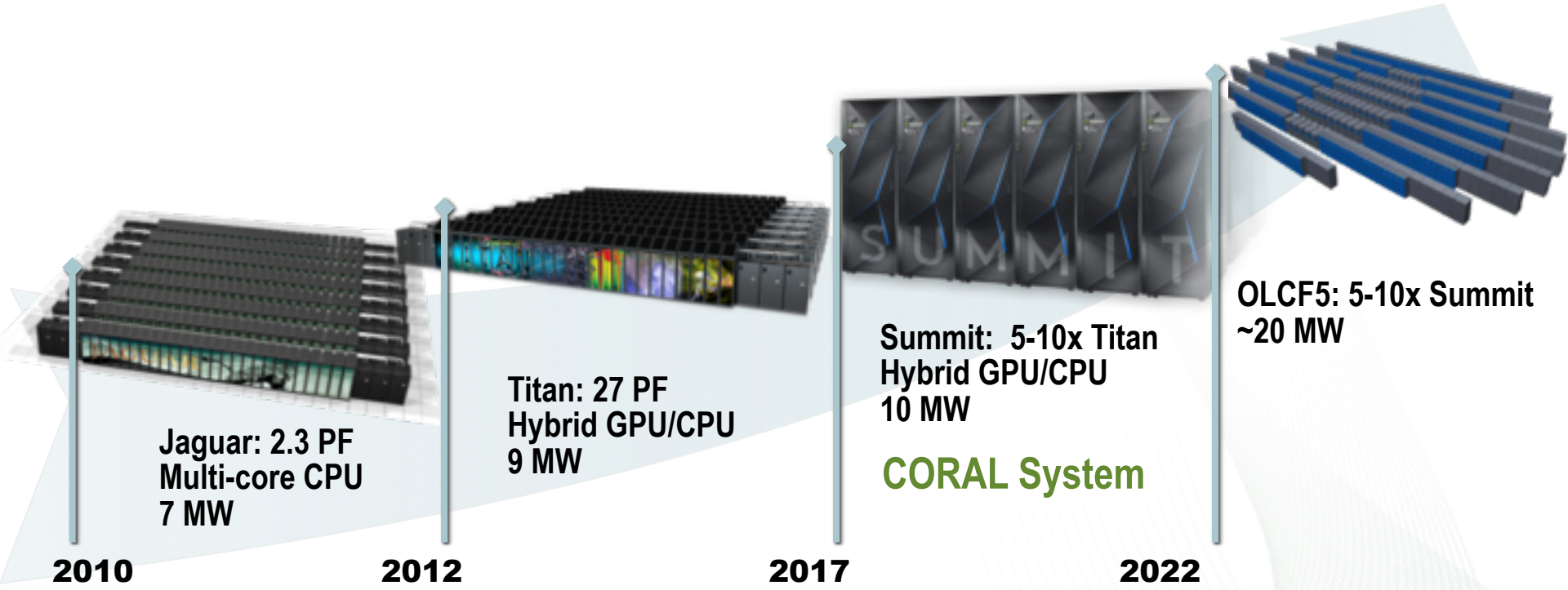
Physics: Looking Forward

- sd-shell CCEI gives good agreement with experiment.
- A-dependence is mitigated by increasing size of CC model space.
- For sdpf interactions and the island of inversion, we need a comparison of different model spaces, e.g. with an ^{16}O, ^{22}O, and ^{24}O core.

Computation: Looking Forward

Since clock-rate scaling ended in 2003, HPC performance has been achieved through increased CPU parallelism and, recently, accelerators.

Titan and beyond deliver heterogeneous architectures in the form of very powerful nodes with MPI and openMP parallelism and GPU accelerators.



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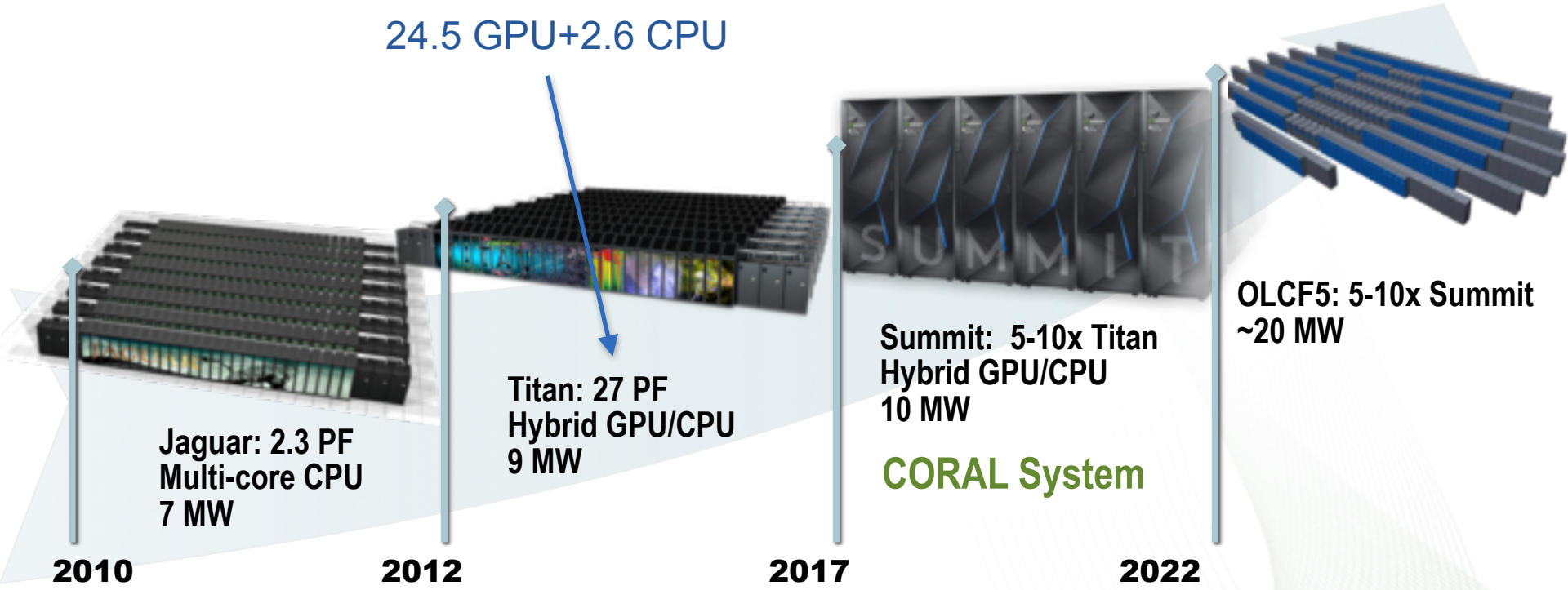

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  - IBM CoE is working on libraries for us

Questions?

Thank you