Structure and electric dipole response of open-shell nuclei from coupled-cluster theory

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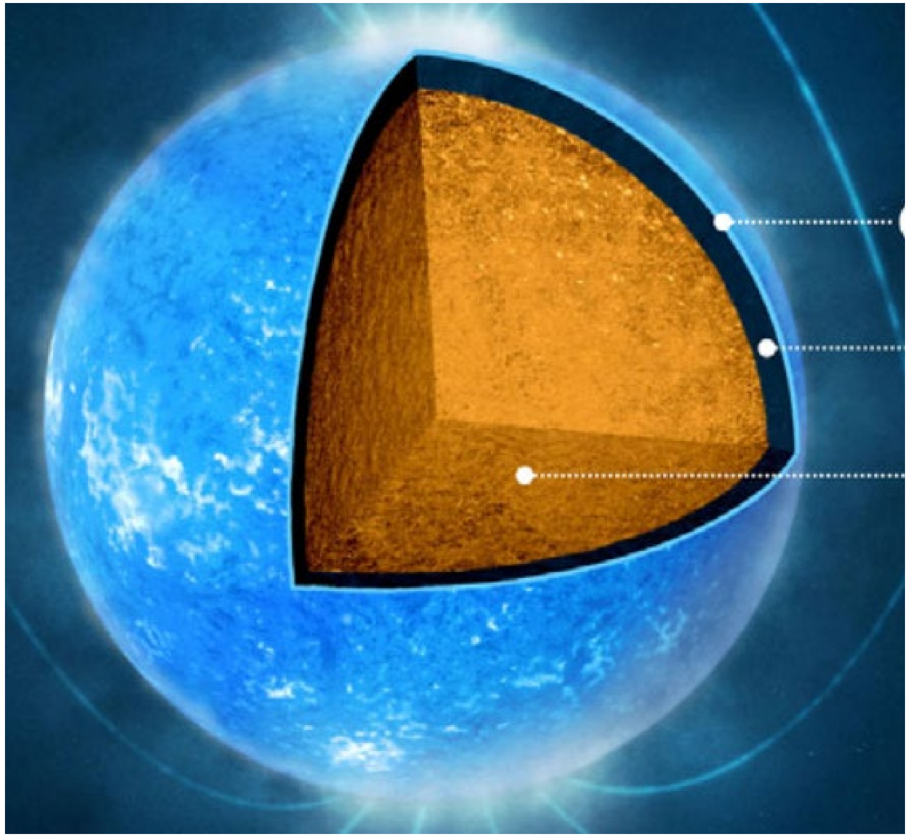
Johannes Gutenberg-Universität Mainz

14th International Spring Seminar on Nuclear Physics, Ischia, Italy

Nuclear matter

Neutron star



Watts et al., Rev. Mod. Phys. **88**, 021001 (2016)

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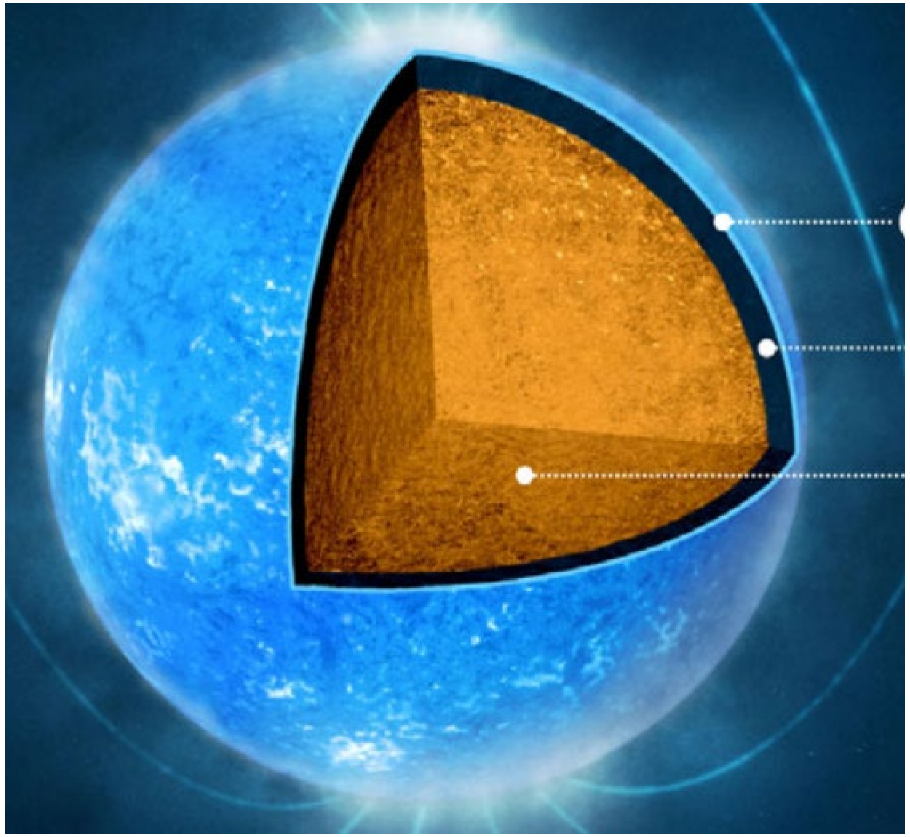
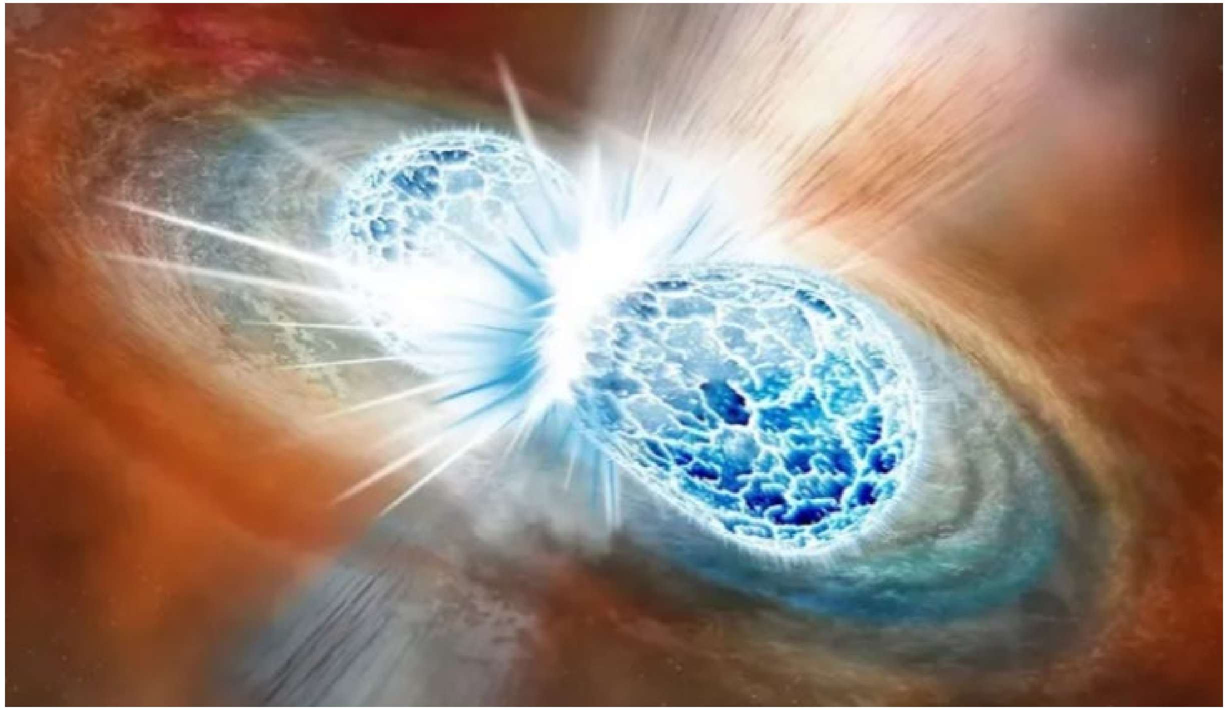


Neutron stars merger



Watts et al., Rev. Mod. Phys. **88**, 021001 (2016)

Nuclear matter equation of state

$$\frac{E}{A}(\rho,\beta) = \frac{E}{A}(\rho,0) + S(\rho)\beta^2 + O(\beta^4)$$

$$\rho = \rho_n + \rho_p$$

$$\beta = \frac{\rho_n - \rho_p}{\rho}$$

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Symmetry energy

$$S(\rho) = J \; + \; \frac{\rho - \rho_0}{3\rho_0} L$$

$$\rho_0 = 0.16 \text{ fm}^{-3}$$

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J: symmetry energy
at saturation density

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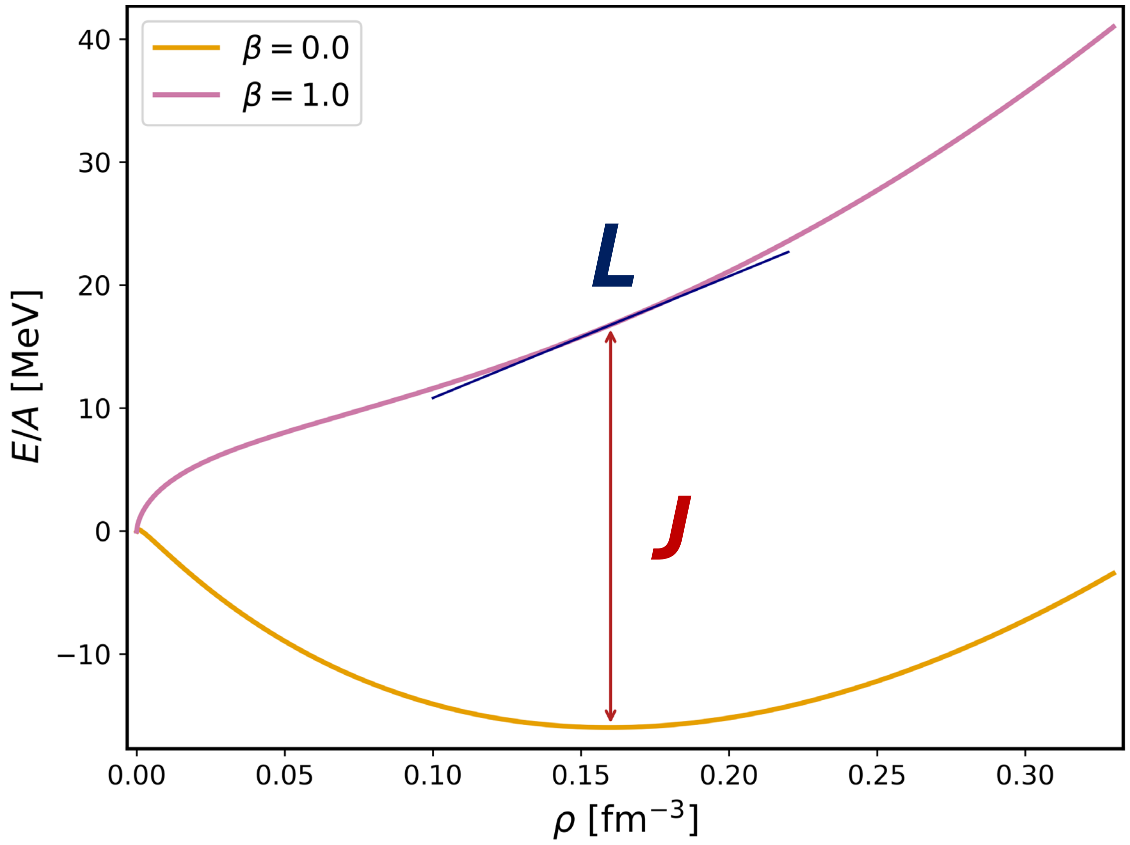
Symmetry energy

$$S(\rho) = \boxed{J} + \frac{\rho-\rho_0}{3\rho_0}\boxed{L}$$

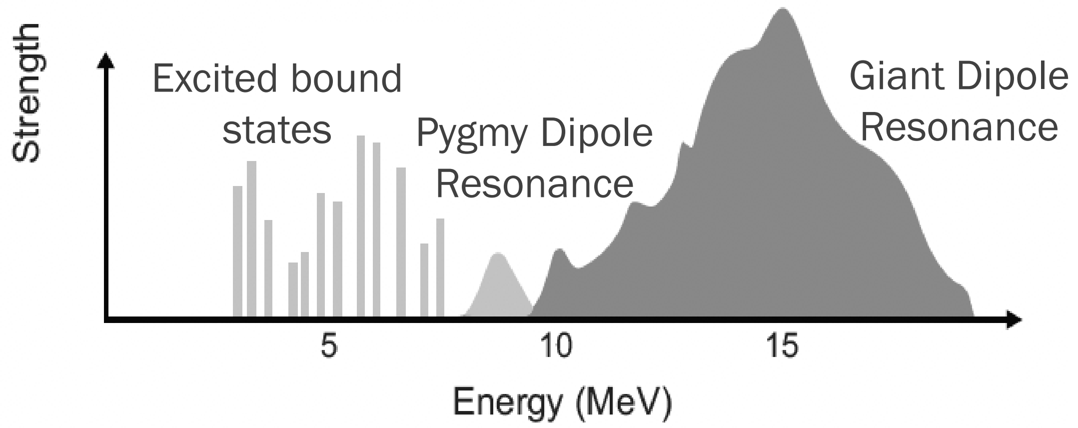
J: symmetry energy at saturation density

L: slope parameter



How to constrain L?

Response function $R(\omega)$



Electric dipole response

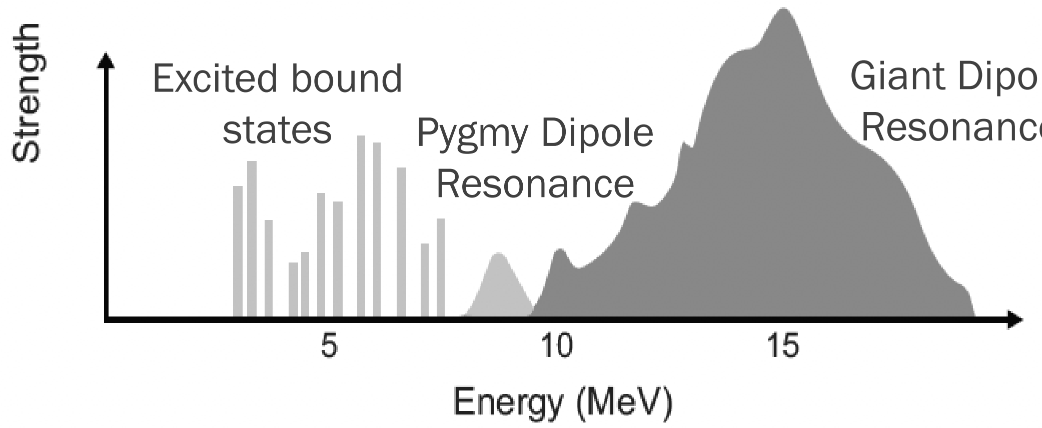
Electric dipole polarizability

$$\alpha_D = 2\alpha \int d\omega \frac{R(\omega)}{\omega}$$

How to constrain L?

Electric dipole response

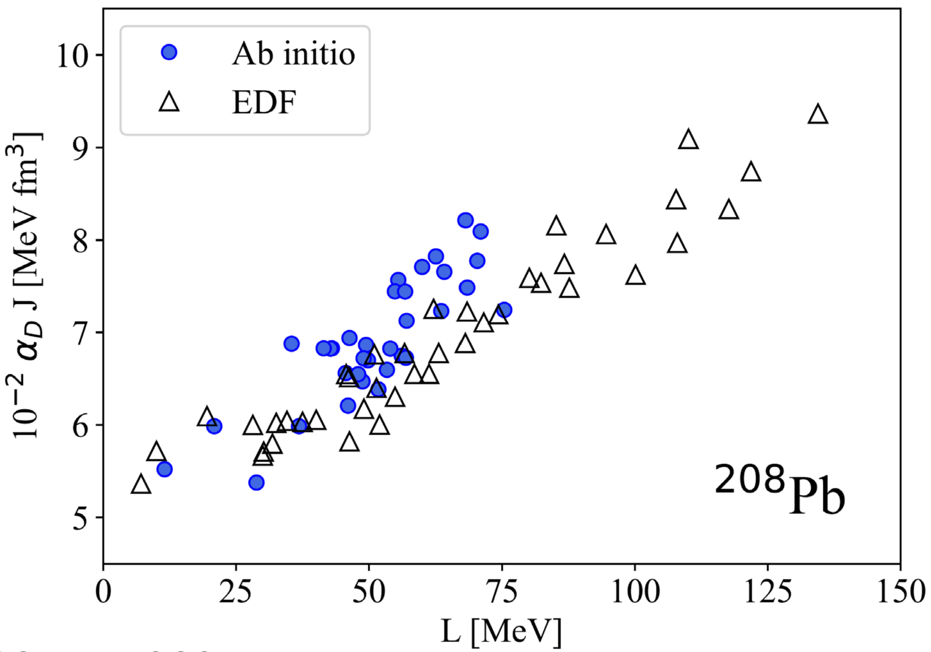
Response function $R(\omega)$



Electric dipole polarizability

$$\alpha_D = 2\alpha \int d\omega \frac{R(\omega)}{\omega}$$

Courtesy: Francesca Bonaiti



Strong linear **correlation** between α_D and the **slope** of the symmetry energy L

Coupled-cluster theory

Coupled-cluster (CC) ground-state $$|\Psi_0\rangle = e^T|\Phi_0\rangle$$

Hagen et al., Rep. Prog. Phys. **77**, 096302 (2014)

Coupled-cluster theory

Coupled-cluster (CC) ground-state

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$T \approx T_1 + T_2 + T_3 + \cdots$ *n*-particle *n*-hole amplitudes

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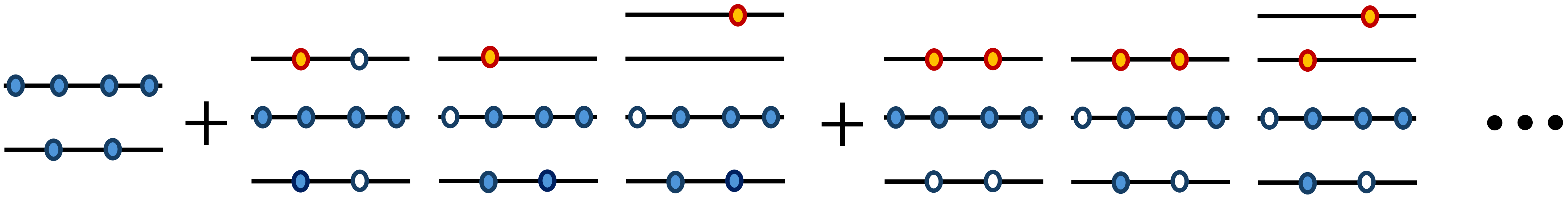
$|\Psi_0\rangle =$



$|\Phi_0\rangle$ $\quad$ $1p1h$ excitations $\quad$ $2p2h$ excitations

Hagen et al., Rep. Prog. Phys. **77**, 096302 (2014)

Coupled-cluster theory

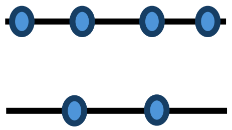
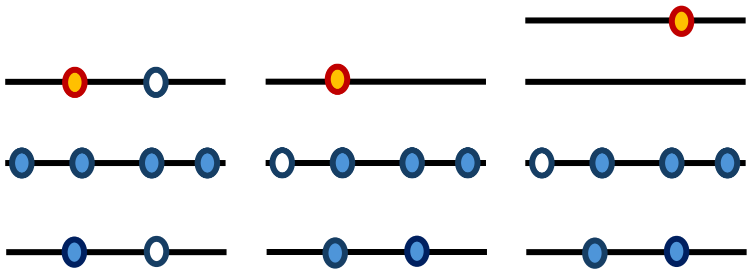
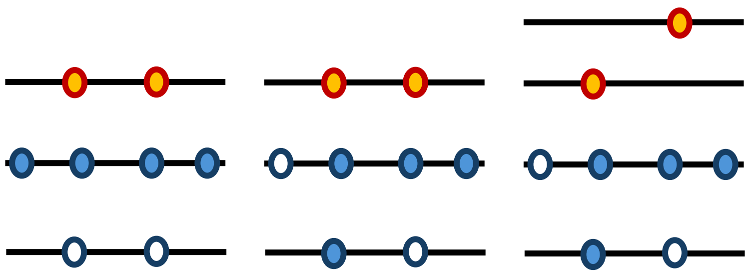
Coupled-cluster (CC) ground-state

$$|\Psi_0\rangle = e^{T}\boxed{|\Phi_0\rangle}$$

$|\Phi_0\rangle$ Reference state

$$T \approx \underbrace{T_1 + T_2}_{\text{CCSD}} + T_3 + \cdots$$

n-particle *n*-hole amplitudes

$|\Psi_0\rangle =$  $+$  $+$  $\cdots$

$|\Phi_0\rangle$ $1p1h$ excitations $2p2h$ excitations

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Coupled-cluster theory

Coupled-cluster (CC) ground-state

$$|\Psi_0\rangle = e^{T}|\Phi_0\rangle$$

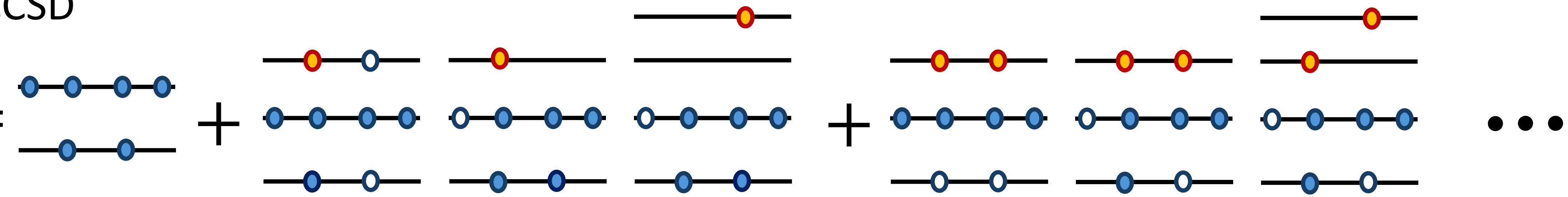
$|\Phi_0\rangle$ Reference state

CCSDT-1: approximate triples

$$T \approx T_1 + T_2 + T_3 + \cdots$$

n-particle *n*-hole amplitudes

CCSD

$|\Psi_0\rangle =$ 

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Challenges

Unified treatment of nuclear **structure** and **response** functions

Open-shell nuclei

Part 1:
Structure of open-shell nuclei

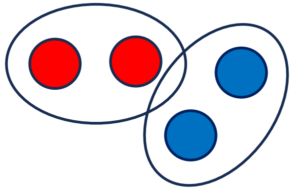
Open-shell nuclei from coupled-cluster theory

Symmetry-breaking approaches

Open-shell nuclei from coupled-cluster theory

Symmetry-breaking approaches

Pairing



Bogoliubov CC

Tichai et al., Phys. Lett. B **851**, 138571 (2024)

Open-shell nuclei from coupled-cluster theory

Symmetry-breaking approaches

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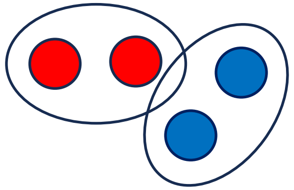
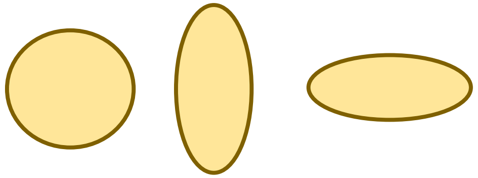


Bogoliubov CC

Deformation



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Hagen et al. Phys. Rev. C **105**, 064311 (2022)

Open-shell nuclei from coupled-cluster theory

Symmetry-breaking approaches

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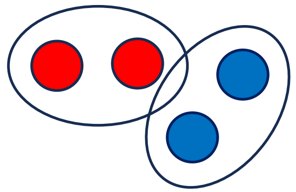

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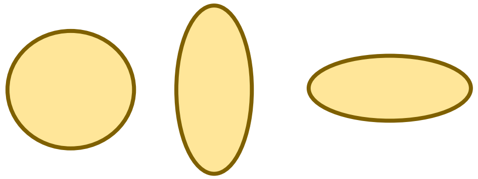

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Equations-of-motion

Open-shell nuclei from coupled-cluster theory

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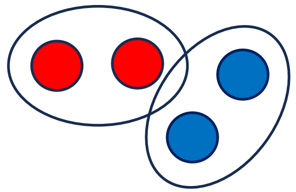

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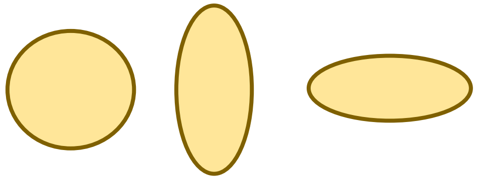

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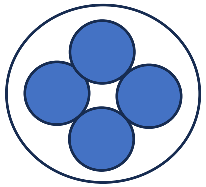
Equations-of-motion

Closed-shell

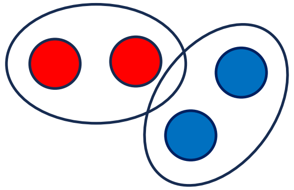


$$|\Psi_0\rangle = e^T|\Phi_0\rangle$$

Open-shell nuclei from coupled-cluster theory

Symmetry-breaking approaches

Pairing



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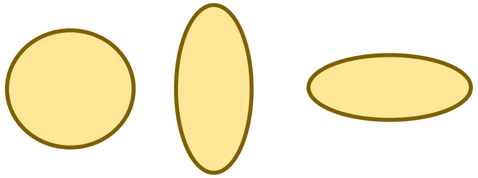

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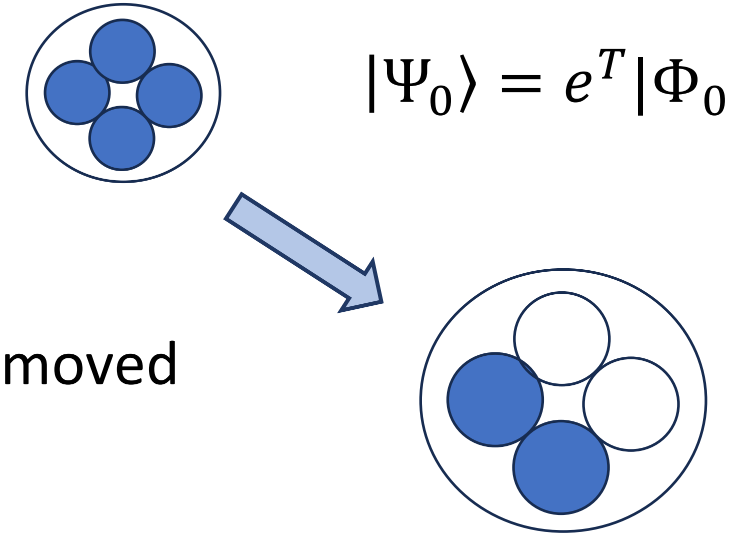


$$|\Psi_0\rangle = e^T|\Phi_0\rangle$$

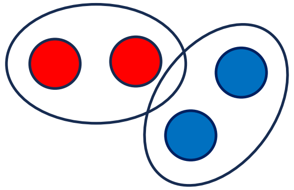
Two-particle-removed (2PR) nucleus

$$|\Psi_f^{(A-2)}\rangle = R_f^{(A-2)}|\Psi_0\rangle$$

Open-shell nuclei from coupled-cluster theory

Symmetry-breaking approaches

Pairing



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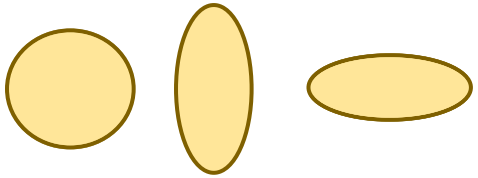

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Equations-of-motion

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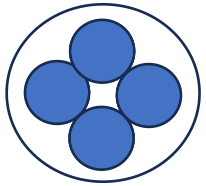
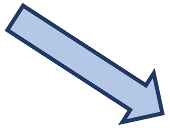


$$|\Psi_0\rangle = e^T|\Phi_0\rangle$$



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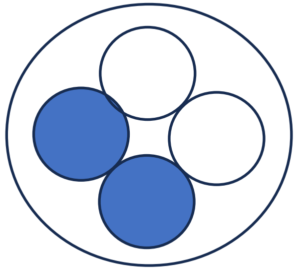
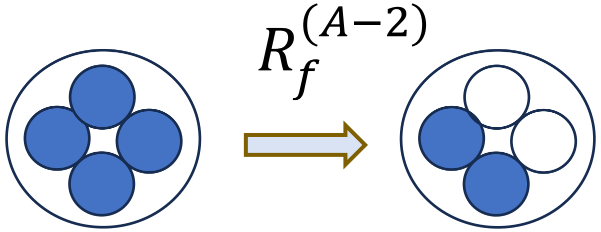


Excitation operator

$$|\Psi_f^{(A-2)}\rangle = R_f^{(A-2)}|\Psi_0\rangle$$

Two-particle-removed coupled-cluster



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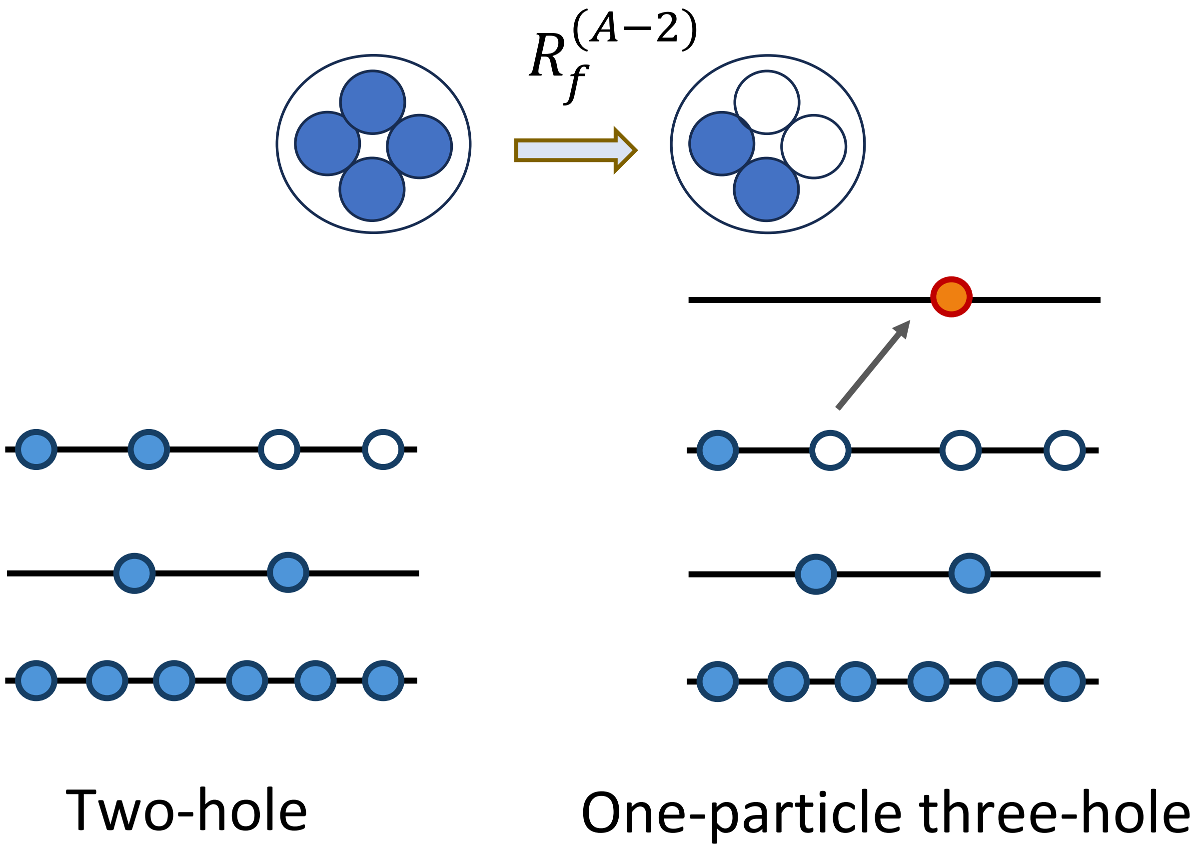
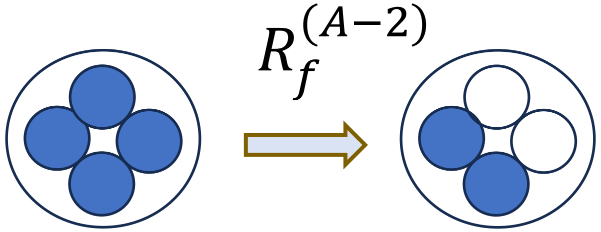
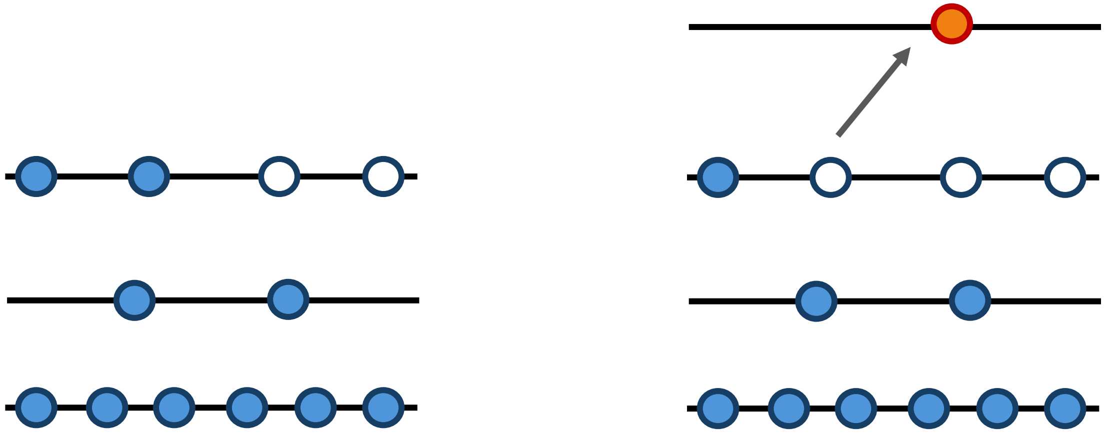


$$R_f^{(A-2)} = \frac{1}{2}\sum_{ij} r_{ij} c_j c_i + \frac{1}{6}\sum_{ijka} r_{ijk}^{a}\, c_a^{\dagger} c_k c_j c_i$$

Two-particle-removed coupled-cluster





Two-hole

One-particle three-hole

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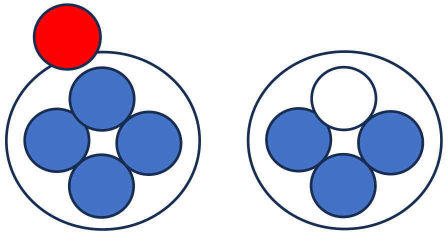
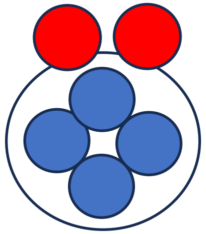
See also



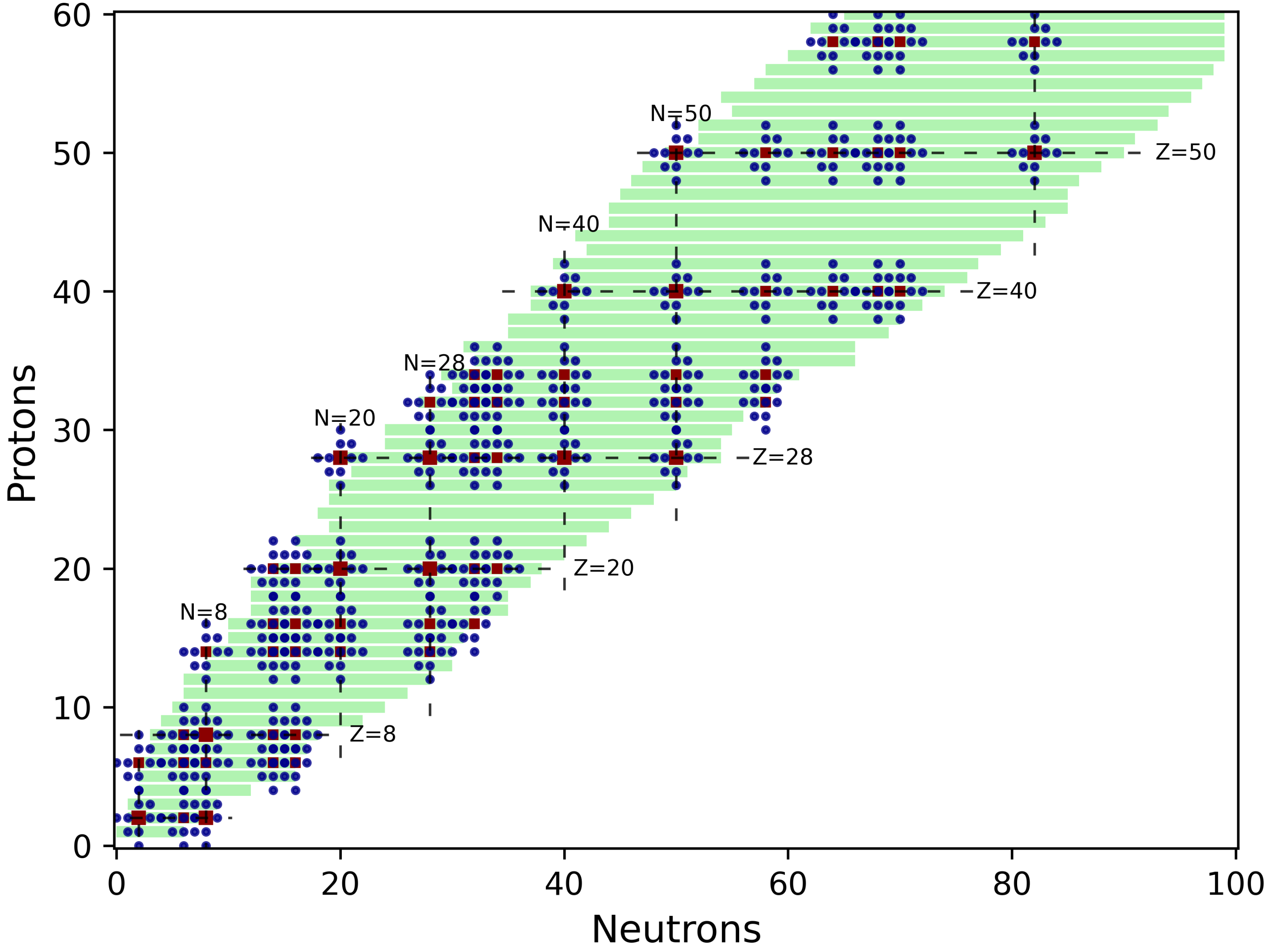
One-particle-attached/ removed (1PA/1PR)



Two-particle-attached (2PA)

Jansen, Phys. Rev. C **88**, 024305 (2013)
Bonaiti et al., PRC **110**, 044306 (2024)

Two-particle-removed coupled-cluster



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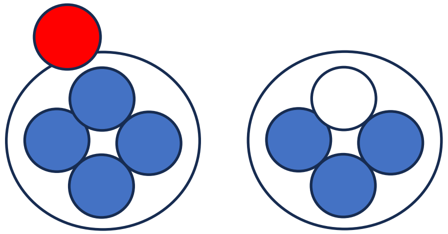

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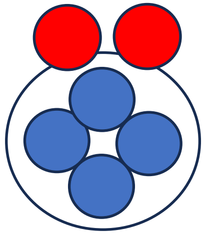

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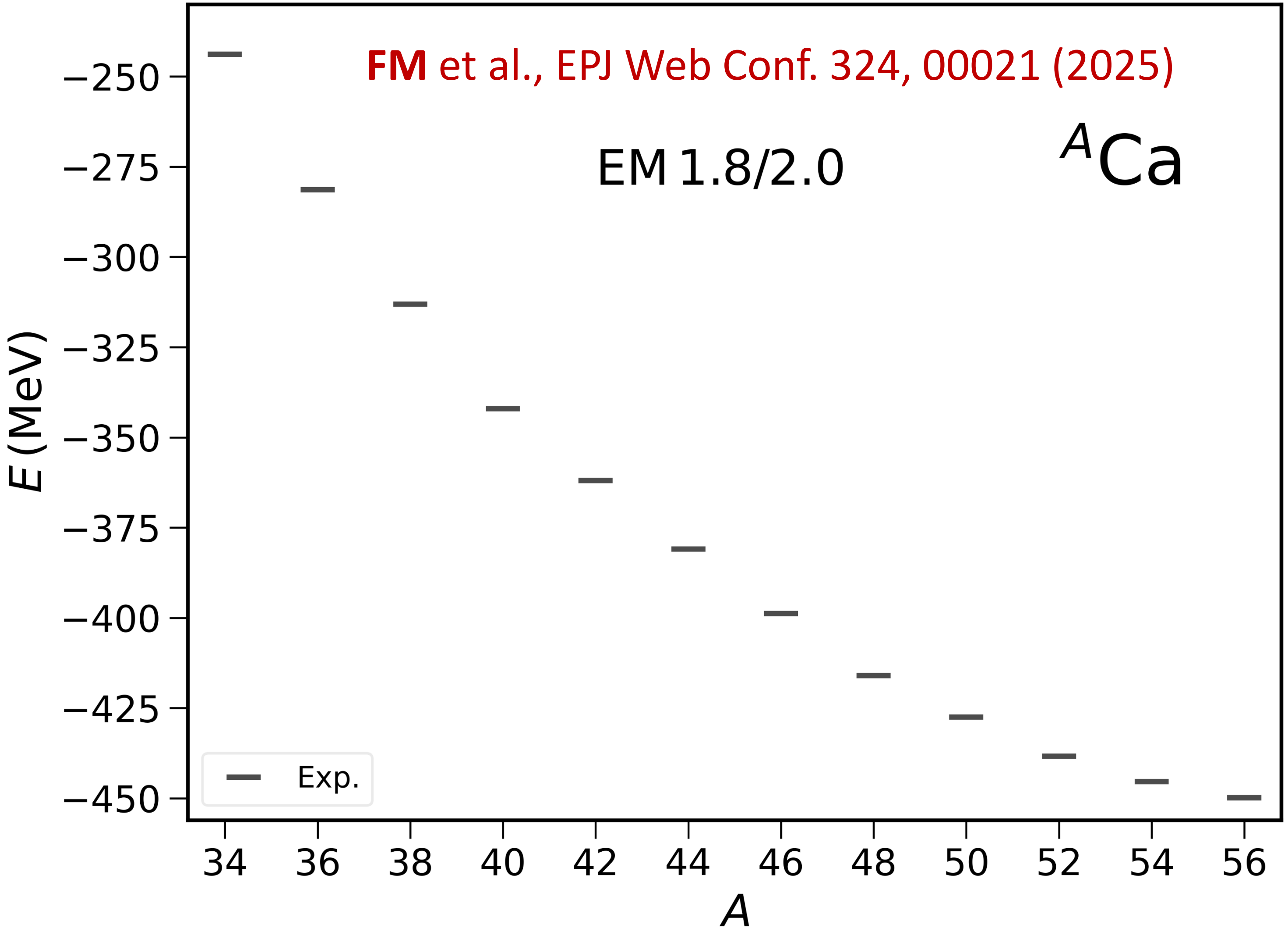
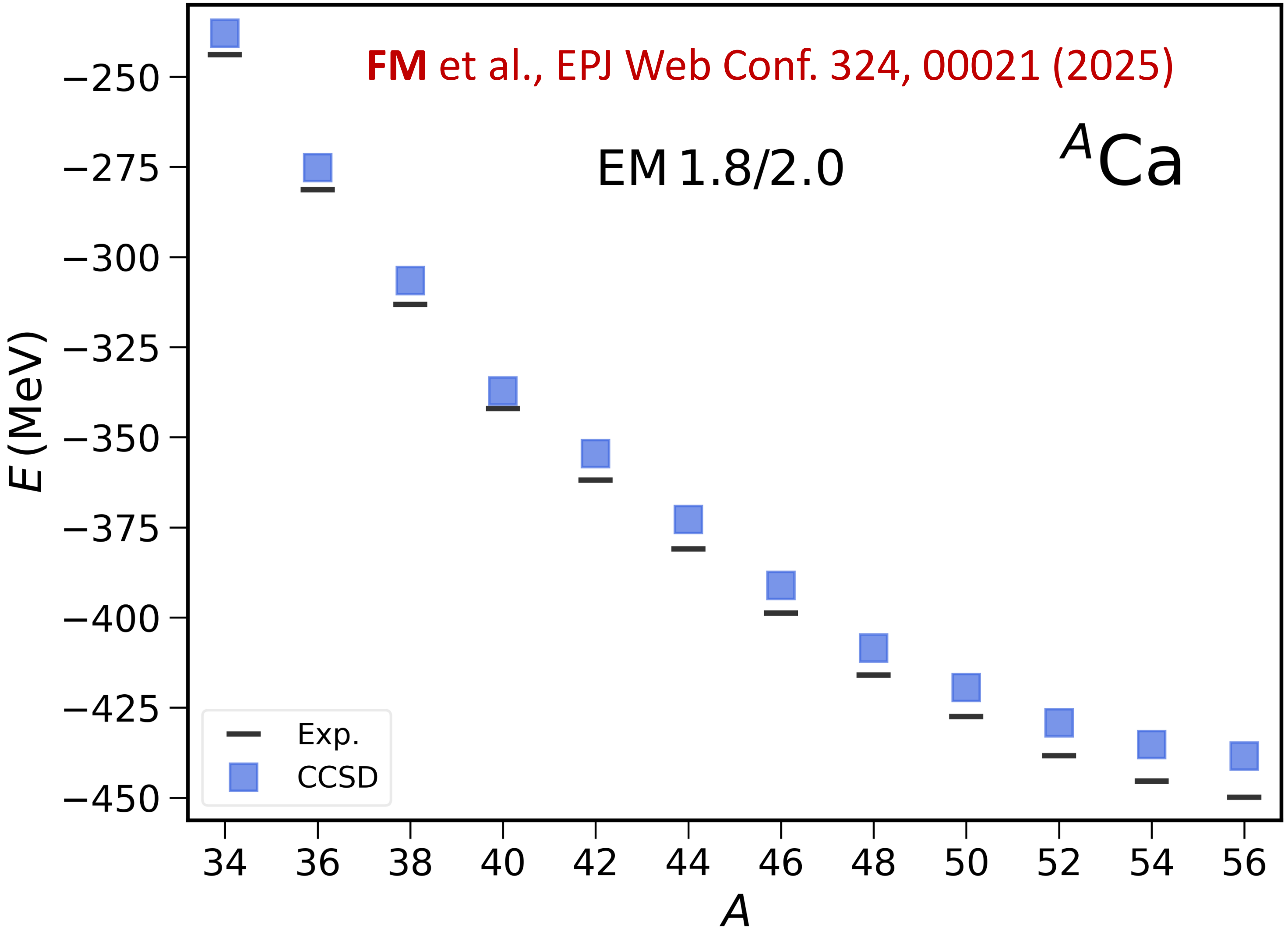
Binding energies - validation



Experiment

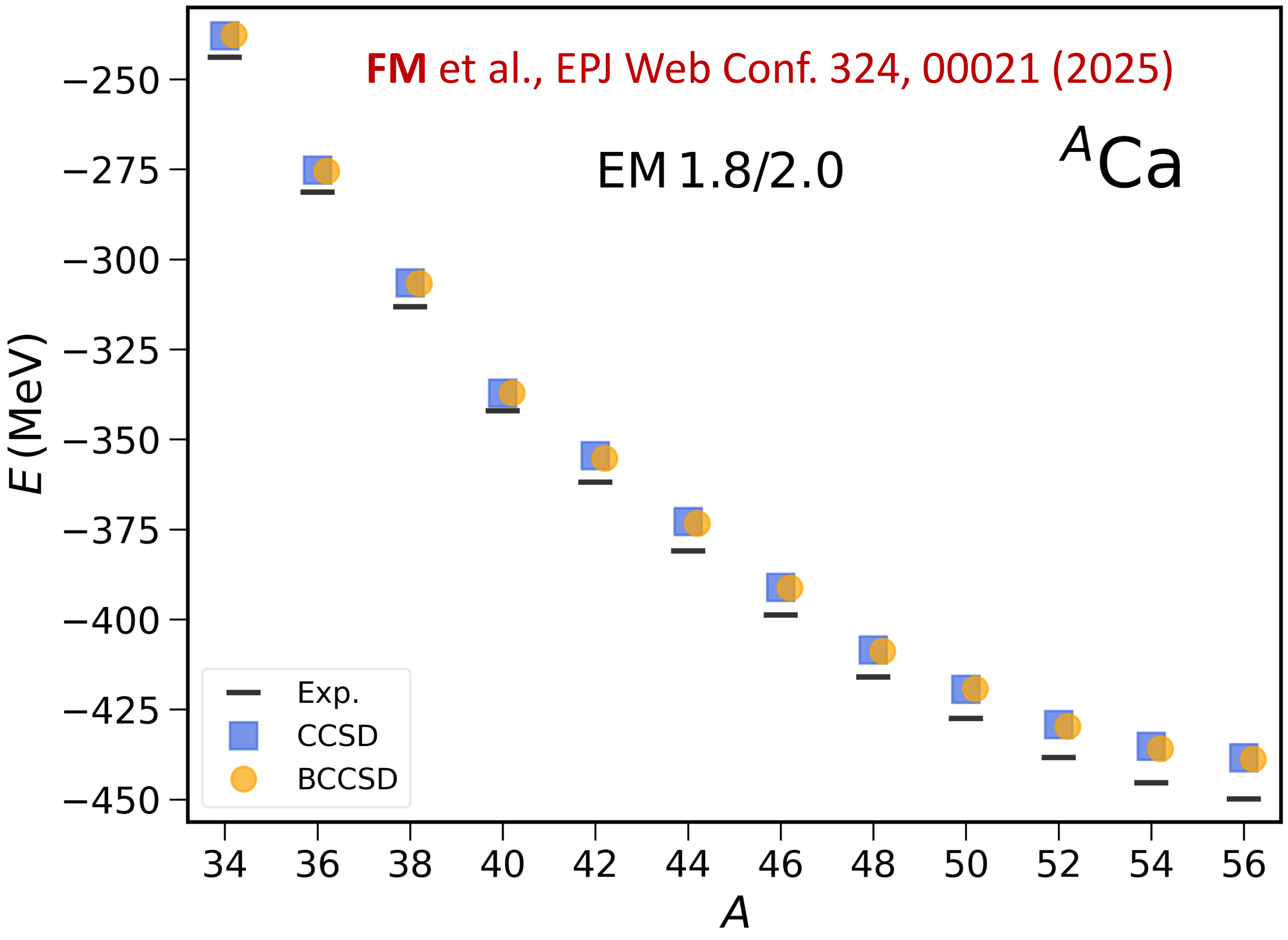
Binding energies - validation

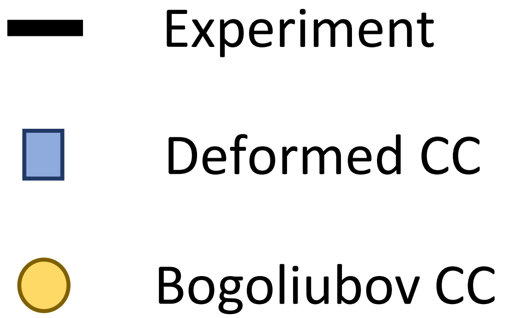


Experiment

Deformed CC

Binding energies - validation





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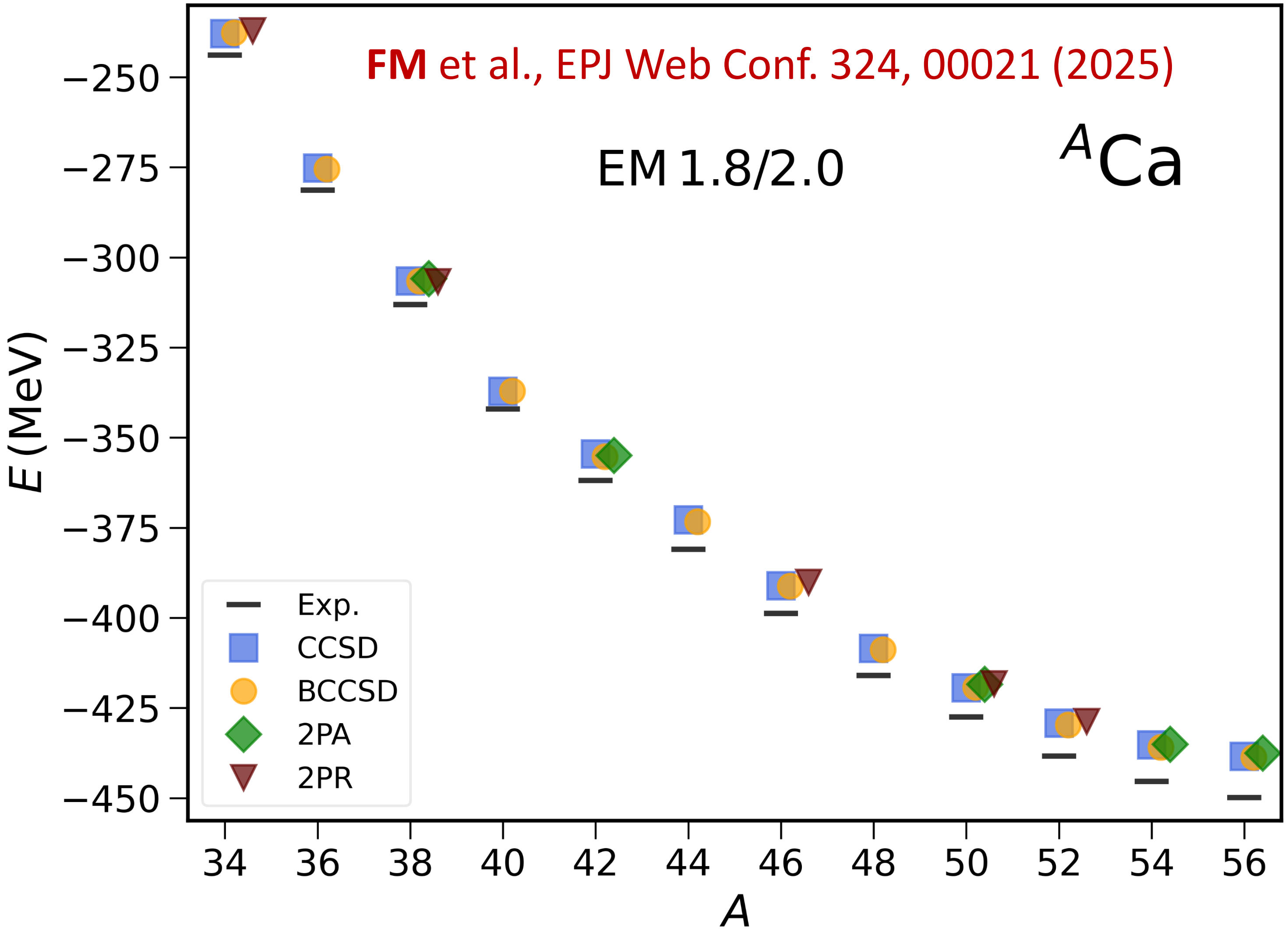
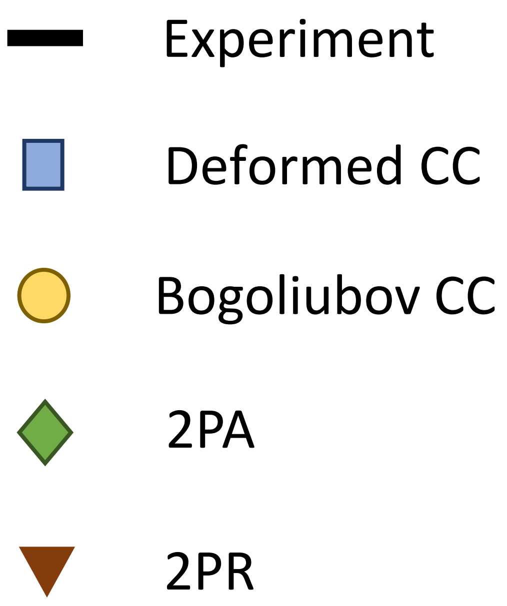
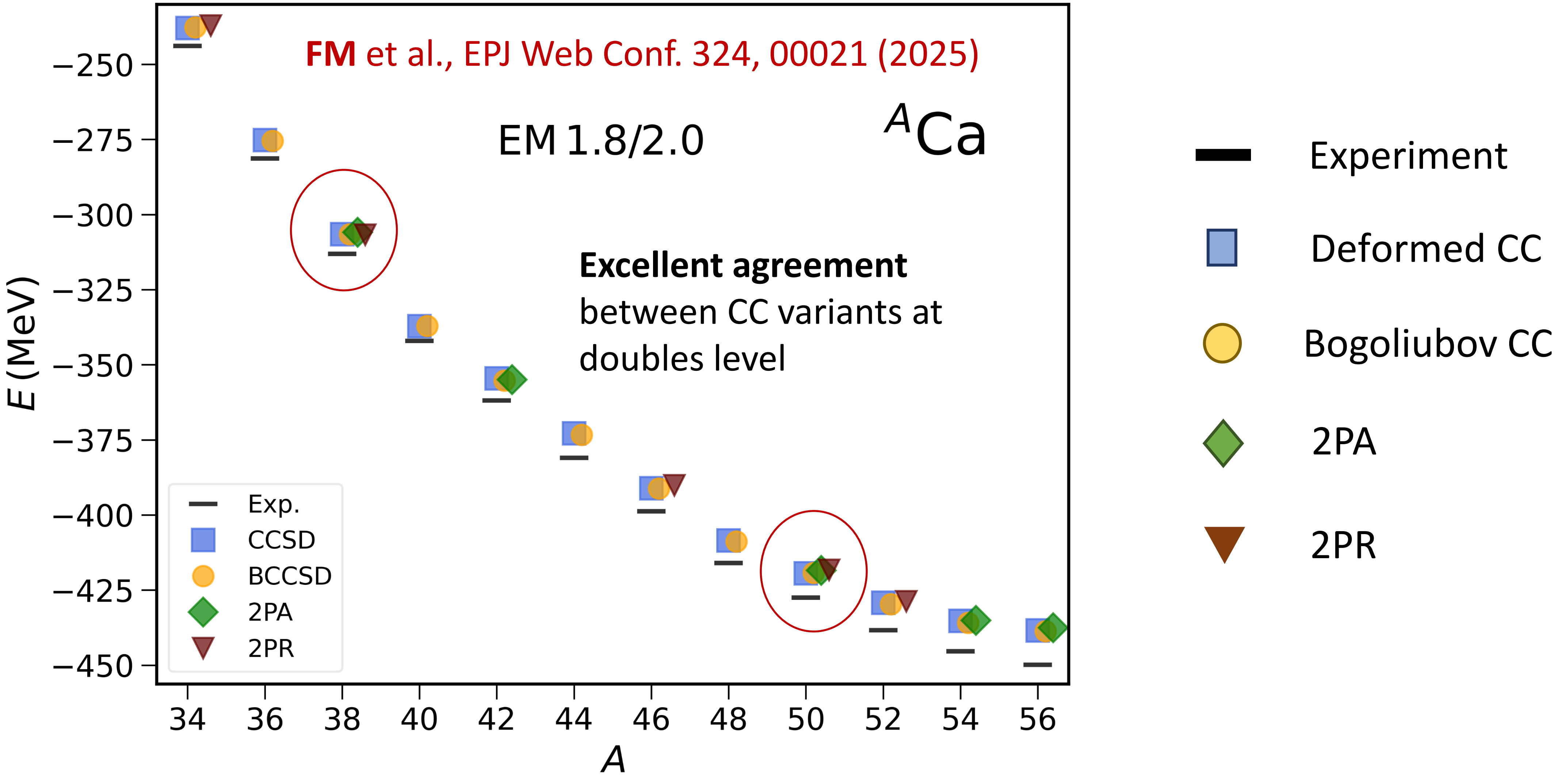
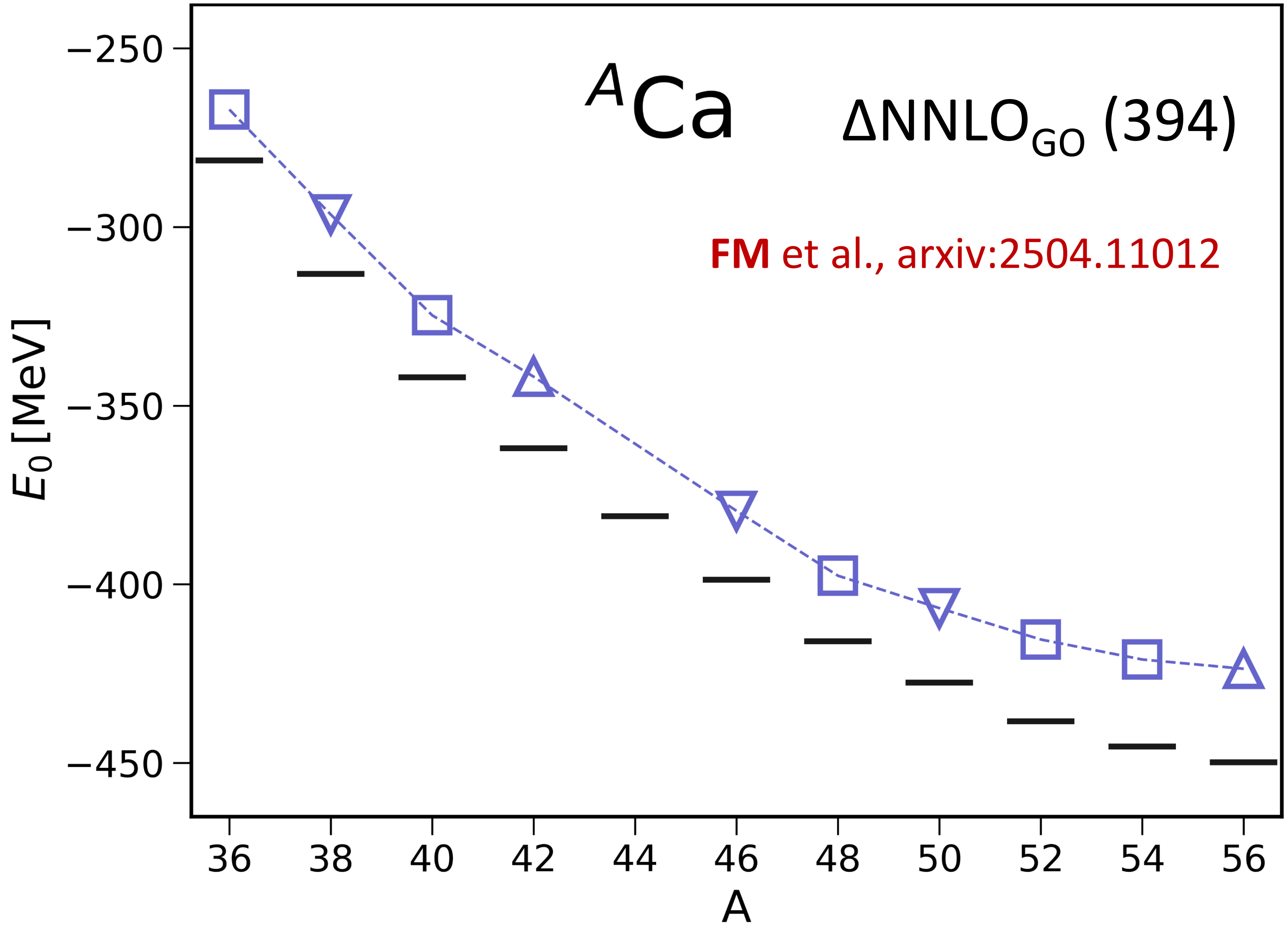




Binding energies - validation



Binding energies in Ca chain



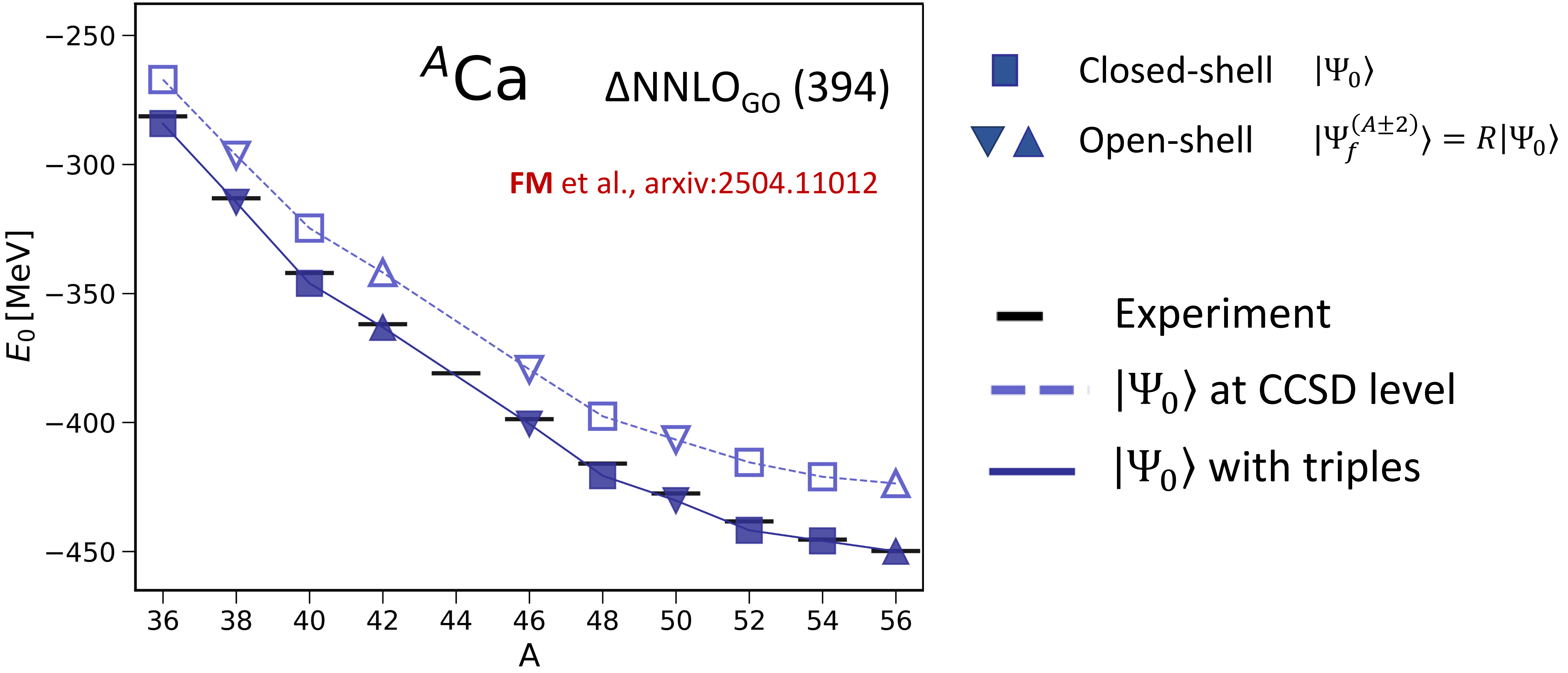
Closed-shell $|\Psi_0\rangle$

Open-shell $|\Psi_f^{(A\pm 2)}\rangle = R|\Psi_0\rangle$

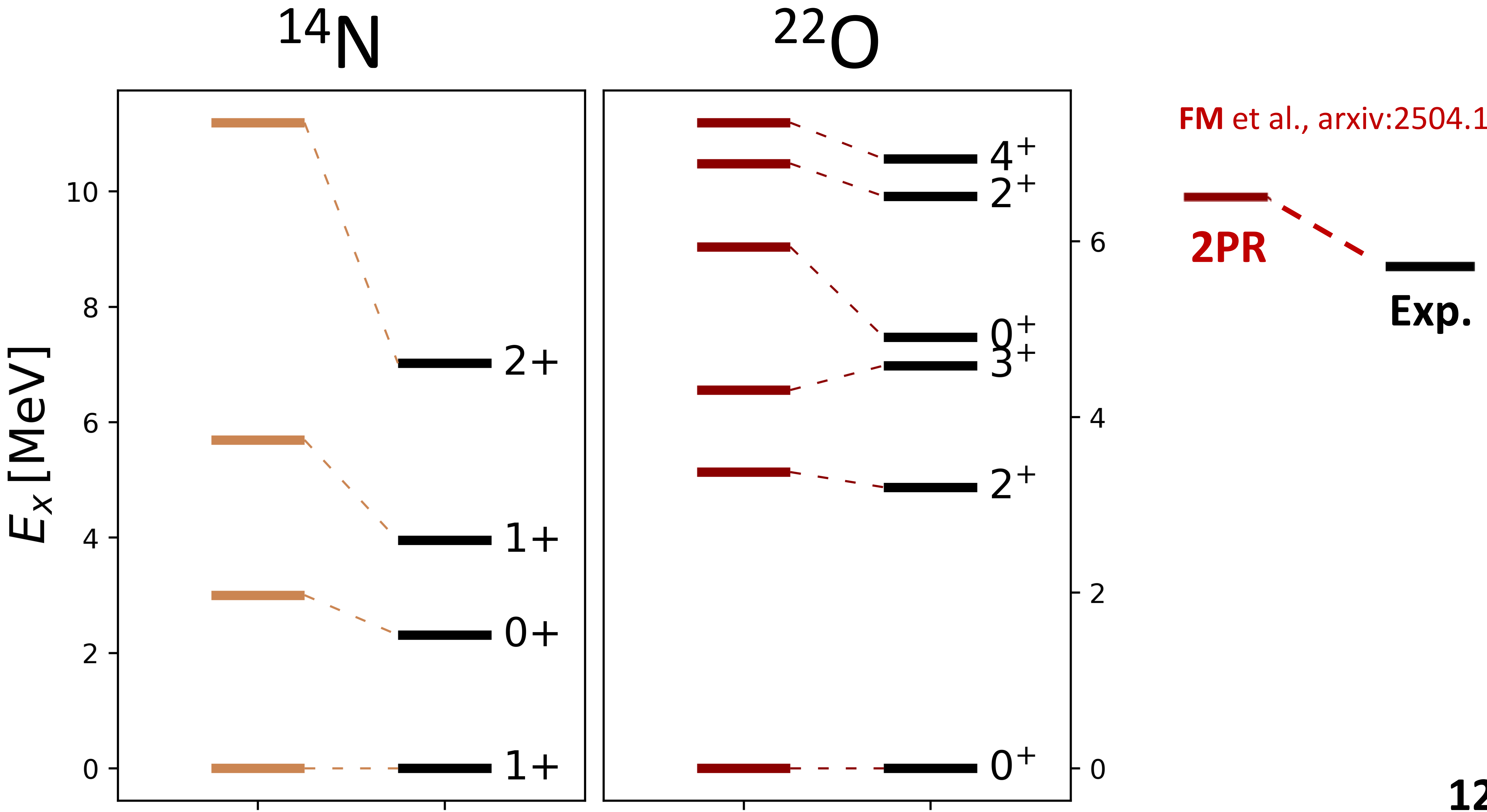
Experiment

$|\Psi_0\rangle$ at CCSD level

Binding energies in Ca chain

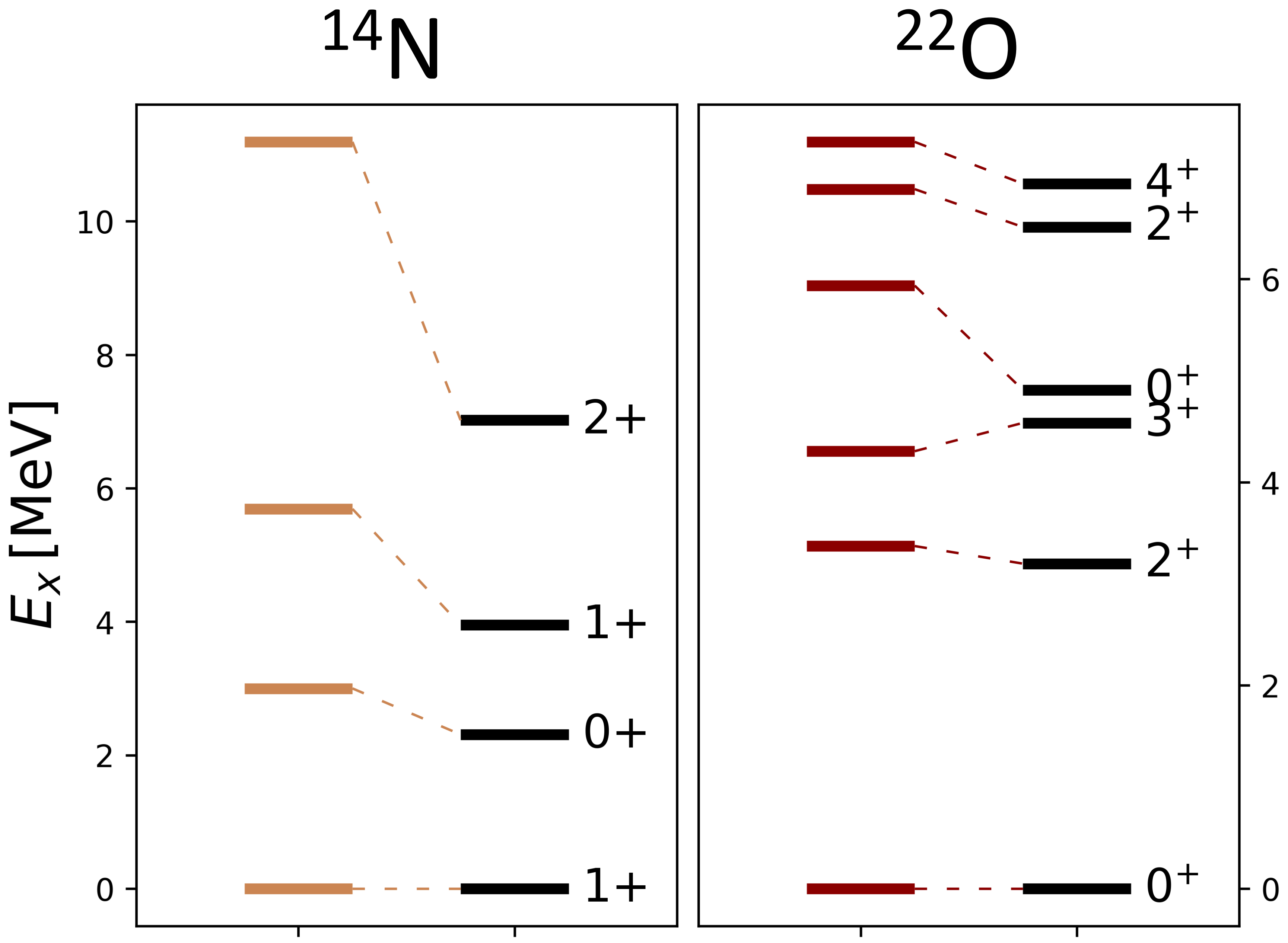


Excited states



FM et al., arxiv:2504.11012

Excited states



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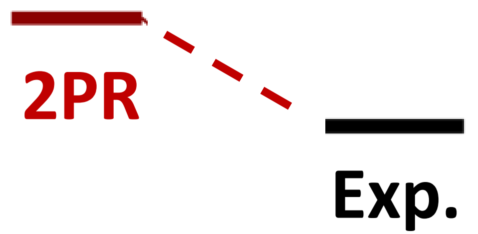


2PR with the $\Delta NNLO_{GO}$ (394) interaction describes well several **excited states**

Part 2:
Electric dipole polarizability

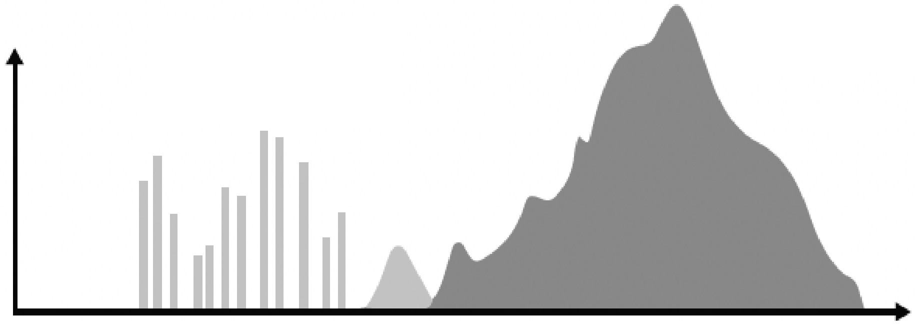
Dipole response functions

$$R(\omega) = \sum_f \left| \langle \Psi_f | \Theta | \Psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$

Dipole response functions

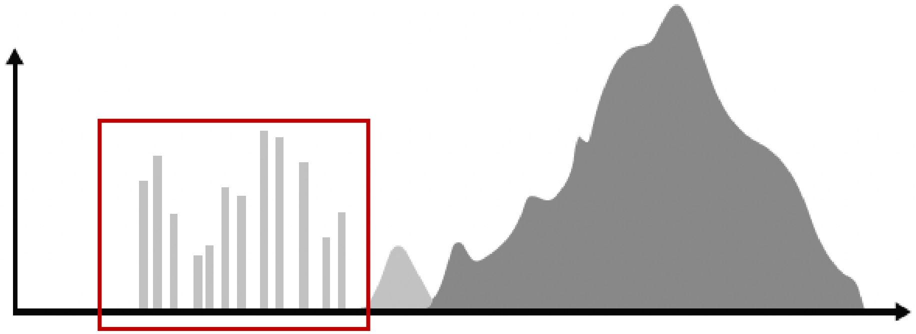
$$R(\omega) = \sum_f \left|\langle \Psi_f \boxed{|\Theta|} \Psi_0 \rangle\right|^2 \delta(E_f - E_0 - \omega)$$

Θ: excitation operator



Dipole response functions

$$R(\omega) = \sum_f \left| \langle \Psi_f \boxed{|\Theta|} \Psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$



Θ: excitation operator

Dipole response functions

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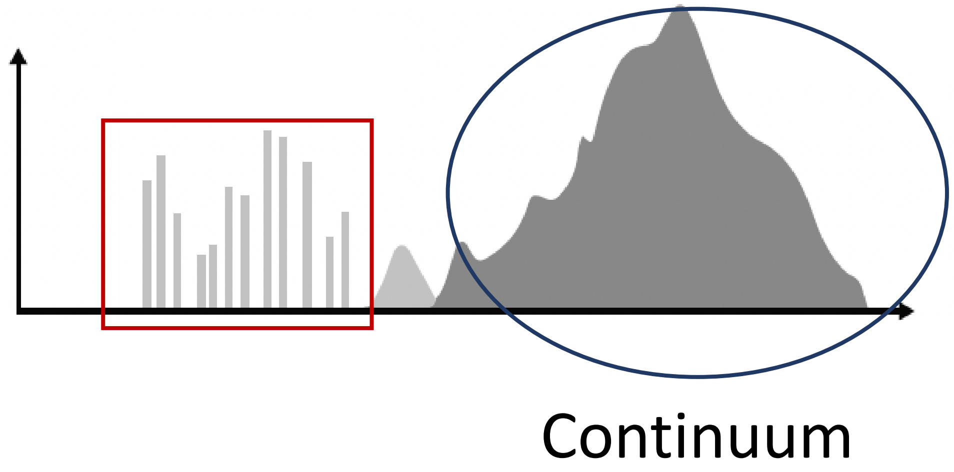

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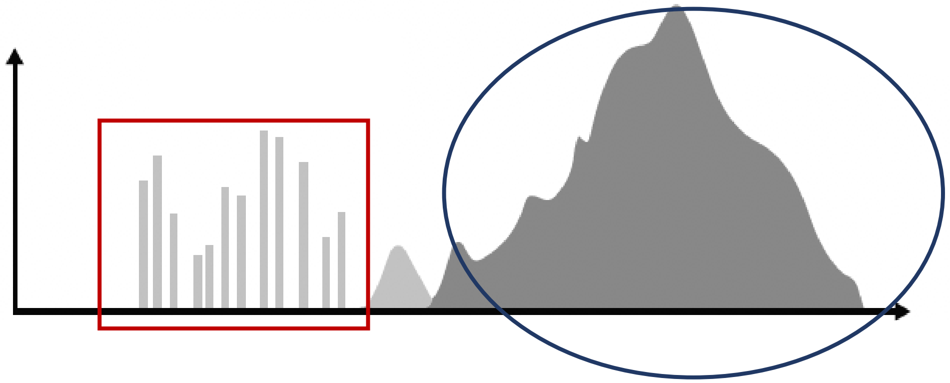
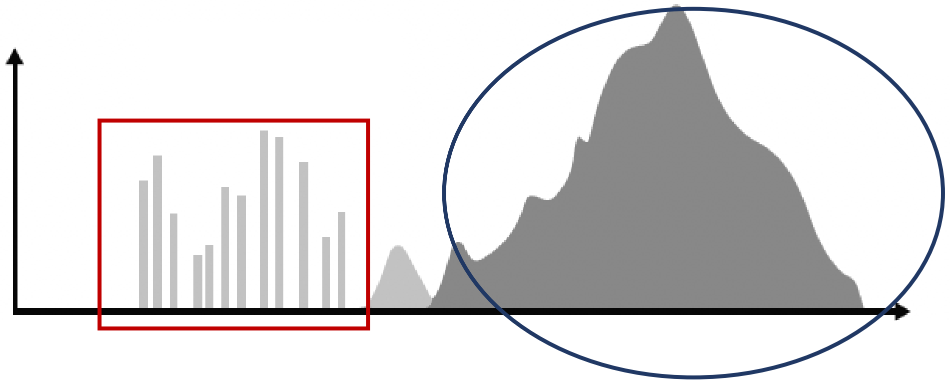


Lorentz integral transform (LIT)

$$L(\sigma, \Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \frac{\Gamma}{\pi} \langle \widetilde{\Psi}_L | \widetilde{\Psi}_R \rangle$$

Dipole response functions

$$R(\omega) = \sum_f \left|\langle \Psi_f \boxed{|\Theta|} \Psi_0 \rangle\right|^2 \delta(E_f - E_0 - \omega)$$



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Bound pseudo-state $|\widetilde{\Psi}_R\rangle$

Dipole response functions

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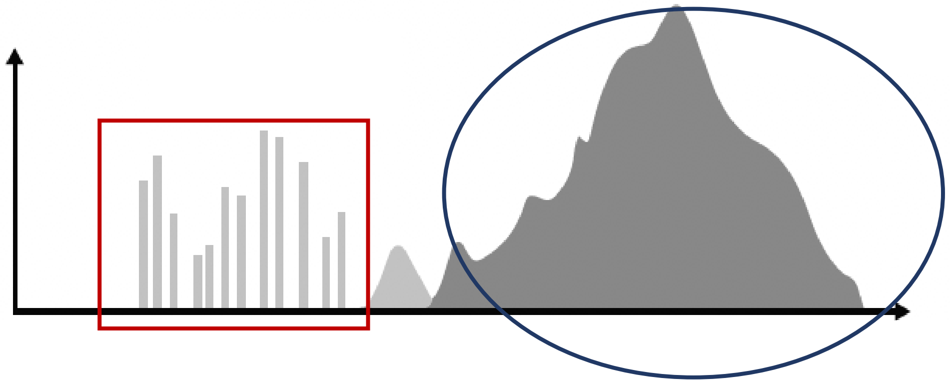
Θ: excitation operator



Continuum

Lorentz integral transform (LIT)

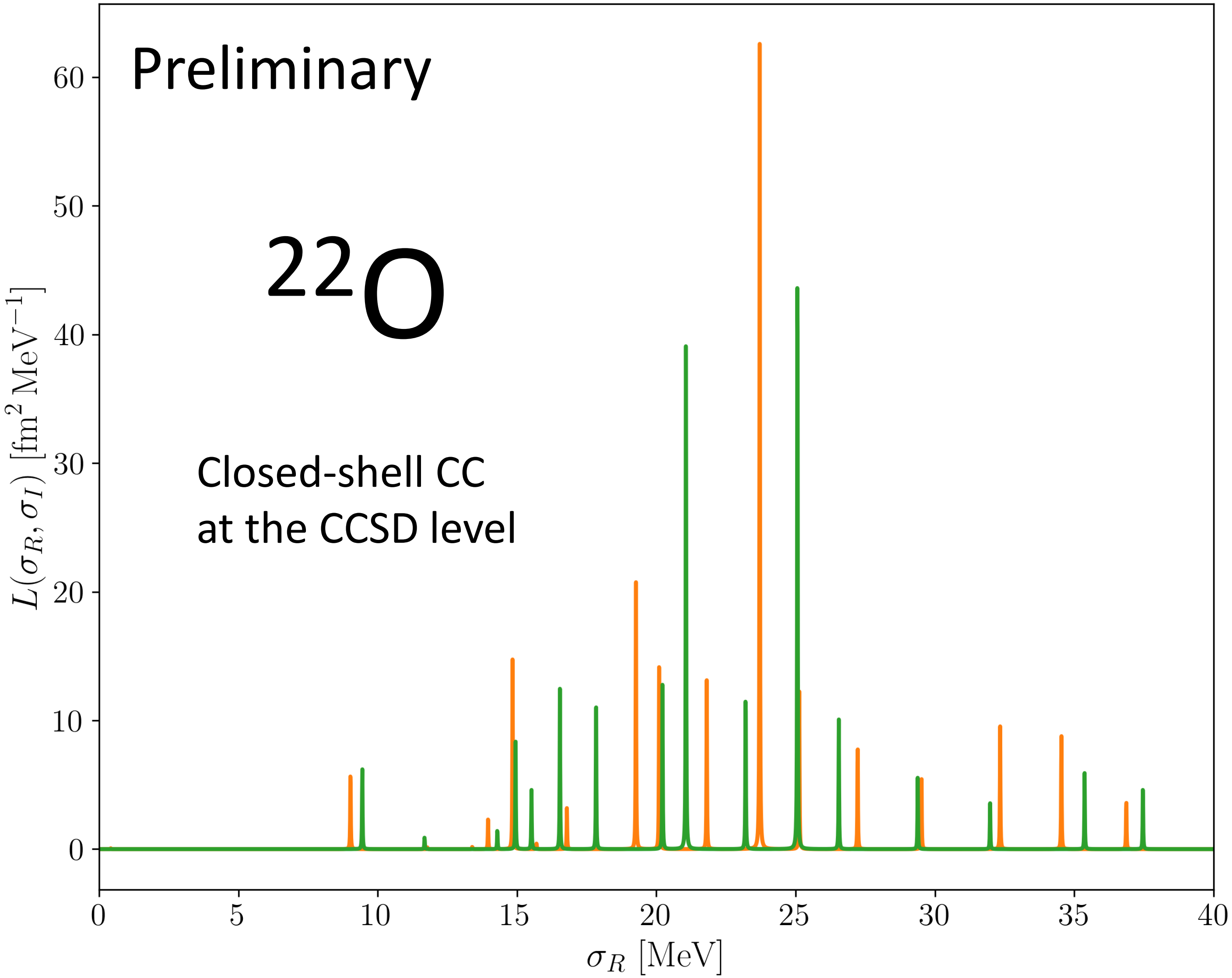
$$L(\sigma, \Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \frac{\Gamma}{\pi} \langle \widetilde{\Psi}_L | \widetilde{\Psi}_R \rangle$$

Bound pseudo-state $|\widetilde{\Psi}_R\rangle$

LIT-CC ansatz

$$\boxed{\left| \widetilde{\Psi}_R^{(A-2)} \right\rangle = \mathcal{R}^{(A-2)} |\Phi_0\rangle}$$

Discretized response function



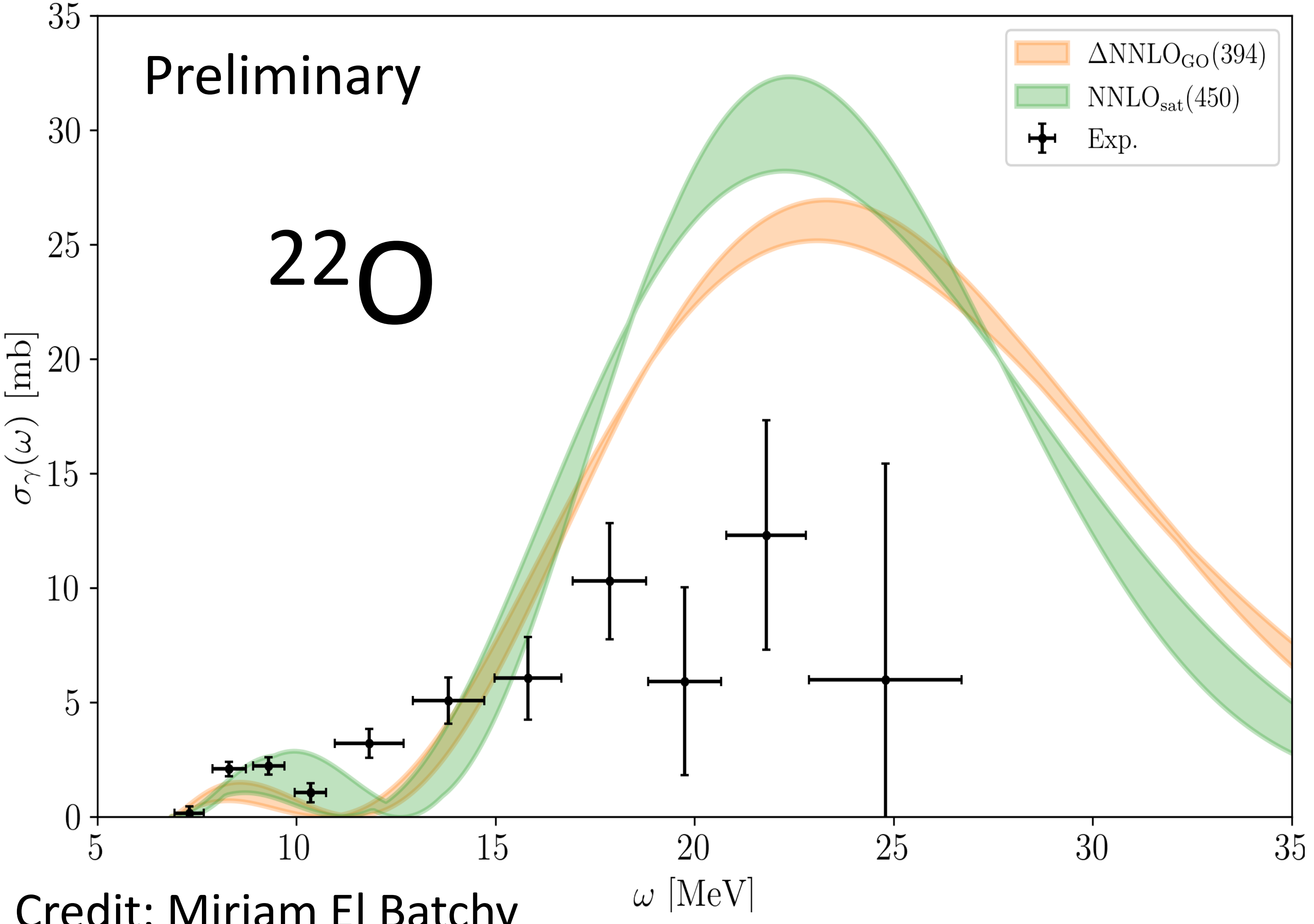
$$L(\sigma, \Gamma \to 0)$$

$\Delta NNLO_{GO}$ (394)

$NNLO_{sat}$ (450)

Francesco Marino – Ischia, 20 May 2025

Photoneutron cross sections



Credit: Miriam El Batchy

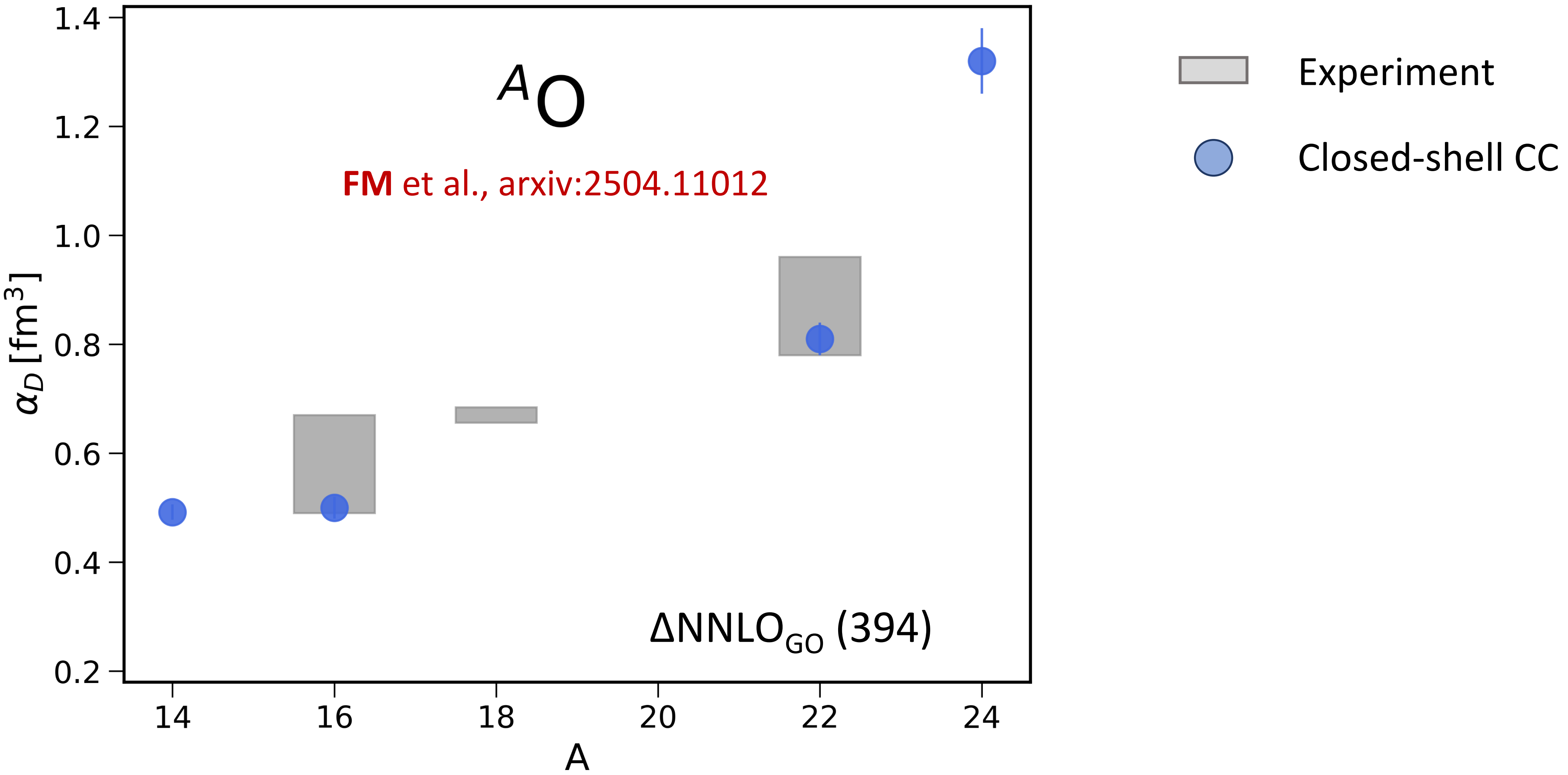
$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega R(\omega)$$

Cross sections with quantified **uncertainties** from the **inversion** of the LIT

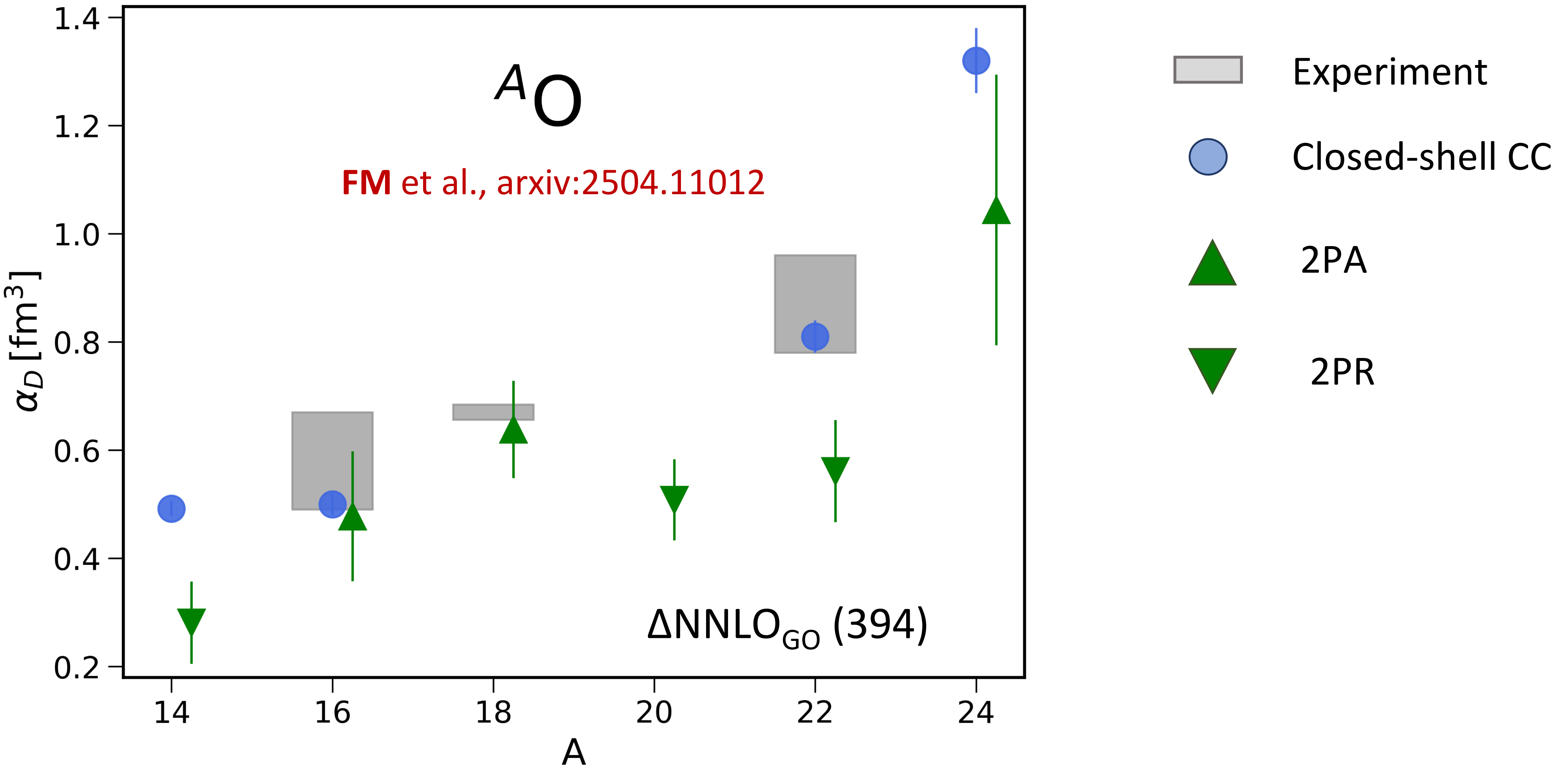
Exp. data from

Leistenschneider et al, Phys. Rev. Lett. **86**, 5442 (2001)

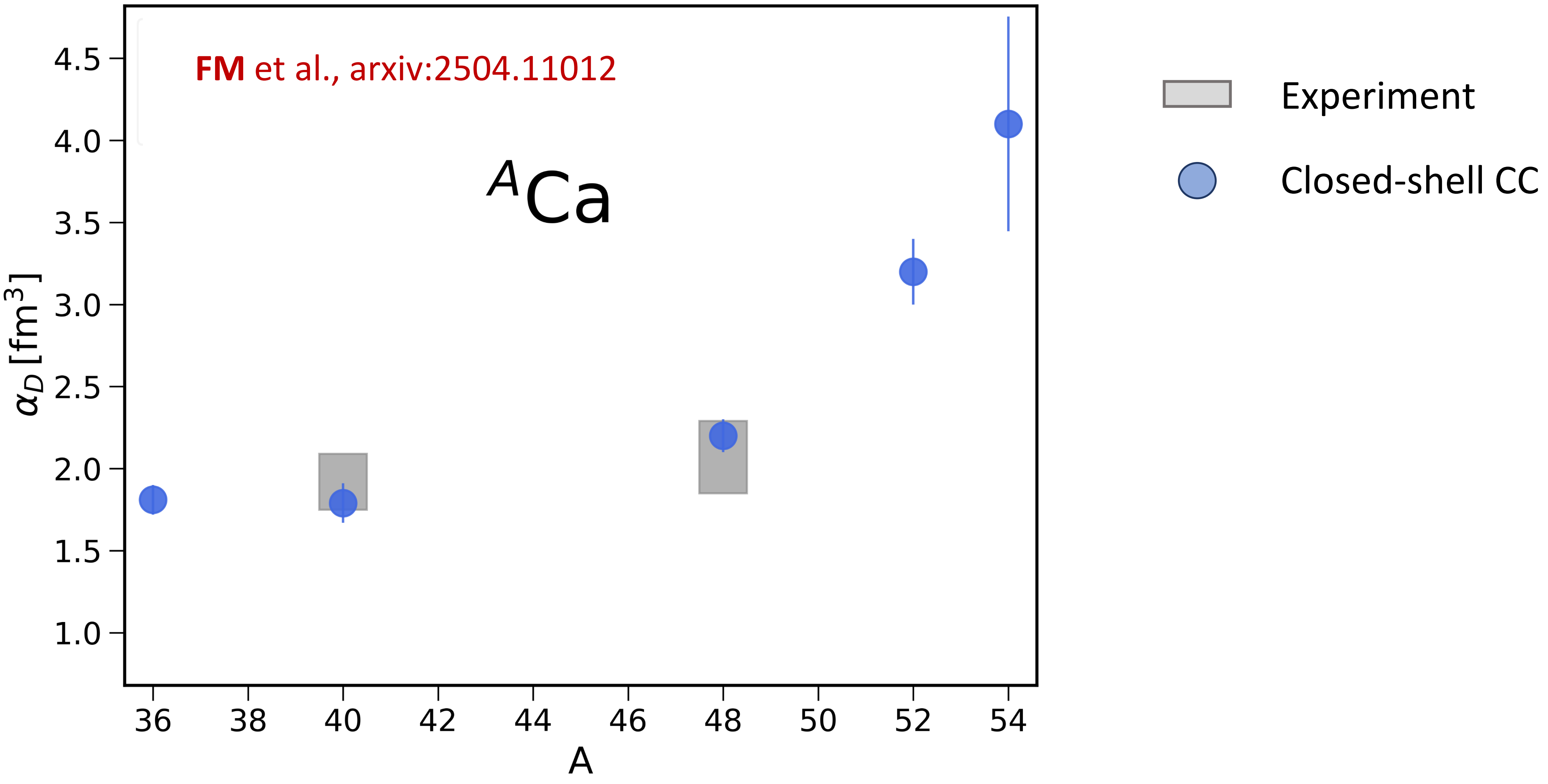
Electric dipole polarizability in O isotopes



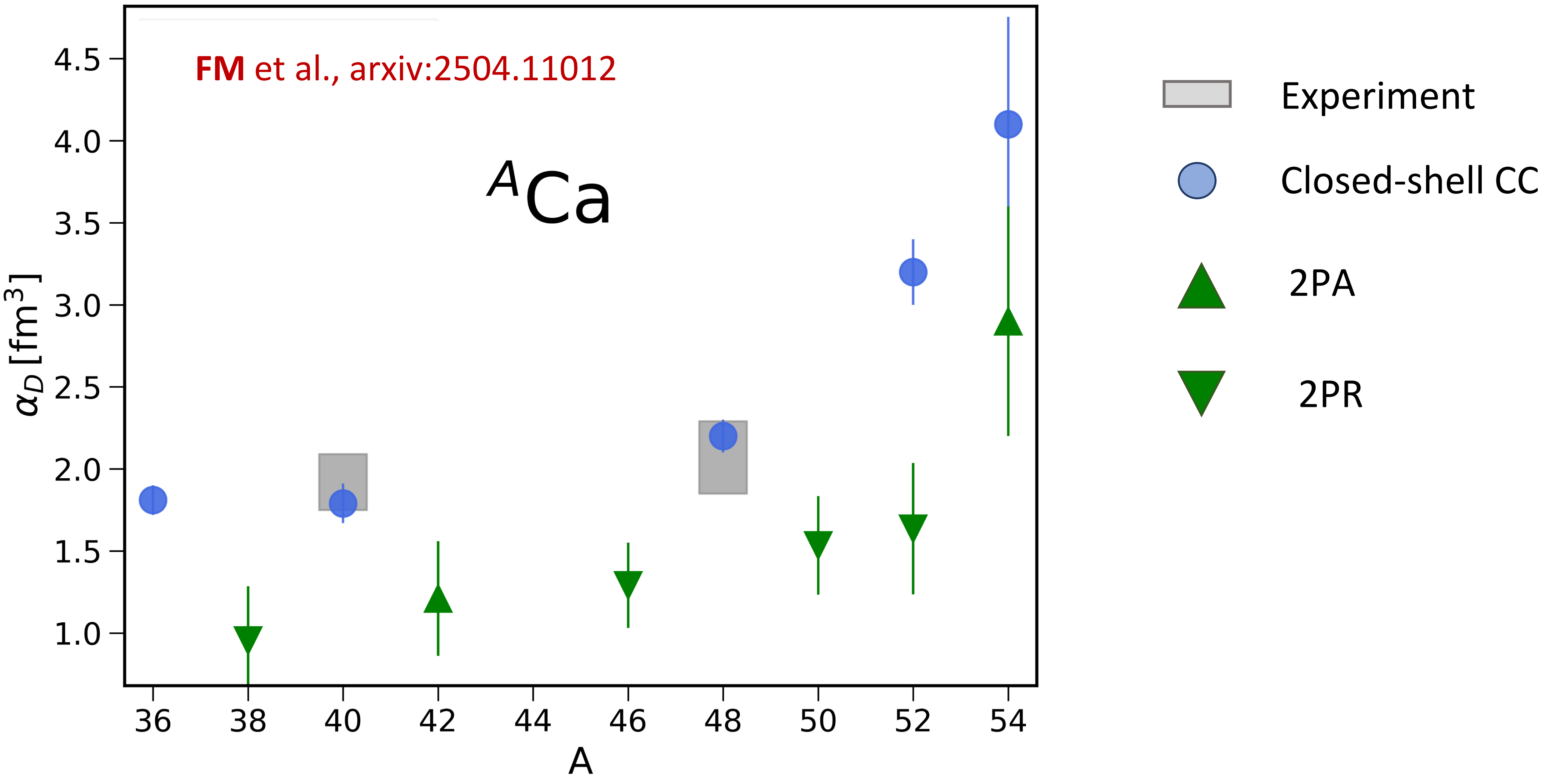
Electric dipole polarizability in O isotopes



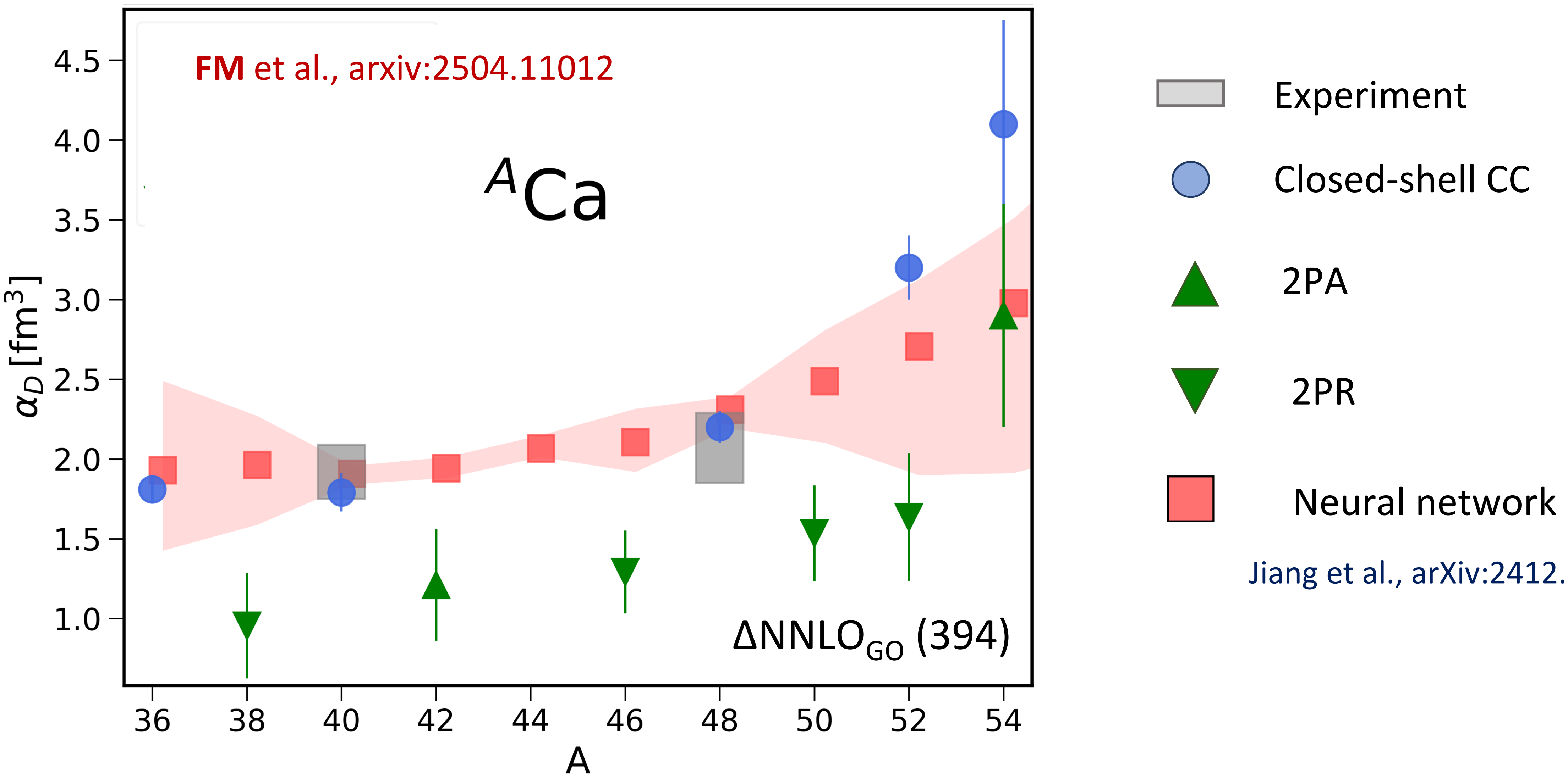
Electric dipole polarizability in Ca isotopes



Electric dipole polarizability in Ca isotopes



Electric dipole polarizability in Ca isotopes



Jiang et al., arXiv:2412.02876

Conclusions and perspectives

- We have applied coupled-cluster theory to study the ground state, excited states and electric dipole polarizability of **open-shell** nuclei close to magicity

- Binding energies and selected excited states are well reproduced. A tendency to underestimate the electric dipole polarizability appears

- Future developments: higher-order truncations, response of odd nuclei, response functions with theory uncertainties …

Thank you for your attention!

Collaborators

Darmstadt:	Alex Tichai
FRIB/Oak Ridge:	Francesca Bonaiti
Mainz:	Sonia Bacca
Oak Ridge:	Gaute Hagen, Gustav Jansen

… and save the date!

Many-body Theory:
Nuclear Physics Meets Quantum Chemistry

Aug 24th – Sep 4th 2026

Mainz Institute for Theoretical Physics

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