Recent progress on IMSRG calculations with 3-body operators

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with Jan Hoppe, Takayuki Miyagi, Alexander Tichai, Ragnar Stroberg, Kai Hebeler, Achim Schwenk

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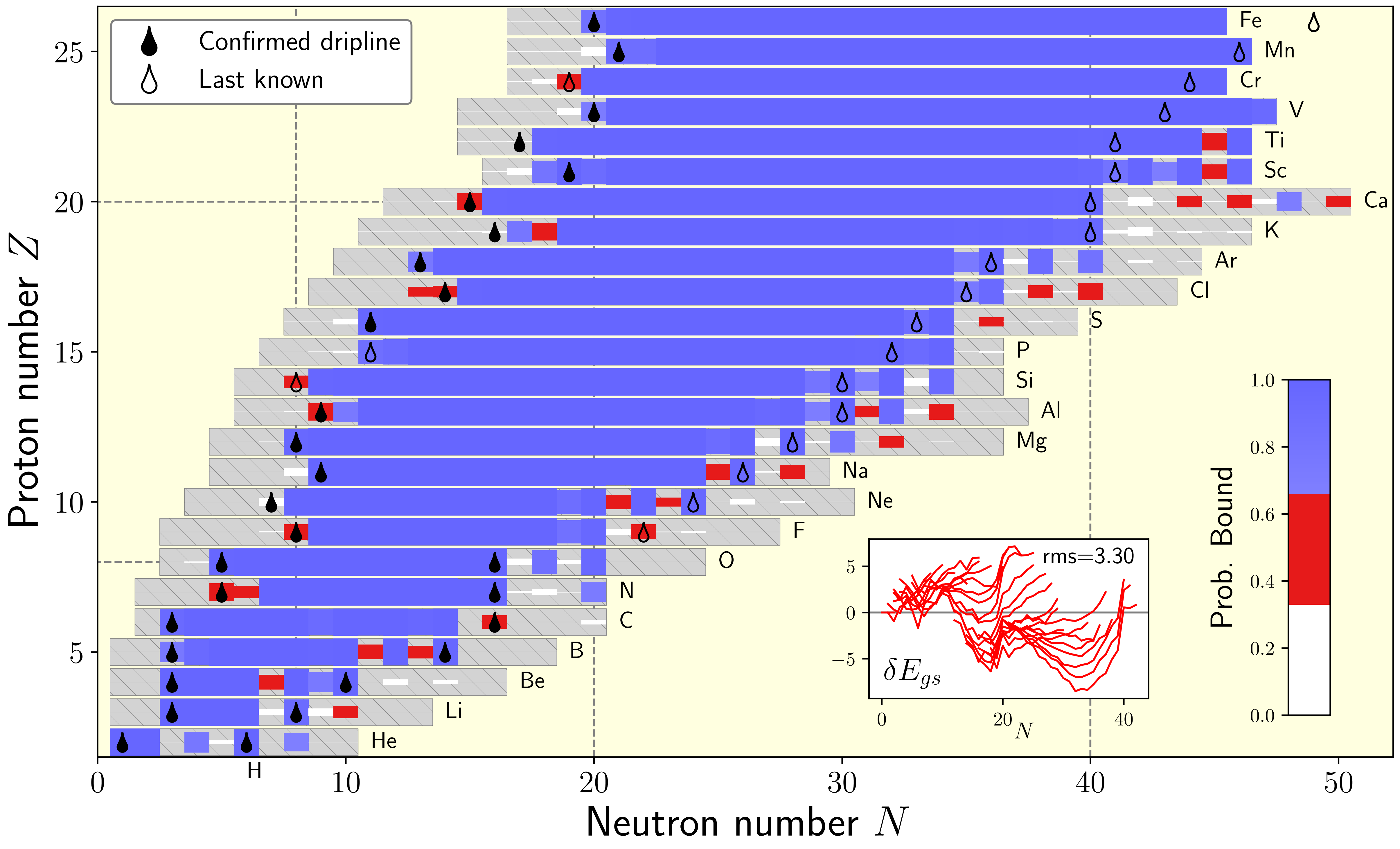
Setting the stage...

Ab initio ingredients:

- Hamiltonian with 2B and 3B forces
- Systematically improvable many-body method

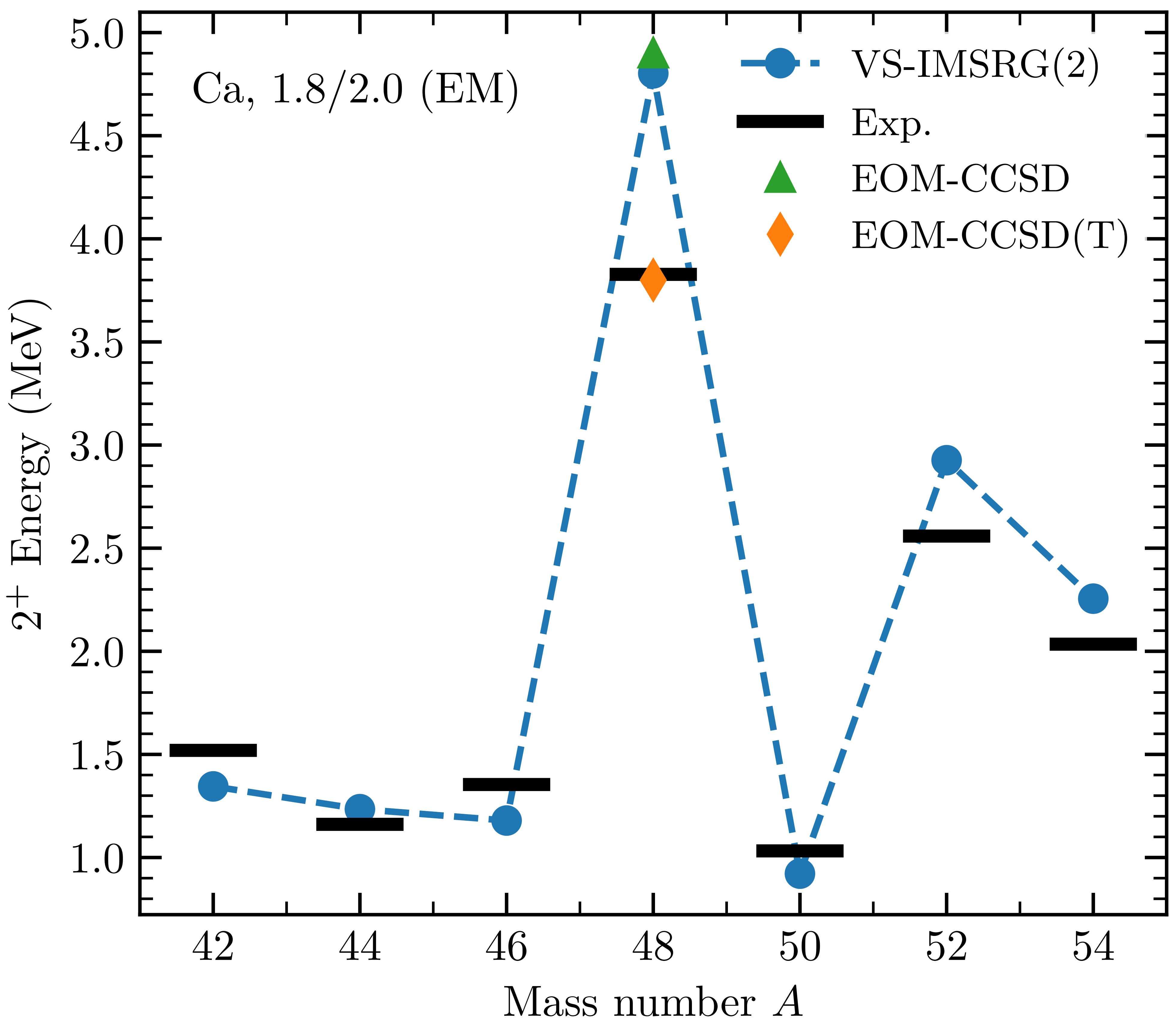
IMSRG:

- Polynomially scaling many-body method
- Open-shell systems via MR-IMSRG and **VS-IMSRG**
- Standard: truncate at IMSRG(2) level



Stroberg et al., PRL **126** (2021)

The problem: 2^+ energy of calcium-48



Hagen et al., PRL **117** (2016)

Simonis et al., PRC **96** (2017)

- Success: Description of 2^+ energies across isotopic chain
- Failure: Overprediction of closed-shell structure at calcium-48
- **Can improvements in the IMSRG bring this down into better agreement with experiment and other theories?**

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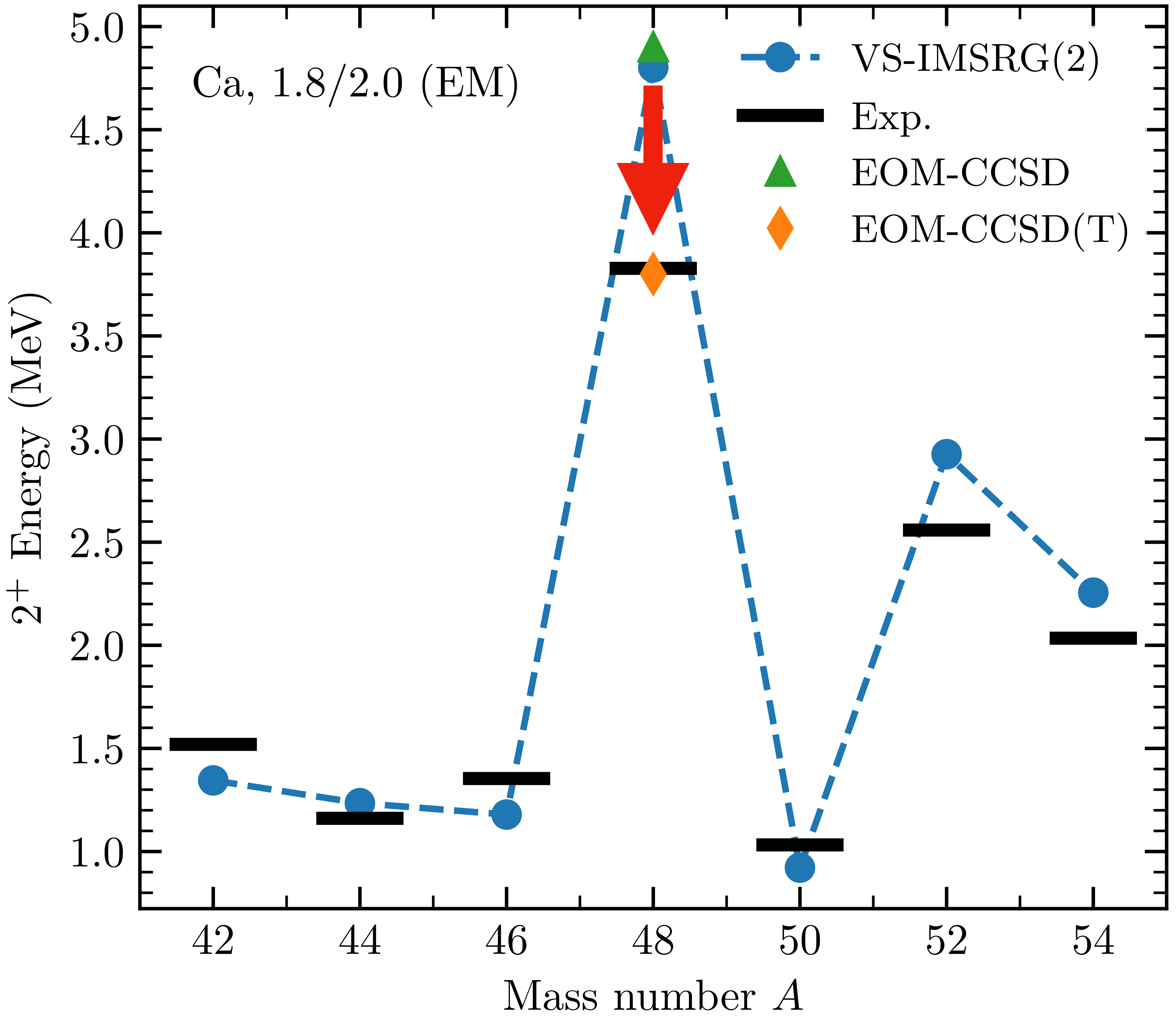

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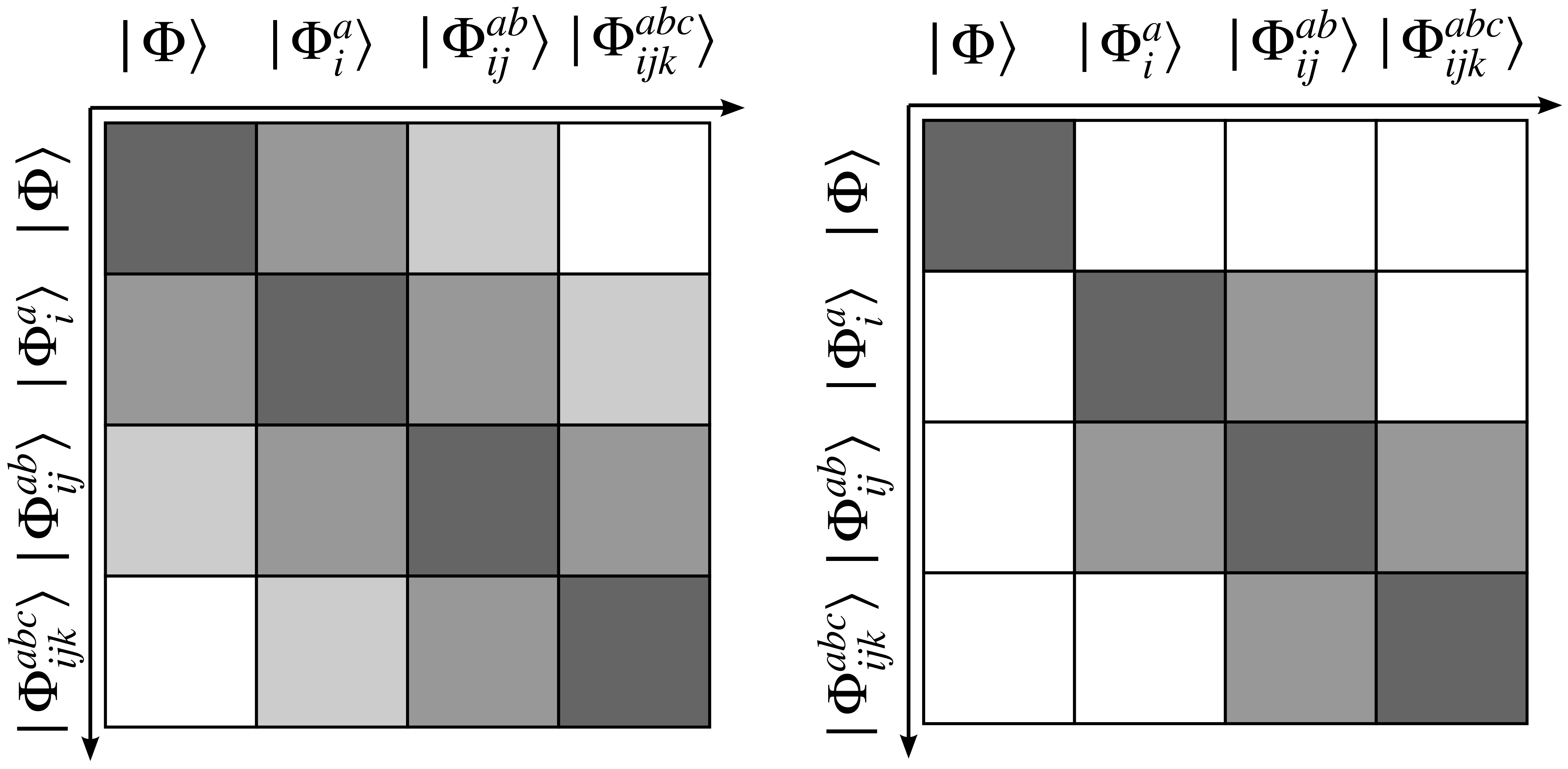
The IMSRG

Tsukiyama et al., PRL **106** (2011)
Hergert et al., Phys. Rep. **621** (2016)

- IMSRG generates unitary transformation of Hamiltonian

$$\frac{dH}{ds} = [\eta, H]$$

- Normal order with respect to $|\Phi\rangle$ approximately handles **induced many-body forces**



initial H transformed H

Hergert et al., Phys. Rep. **621** (2016)

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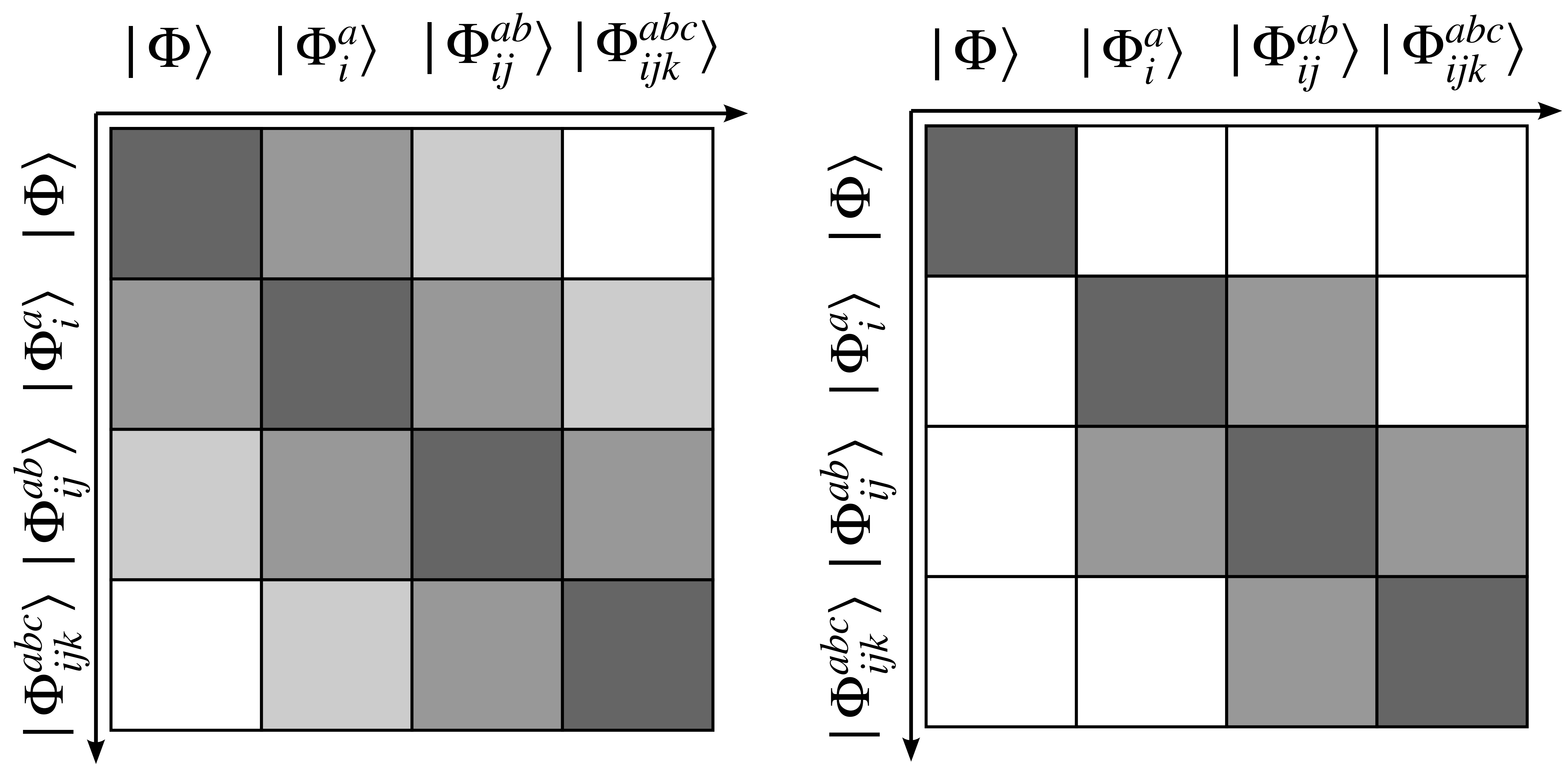


initial H transformed H

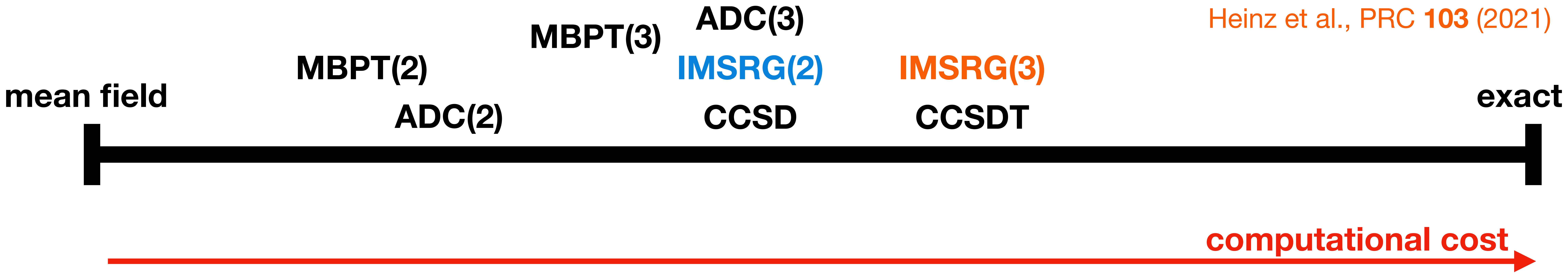
Hergert et al., Phys. Rep. **621** (2016)

Truncation necessary!

- Standard = IMSRG(2) (2-particle excitations, scales like $(o+u)^6 \equiv N^6$)
- More refined = **IMSRG(3)** (N^7 - N^9) Heinz et al., PRC **103** (2021)

Many-body expansion (ab initio picture)

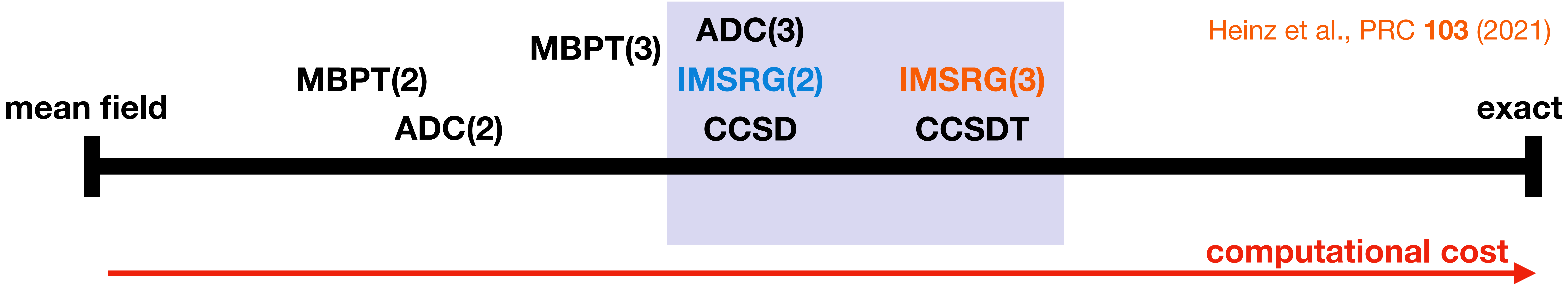
Heinz et al., PRC **103** (2021)



- Systematic expansion to exact result in some limit
- Probe many-body uncertainty by varying many-body truncation
- **IMSRG(3) is a key ingredient here!**

Many-body expansion (ab initio picture)

Heinz et al., PRC **103** (2021)



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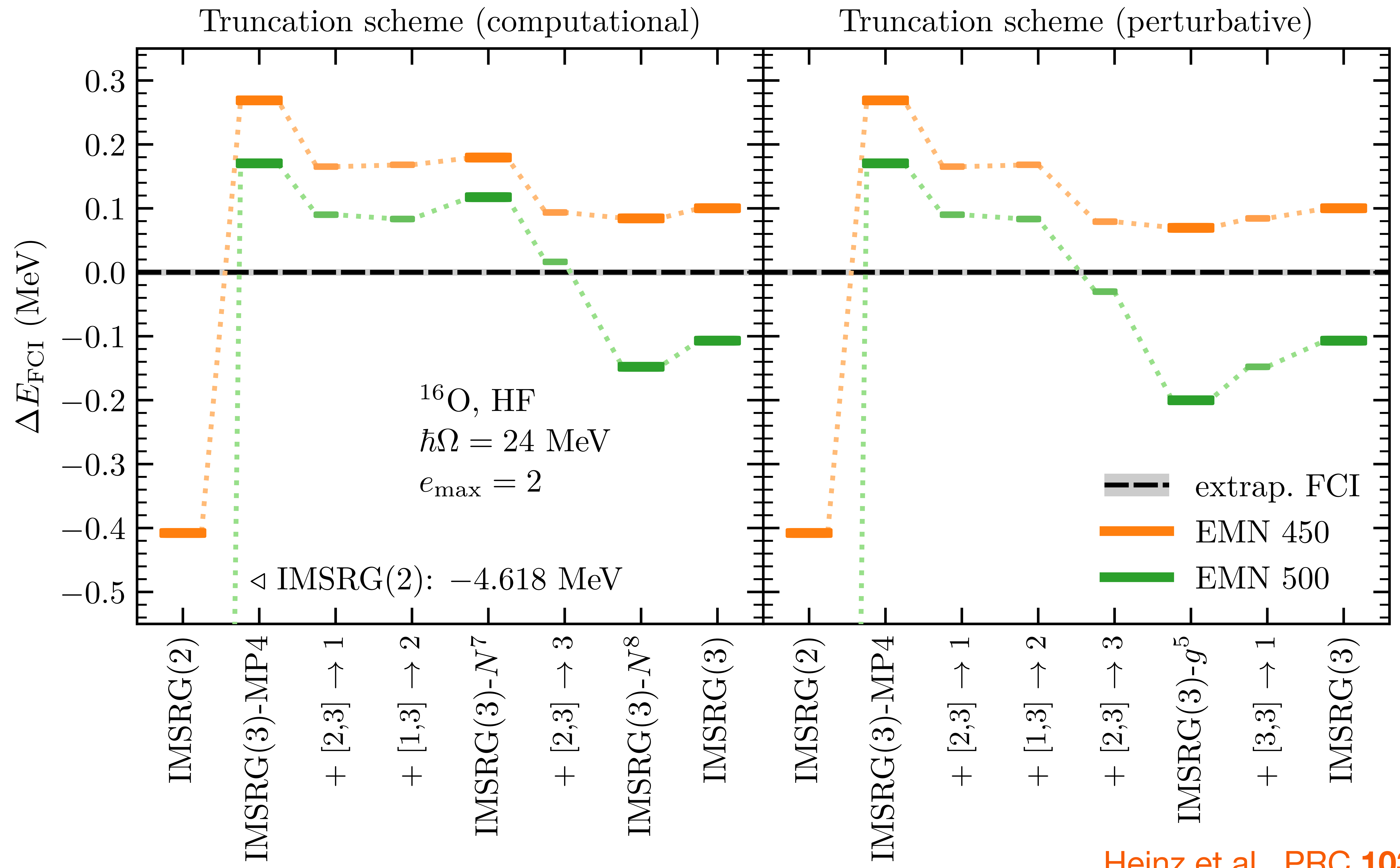
The IMSRG(3) difference



Heinz et al., PRC **103** (2021)

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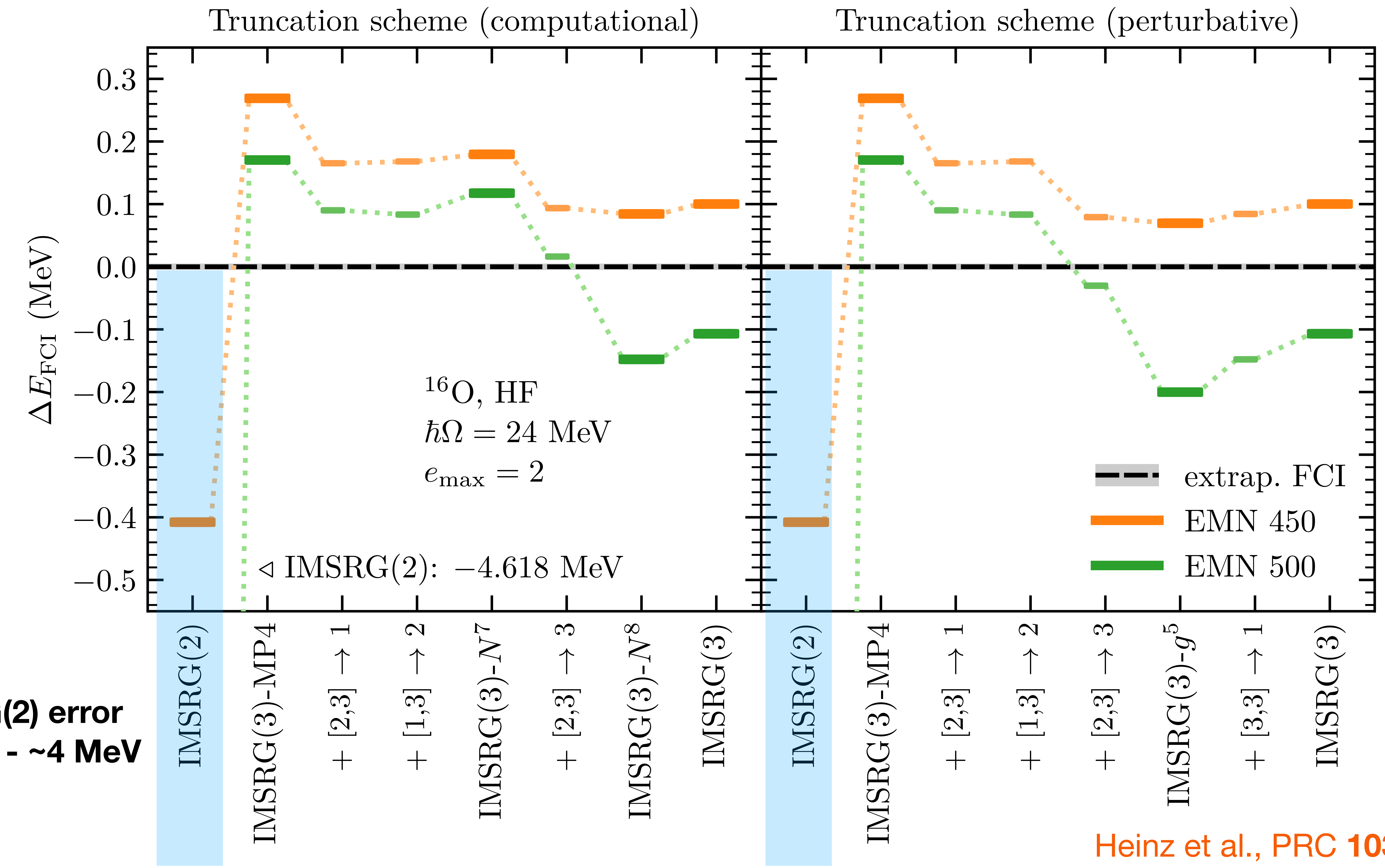
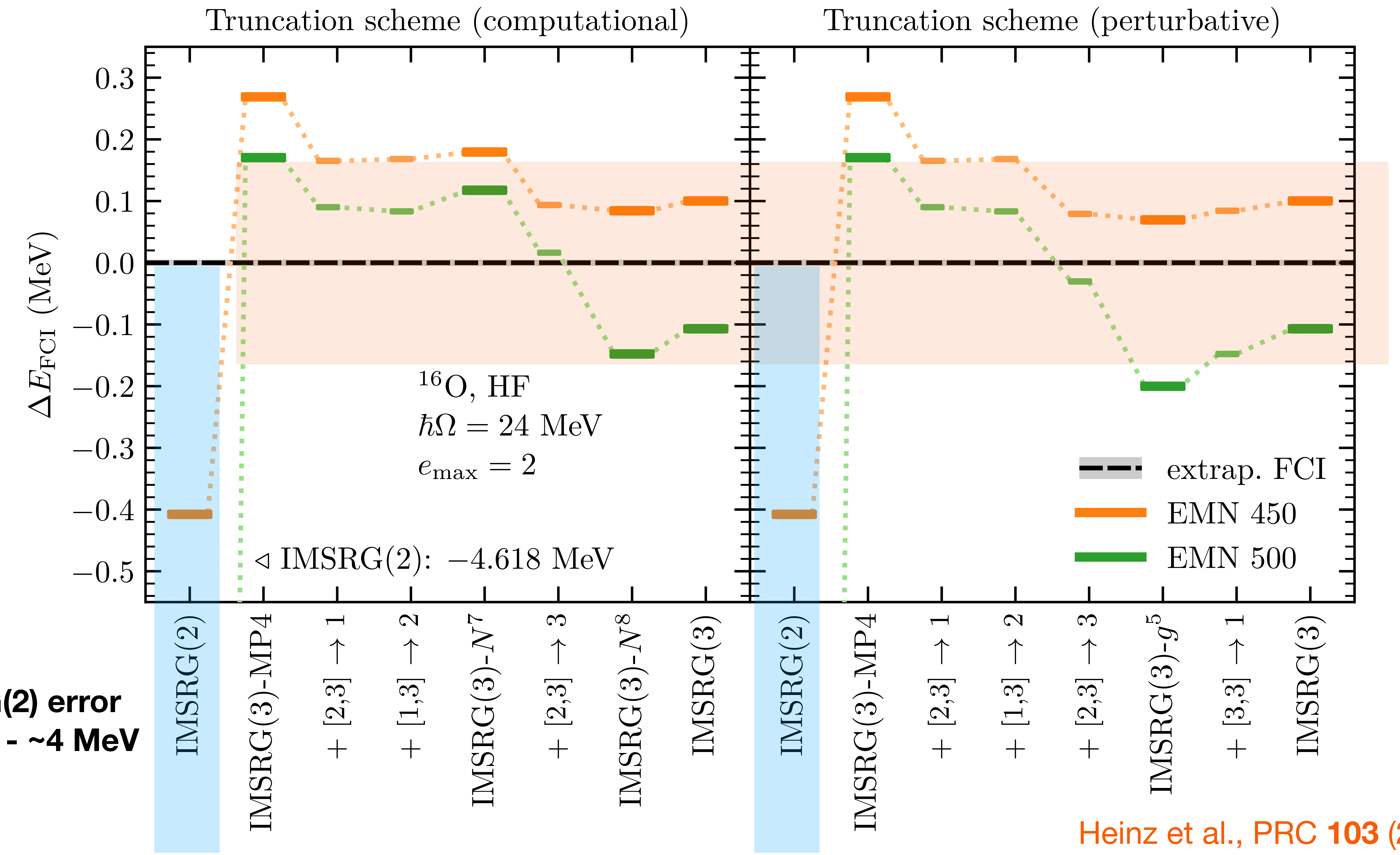


IMSRG(2) error
400 keV - ~4 MeV

Heinz et al., PRC **103** (2021)

The IMSRG(3) difference



IMSRG(3) error ~150 keV

IMSRG(2) error 400 keV - ~4 MeV

Heinz et al., PRC **103** (2021)

The technical details...

- Hamiltonian: EM 1.8/2.0
- NAT basis: $e_{\max}^{\mathrm{NAT}} = 16, E_{3\max}^{\mathrm{NAT}} = 22$
- Truncate to smaller $e_{\max}$ for IMSRG
- NO2B initial Hamiltonian
- Capture induced 3B interactions
  via IMSRG(3): $e_{\max,3\mathrm{b}}, E_{3\max}$
- Employ IMSRG(3)-N^7 truncation

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Pragmatic approach:

Work with converged IMSRG(2) and try to capture 3B effects at minimal computational cost

Goal: Converge 3B w.r.t. $e_{\max,3b}, E_{3\max}$

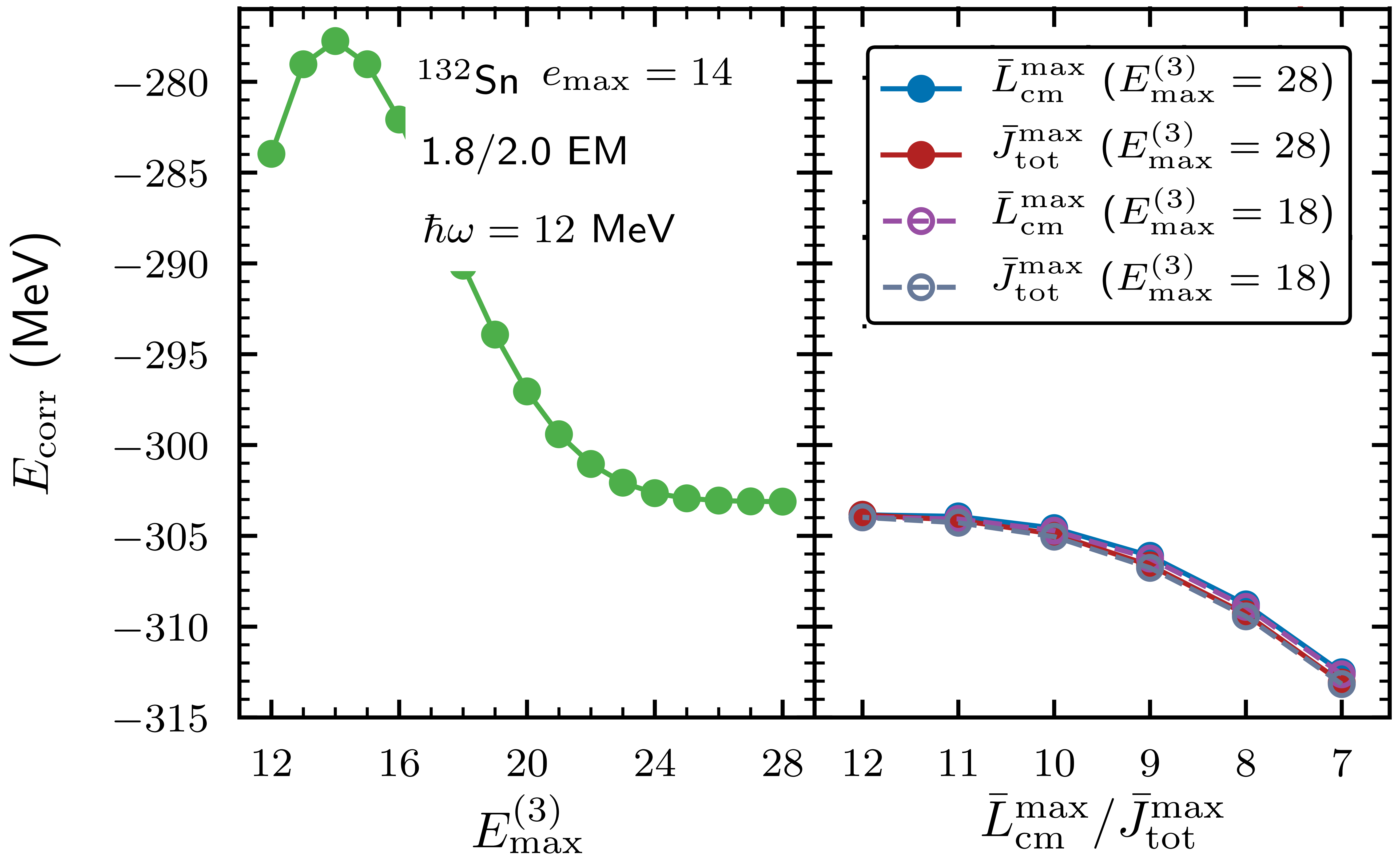
IMSRG(2) as a solid NO2B base

- NAT basis = efficient computational basis

  Tichai et al., PRL **99** (2019)
  Hoppe et al., PRC **103** (2021)
  Novario et al., PRC **102** (2020)

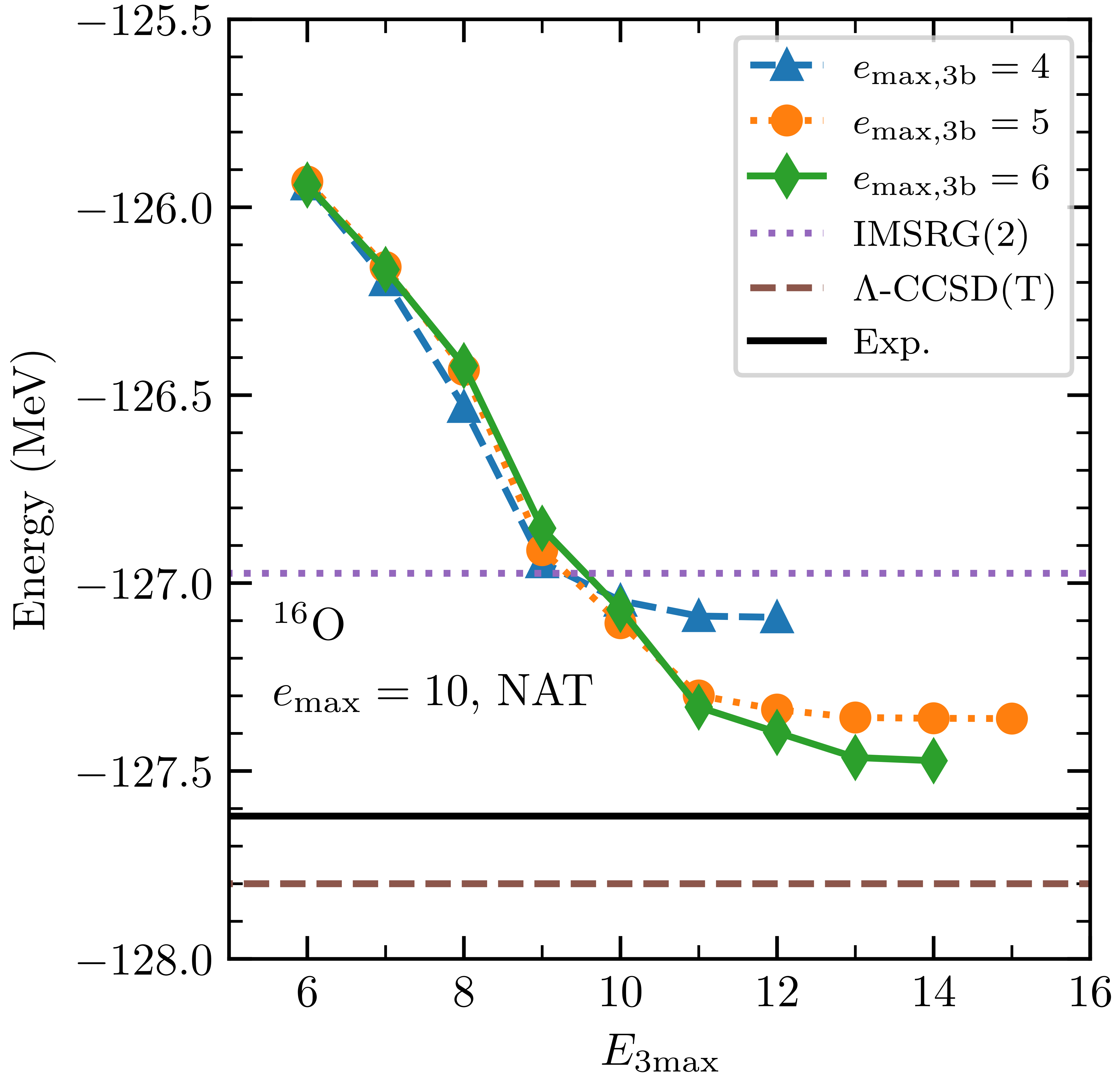
- New treatment of 3N forces in NO2B approximation allow large/no $E_{3\max}$ cut

  Miyagi et al., PRC **105** (2022)
  Hebeler et al., arXiv:2211.16262



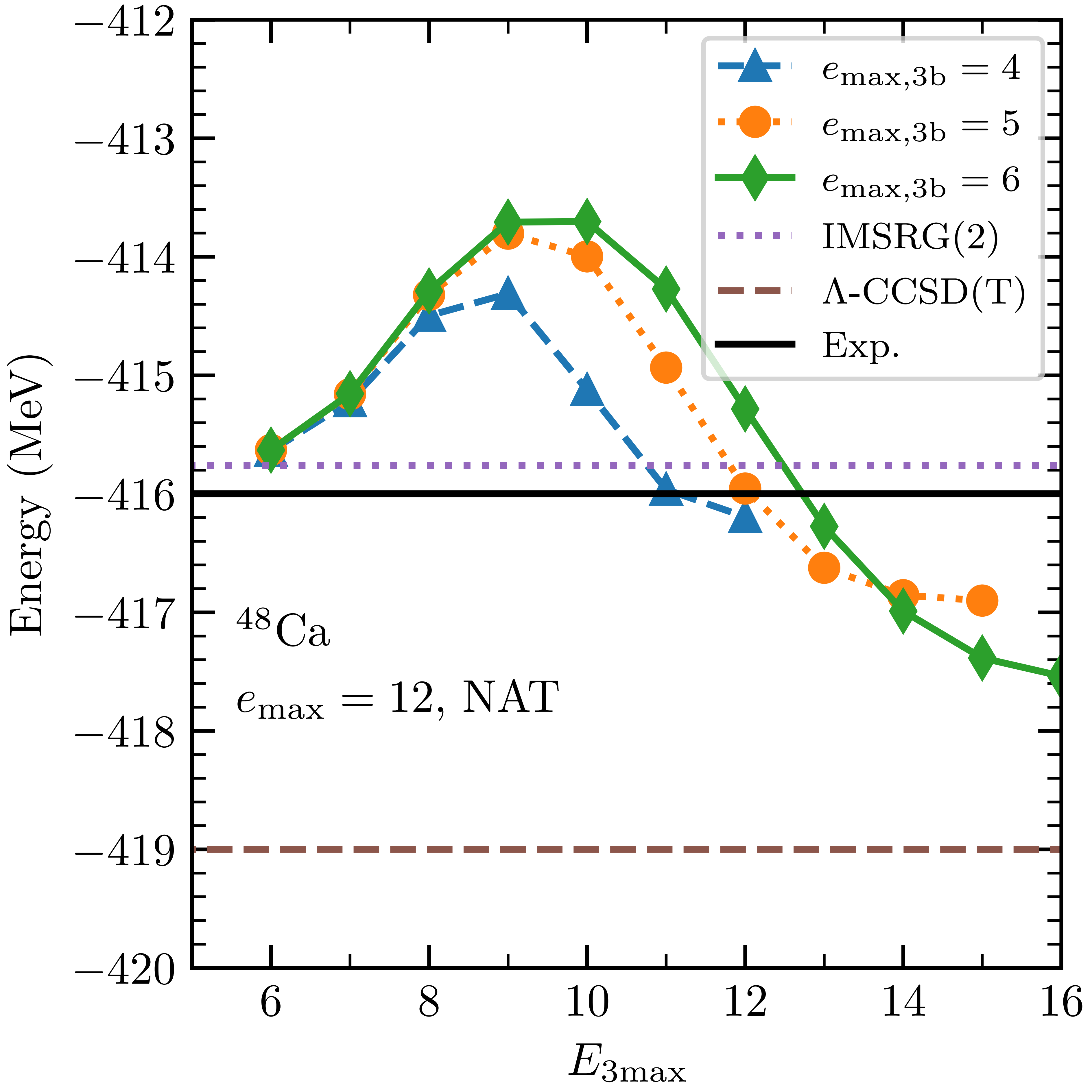
Hebeler et al., arXiv:2211.16262

Oxygen-16: The easy case



- IMSRG(2) converged at $e_{\max} = 10$
- Nice convergence in $E_{3\max}$
- $e_{\max,3b}$ seems converged to ~100 keV
- Apparent consistency with Λ-CCSD(T)

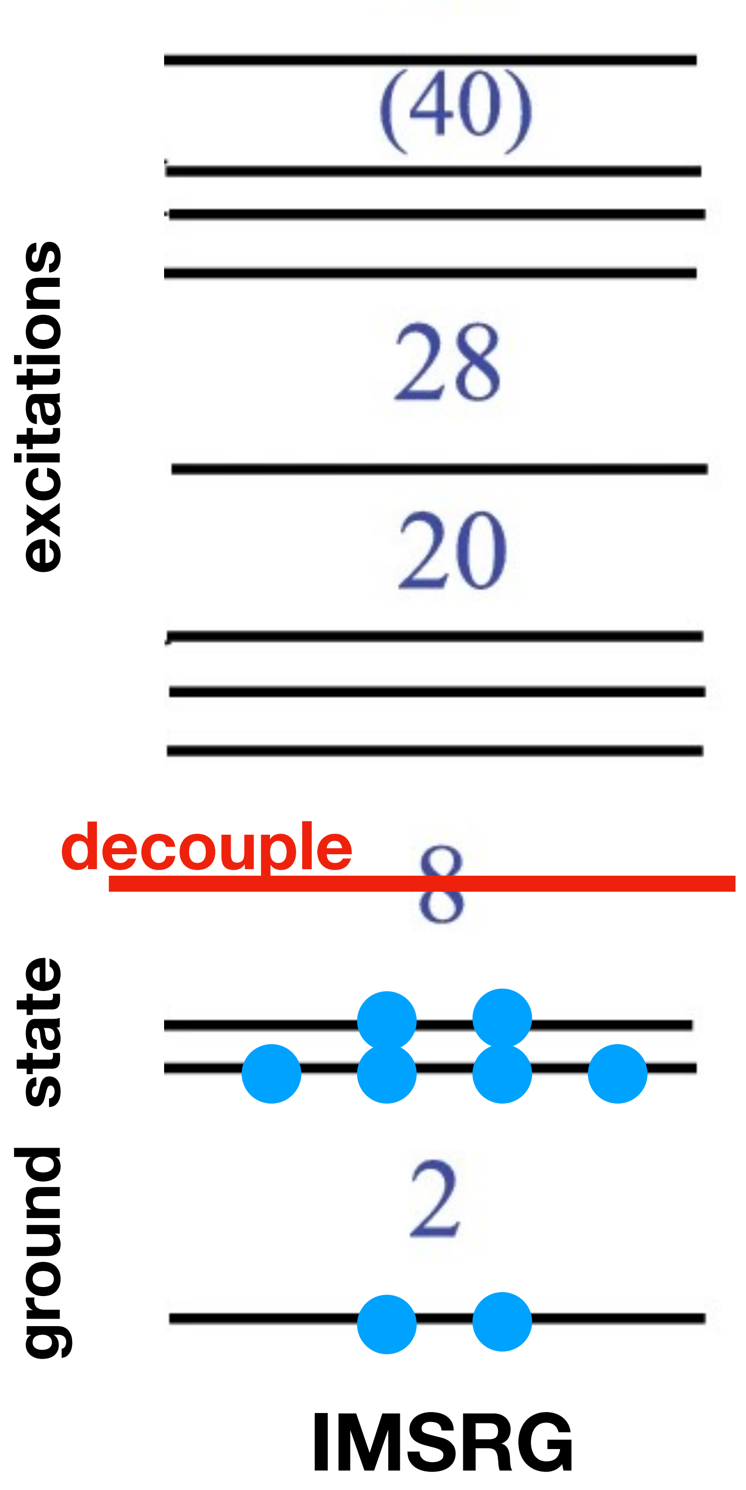
Calcium-48: Not so easy...



- Slow convergence in $e_{\mathrm{max,3b}}$ and $E_{3\mathrm{max}}$
- $E_{3\mathrm{max}} \sim 3e_{\mathrm{max,3b}}$ seems to be required
- Direction of IMSRG(3) corrections consistent with Λ-CCSD(T)

The VS-IMSRG

Stroberg et al., PRL **118** (2017)
Stroberg et al., ARNPS **69** (2019)



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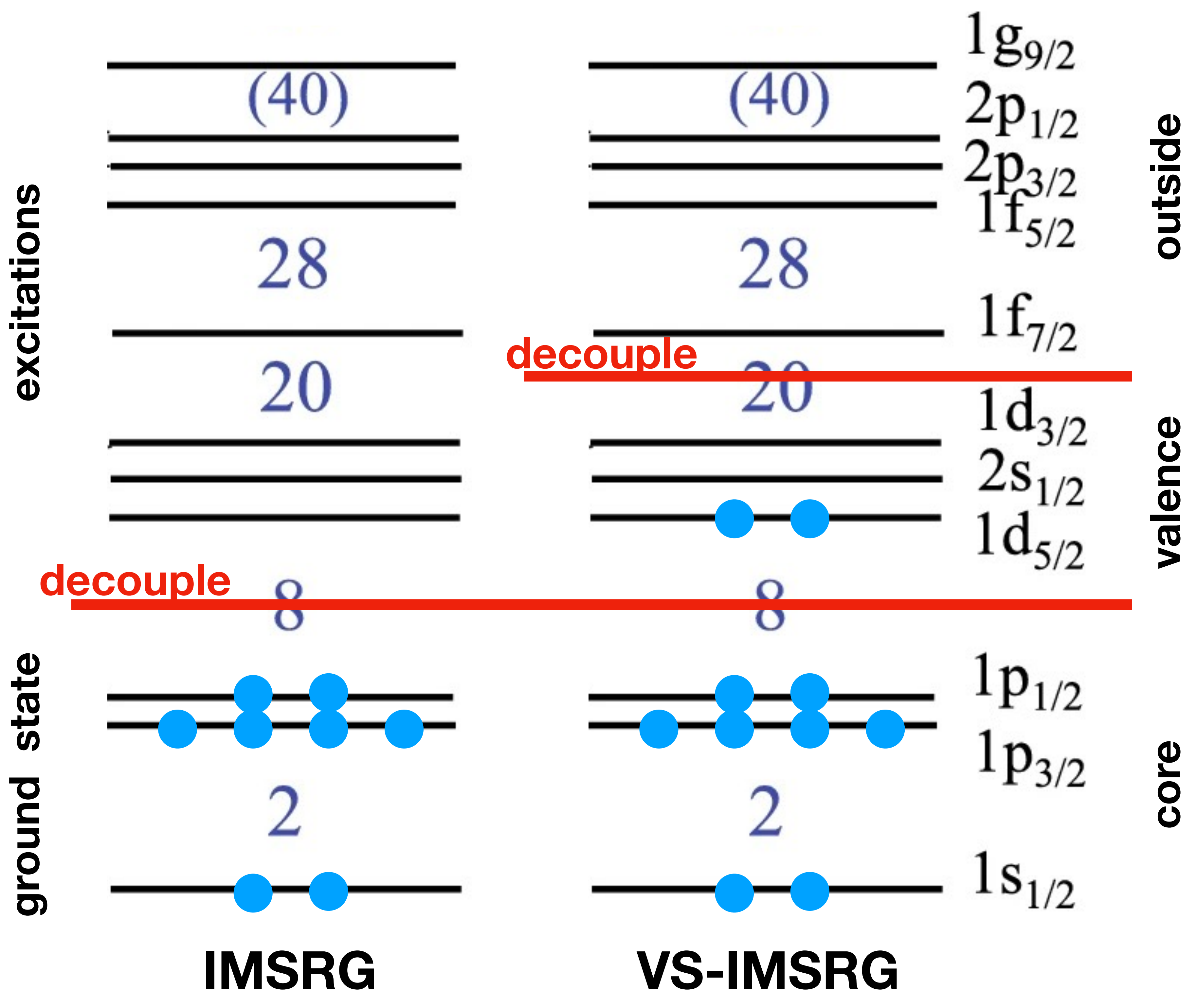

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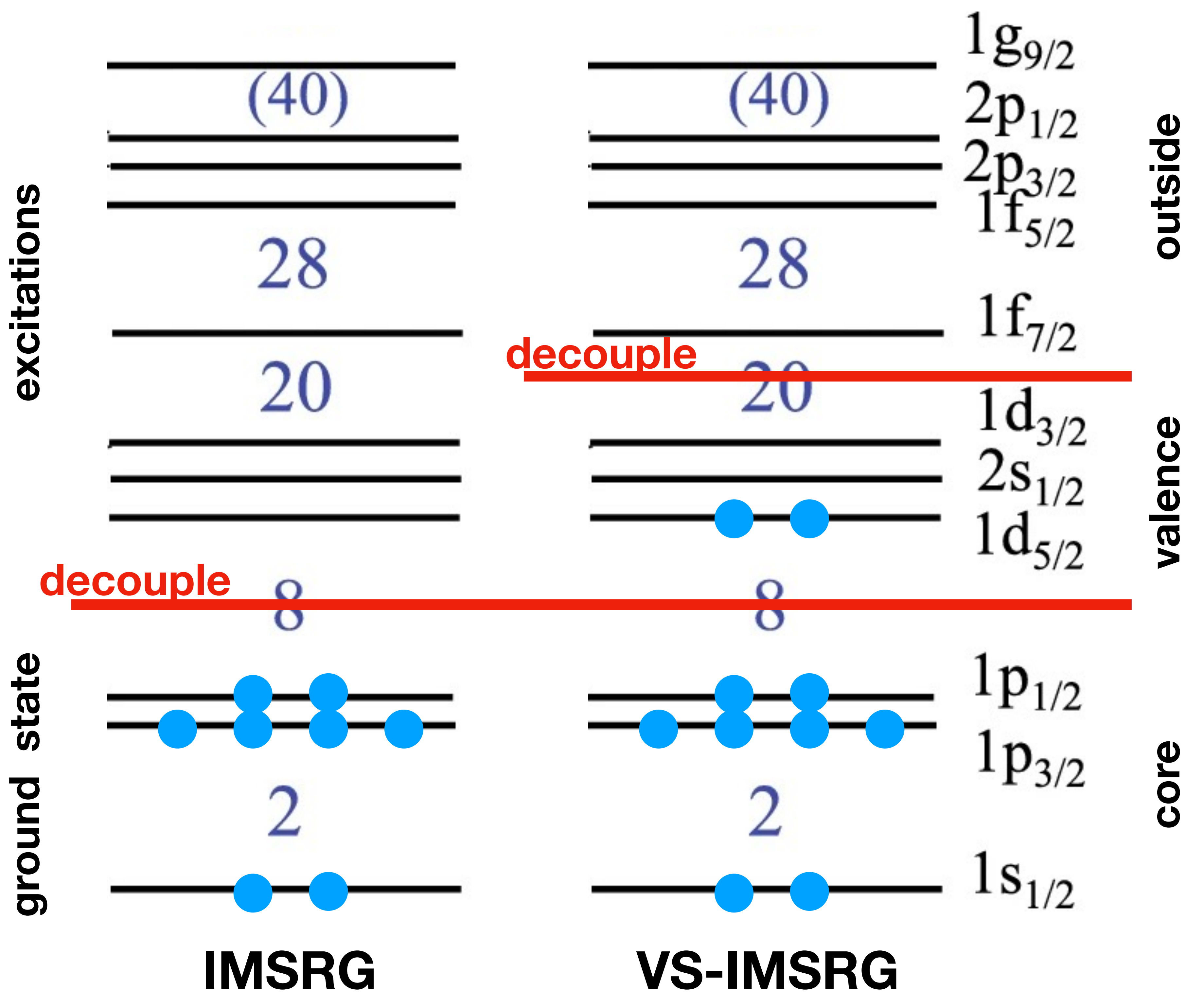

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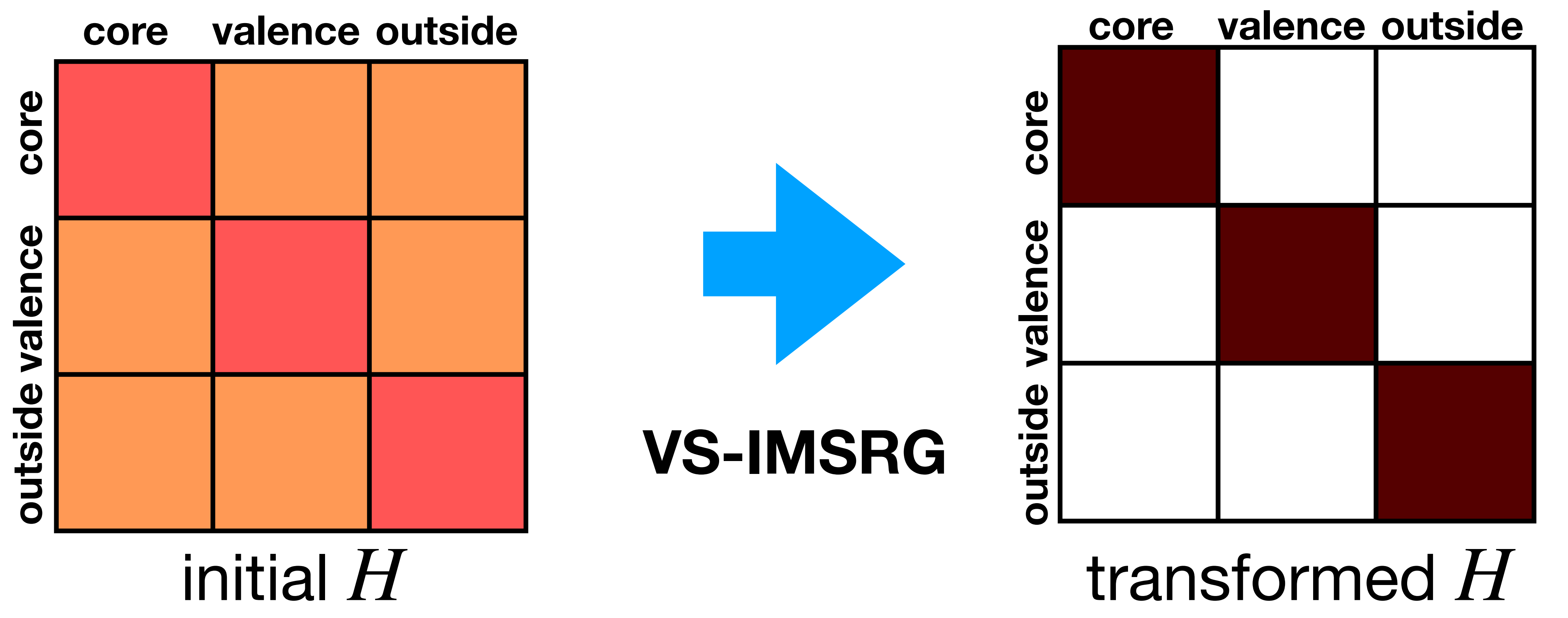
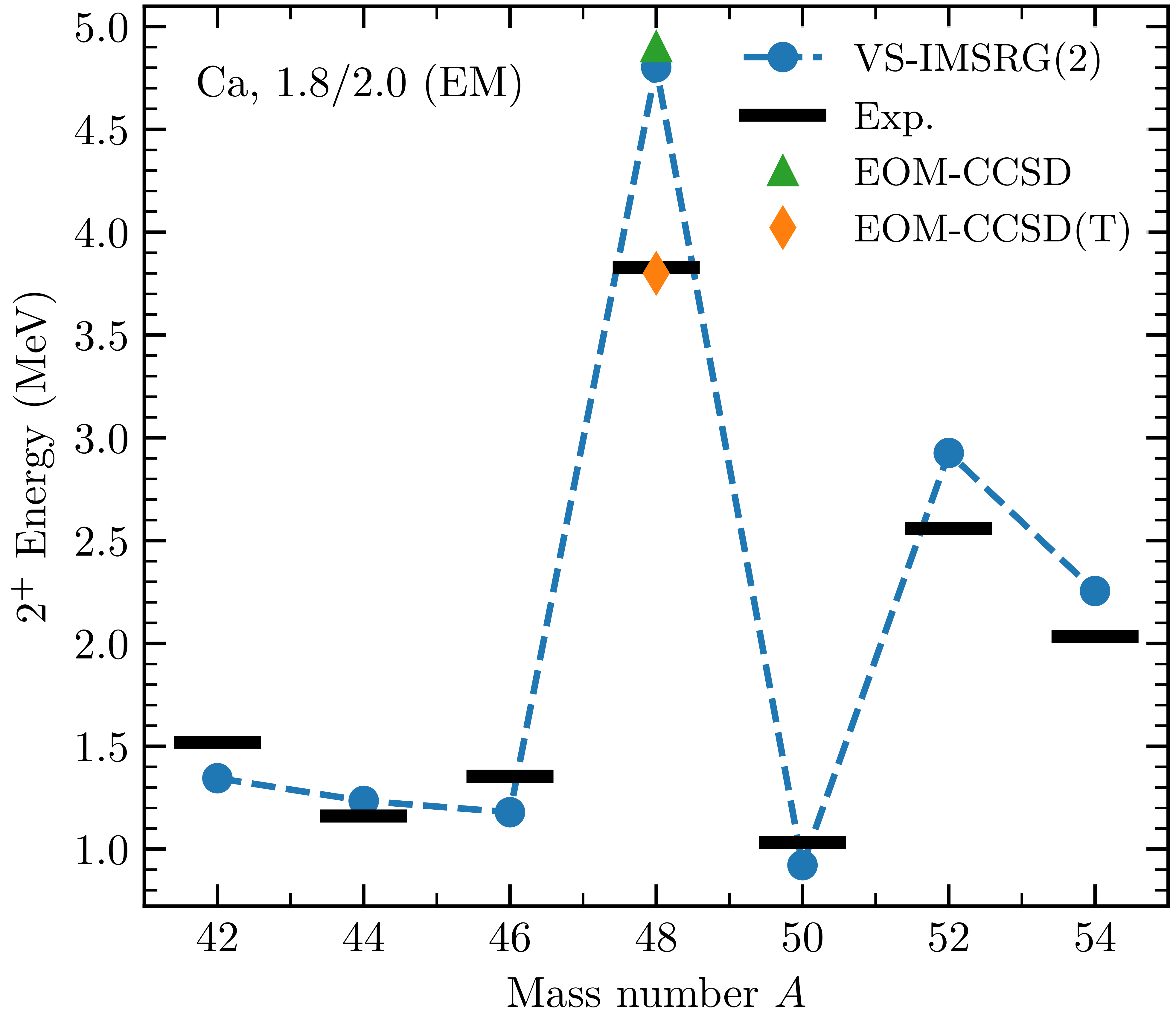


Figure: T. Miyagi

- Decouple core, valence, and outside spaces
- Obtain nucleus-dependent ab initio shell model Hamiltonian
- Can use existing shell model machinery

2^+ energies of calcium-48

- VS-IMSRG(2) overestimates 2^+ energy
- Does VS-IMSRG(3) solve the problem?



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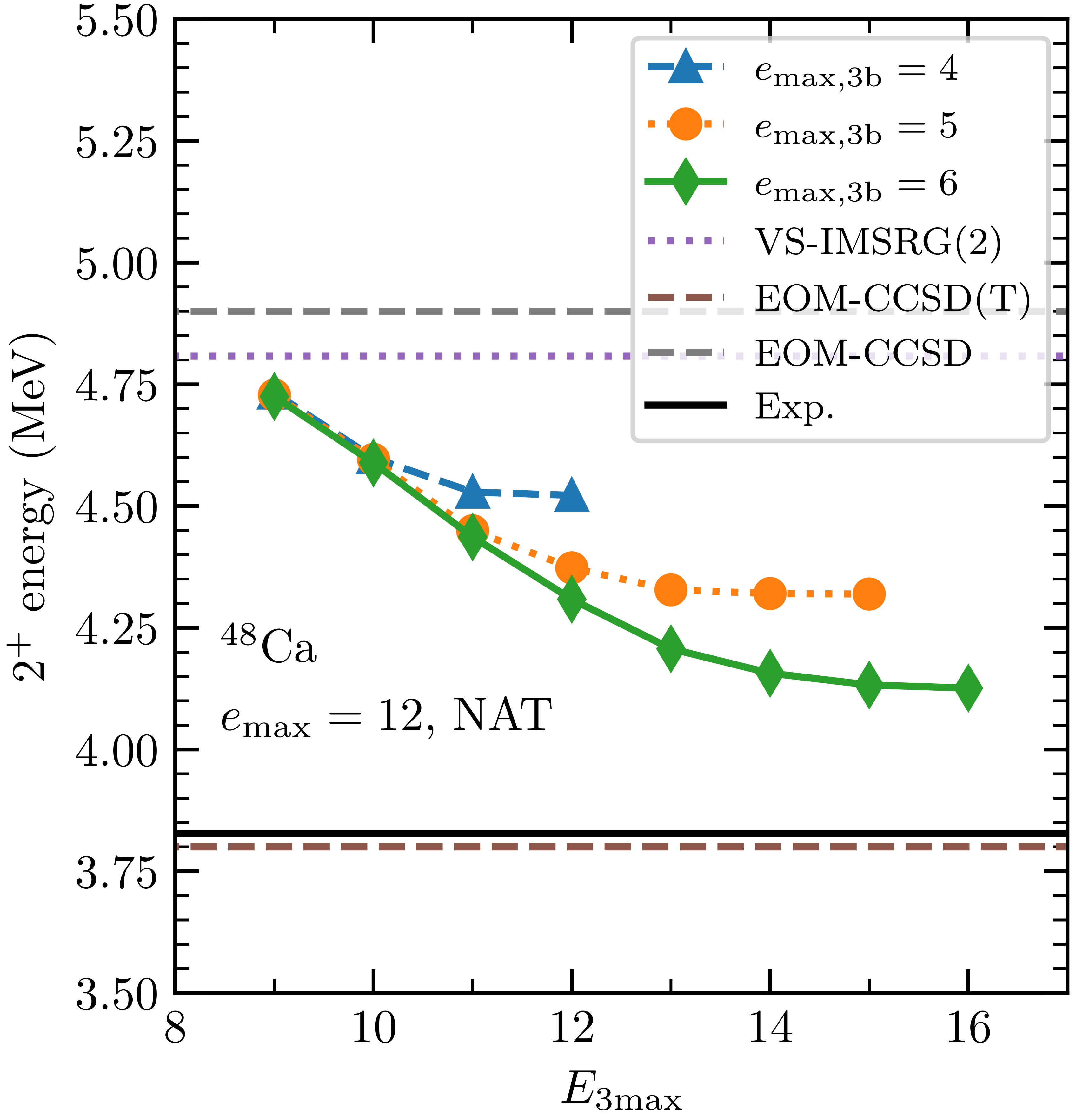
VS-IMSRG(3) convergence: calcium-48



- Corrections improve description of 2^+ energy
- But slow convergence in $e_{\mathrm{max,3b}}$

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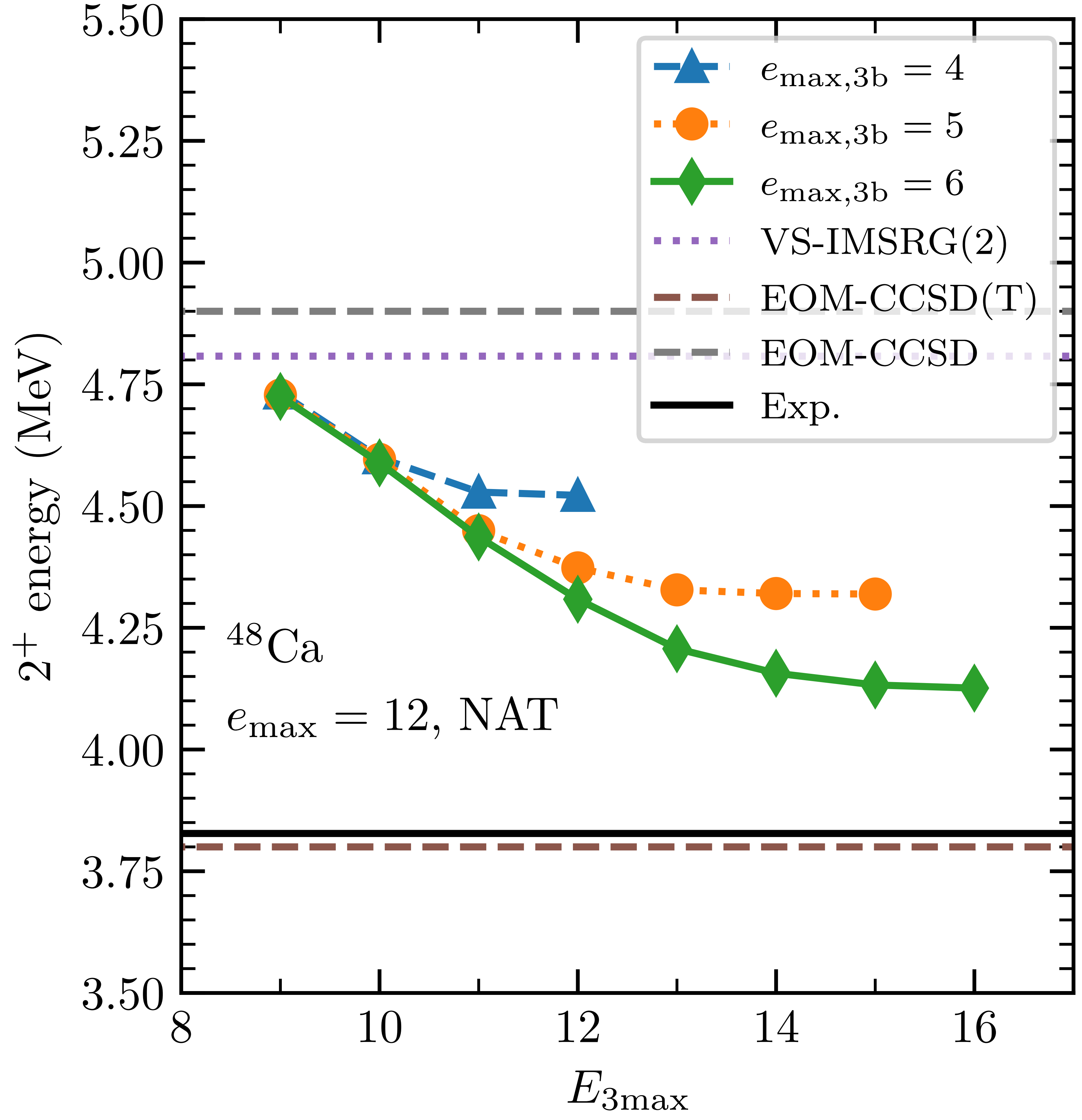


- Corrections improve description of 2^+ energy
- But slow convergence in $e_{\mathrm{max,3b}}$

$e_{\mathrm{max,3b}}$, $E_{3\mathrm{max}}$ seem to be inefficient.

Investigate improved bases for 3-body operators

Novario et al., PRC **102** (2020)

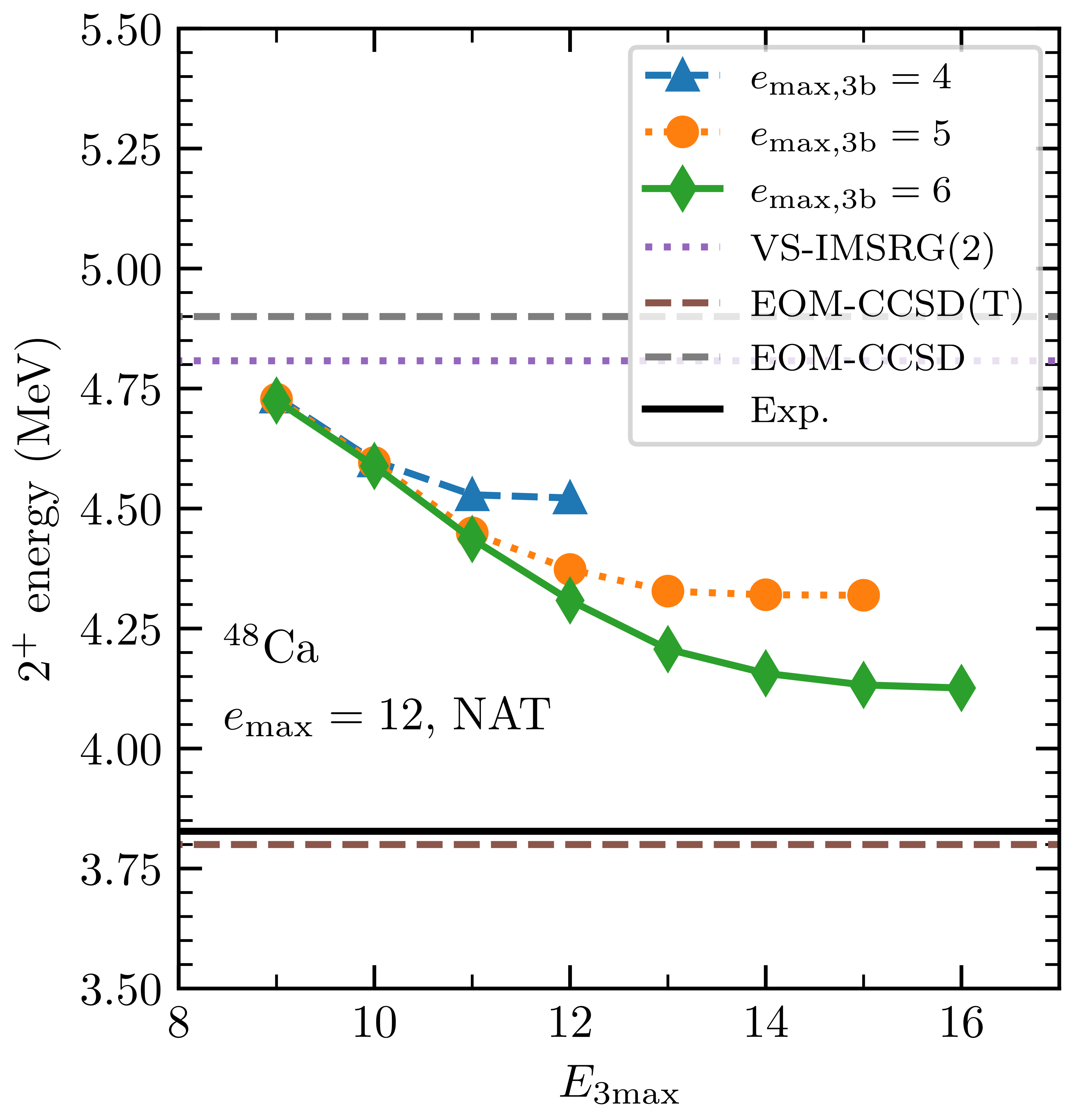
Conclusions and outlook

- Approaching **realistic IMSRG(3) calculations** of medium-mass nuclei

- Small corrections for ground-state energies;
  Larger corrections for 2^+ energies

- Further **optimization** needed
  (basis, numerical implementation)

- Impact of IMSRG(3) in **neutron-rich isotopes**?



Acknowledgments

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- TU Darmstadt "STRONGINT" group
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