Electric dipole polarizability in medium-mass nuclei

FRANCESCA BONAITI, JGU MAINZ

UNCERTAINTY QUANTIFICATION IN NUCLEAR PHYSICS @ MITP

JUNE 26, 2024

In collaboration with:
Sonia Bacca (JGU Mainz)
Francesco Marino (JGU Mainz)
Gaute Hagen (ORNL)
Gustav R. Jansen (ORNL)
Thomas Papenbrock (ORNL/UTK)

When the method uncertainty becomes a challenge

FRANCESCA BONAITI, JGU MAINZ

UNCERTAINTY QUANTIFICATION IN NUCLEAR PHYSICS @ MITP

JUNE 26, 2024

In collaboration with:
Sonia Bacca (JGU Mainz)
Francesco Marino (JGU Mainz)
Gaute Hagen (ORNL)
Gustav R. Jansen (ORNL)
Thomas Papenbrock (ORNL/UTK)

The ab-initio promise

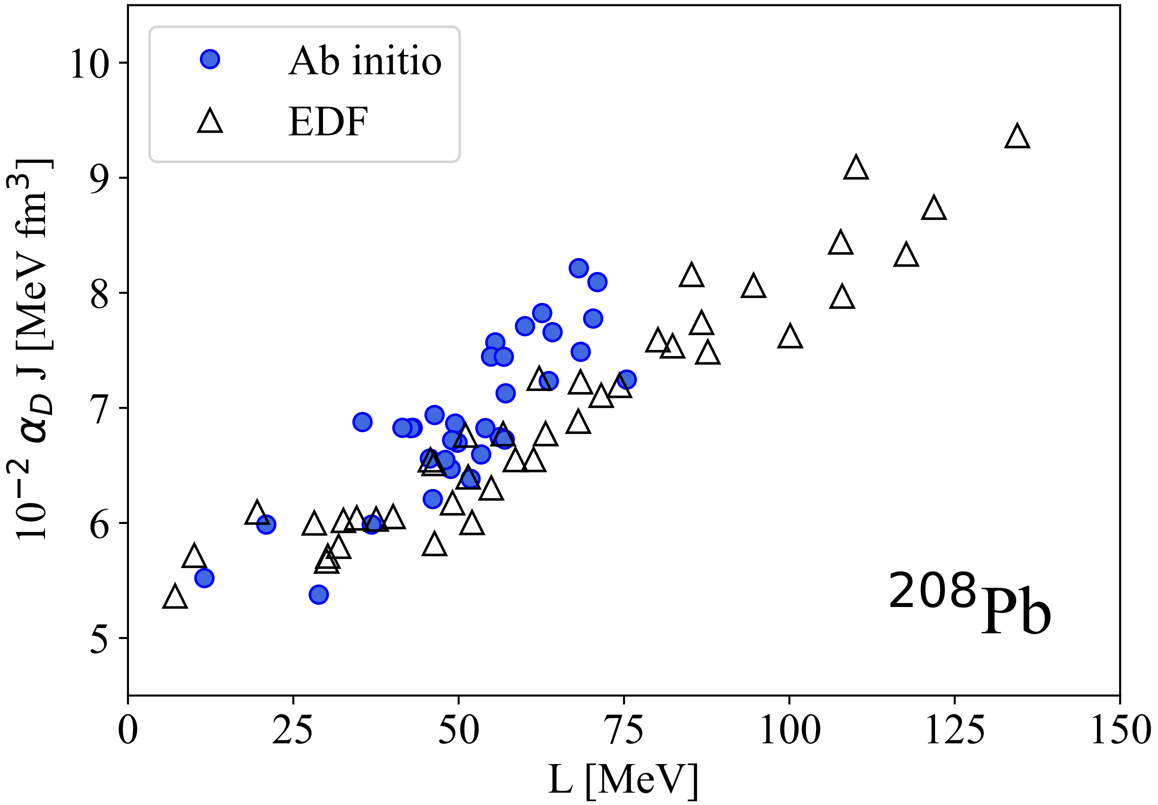
from Christian's talk

$$y_{\mathrm{exp}} = \tilde{y}(\boldsymbol{\alpha}) + \delta y_{\mathrm{EFT}} + \boxed{\delta y_{\mathrm{method}}} + \delta \tilde{y}_{\mathrm{em}} + \delta y_{\mathrm{exp}}$$

Solving the **quantum many-body problem**
in a **systematically improvable way**

But how much are many-body uncertainties **under control**?
see e.g. talks by Christian and Alex

Electric dipole polarizability



Data from X. Roca-Maza et al, PRC 88, 024316 (2013),
B. Hu et al, Nat. Phys. 18, 1196-1200 (2022).

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

It depends on the nuclear response function.
We need:

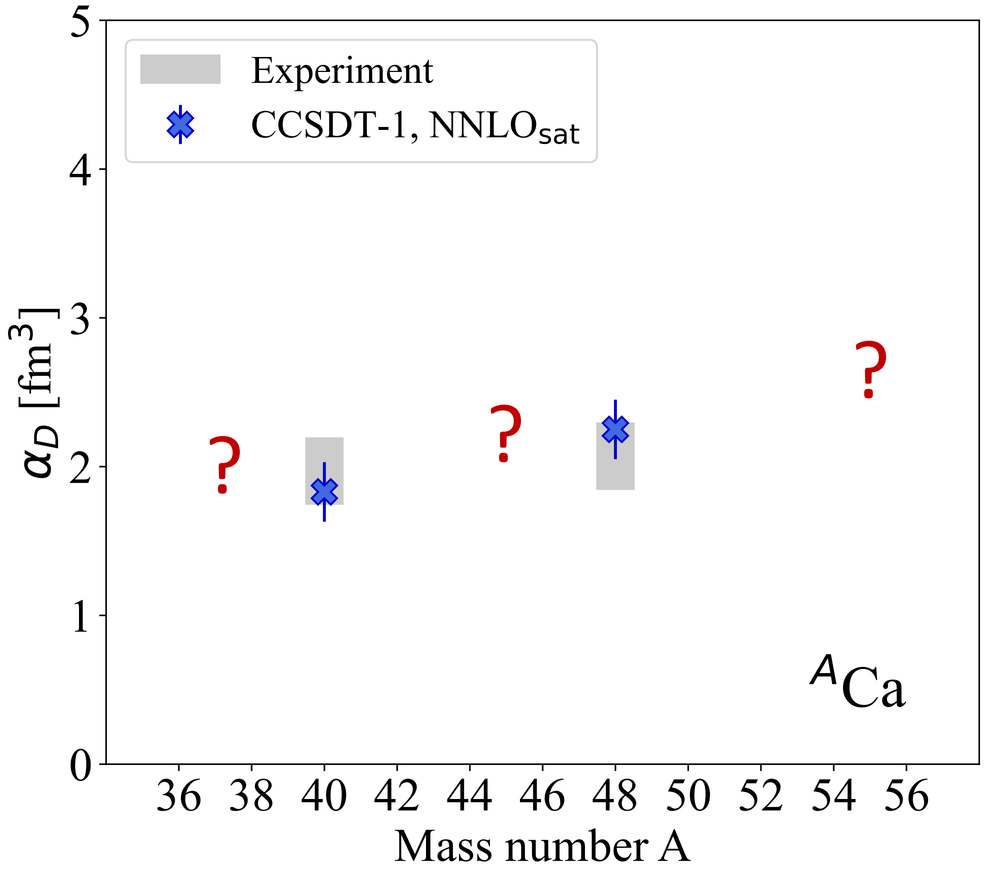
- ❑ Many-body solver: coupled-cluster (CC) theory
  G. Hagen et al, RPP 77, 096302 (2014).

- ❑ Treatment of continuum states: Lorentz Integral Transform (LIT) method
  S. Bacca et al, PRL **111**, 122502 (2013).

⟶ see Sonia's talk

First case study: open-shell nuclei

Happy ending for ^{40,48}Ca... but what's next?



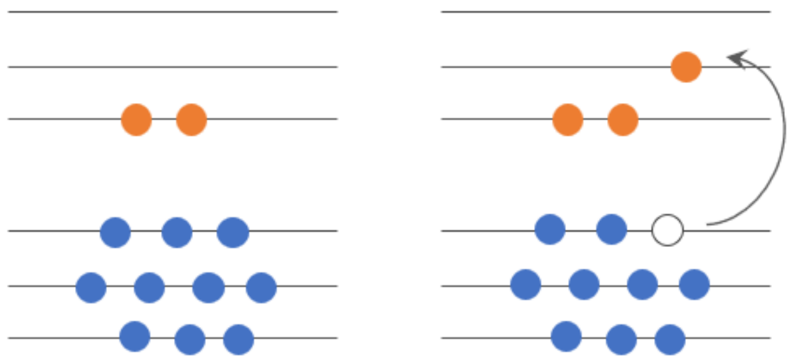
Open-shell nuclei: the 2-Particle-Attached (2PA) case

$$\mathcal{R} = \frac{1}{2}\sum r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i + \ldots$$

$$|\Psi_R\rangle = \mathcal{R}|\Phi_0\rangle$$

2PA LIT state

closed-shell reference



2p-0h 3p-1h

FB et al., arXiv:2405.05608 [nucl-th]

Many-body truncations in LIT-CC

In LIT-CC calculations we employ two CC expansions,

one for the ground-state, one for the excited-state calculation.

"Cooking recipe" for closed-shell nuclei:

- ❑ Vary ground-state scheme between CCSD and CCSDT-1.
- ❑ Consider excited states @ CCSD.

Many-body truncations in LIT-CC

In LIT-CC calculations we employ two CC expansions,

one for the ground-state, one for the excited-state calculation.

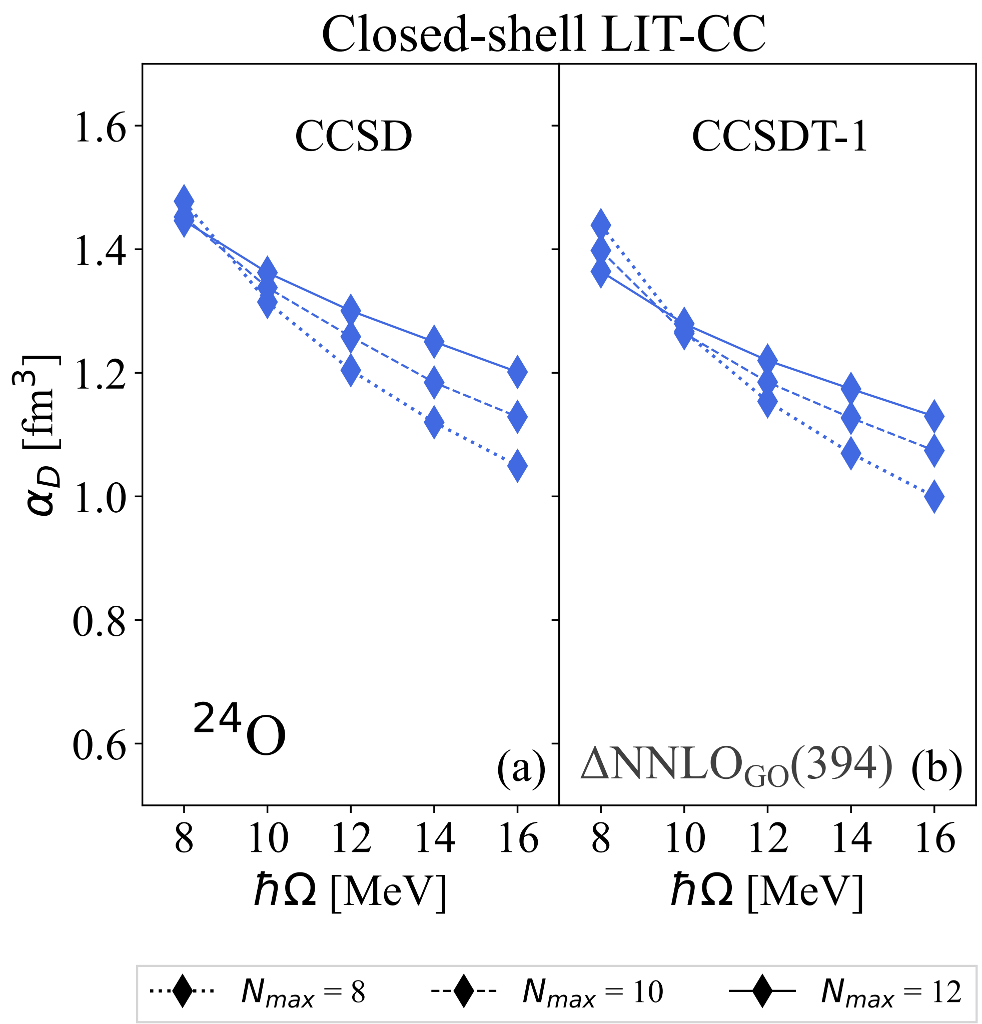
"Cooking recipe" for closed-shell nuclei:

- ❑ Vary ground-state scheme between CCSD and CCSDT-1.
- ❑ Consider excited states @ CCSD.

For 2PA, we are limited to 3p-1h...

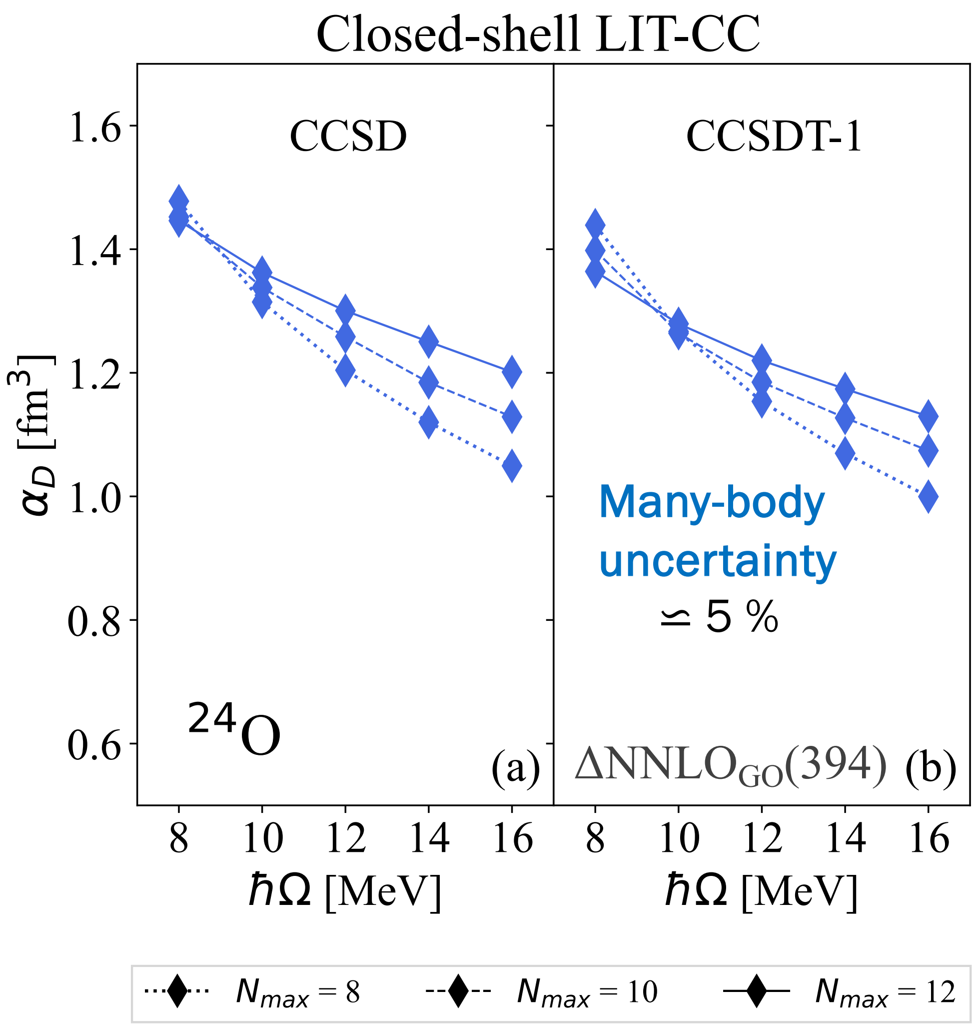
- ❑ Vary ground-state scheme between 2p-0h and 3p-1h.
- ❑ Consider excited states @ 3p-1h.

Electric dipole polarizability of ^{24}O



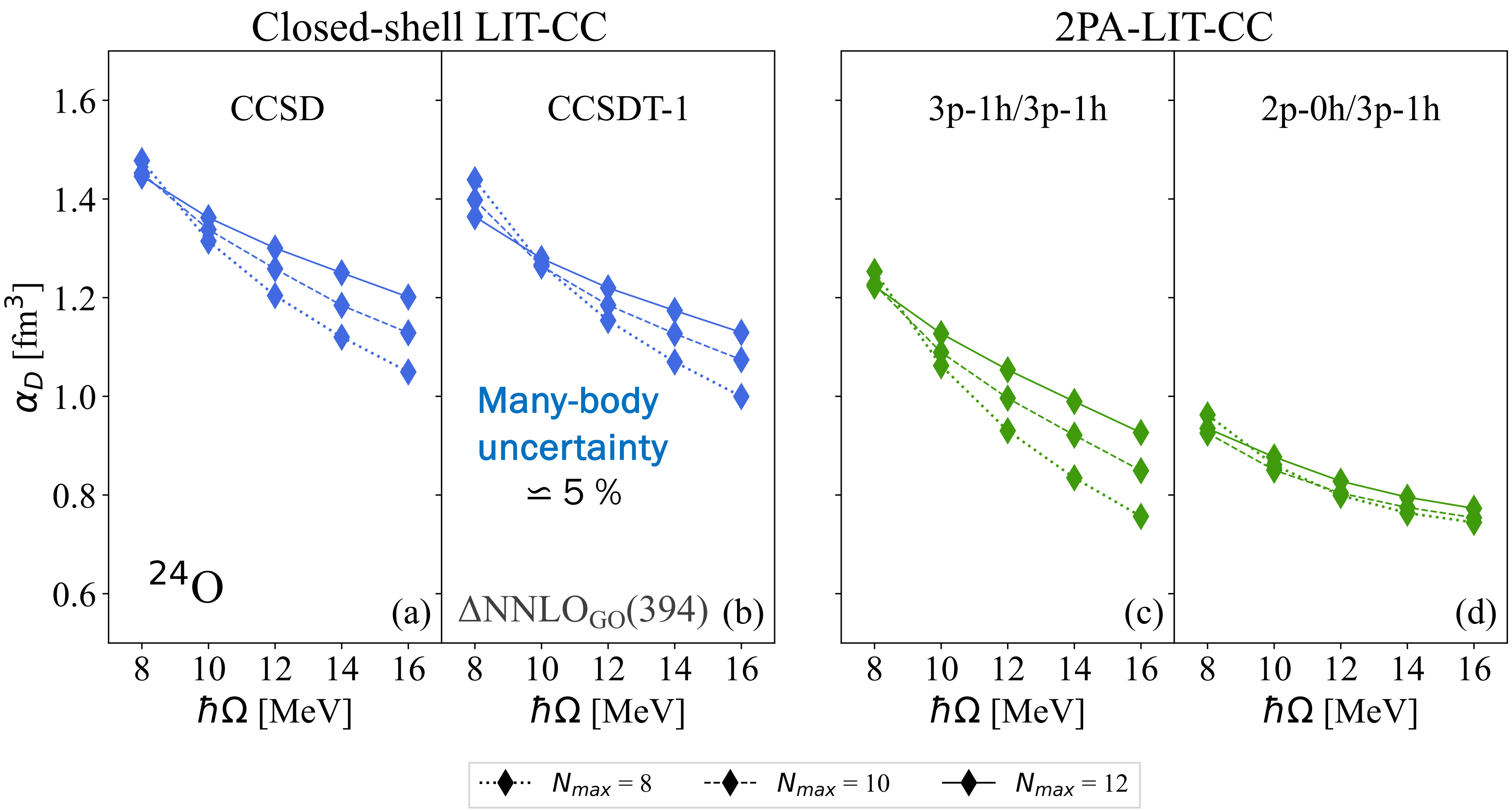
FB et al., arXiv:2405.05608 [nucl-th]

Electric dipole polarizability of ^{24}O



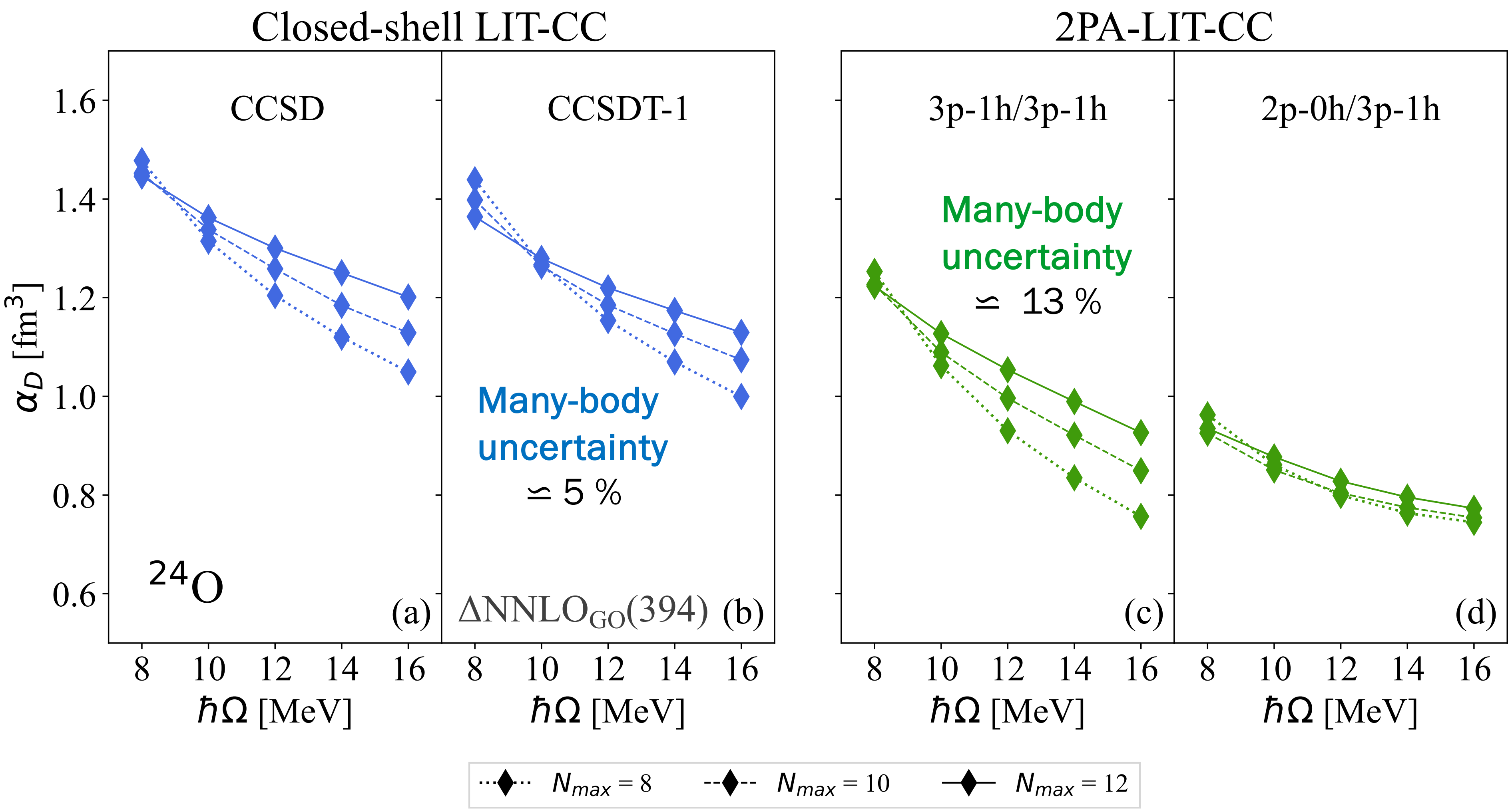
FB et al., arXiv:2405.05608 [nucl-th]

Electric dipole polarizability of ^{24}O



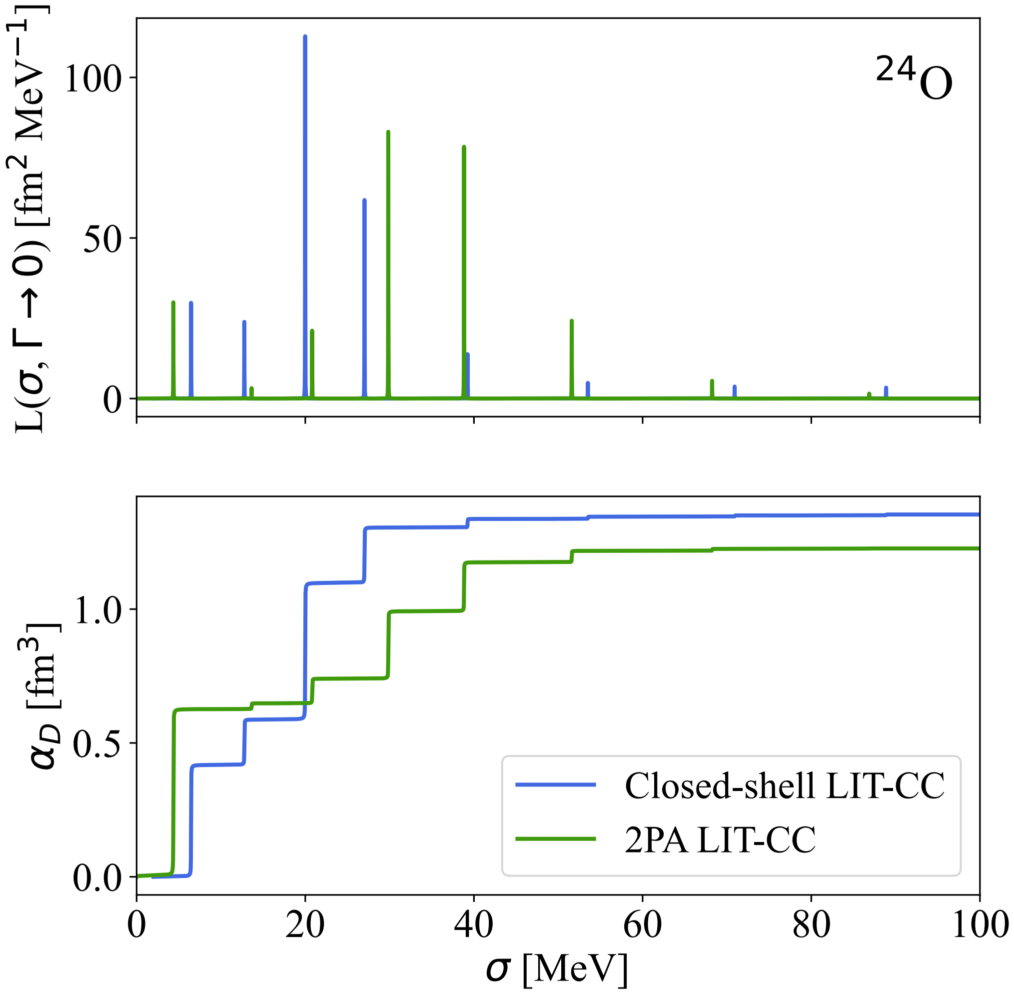
FB et al., arXiv:2405.05608 [nucl-th]

Electric dipole polarizability of ^{24}O



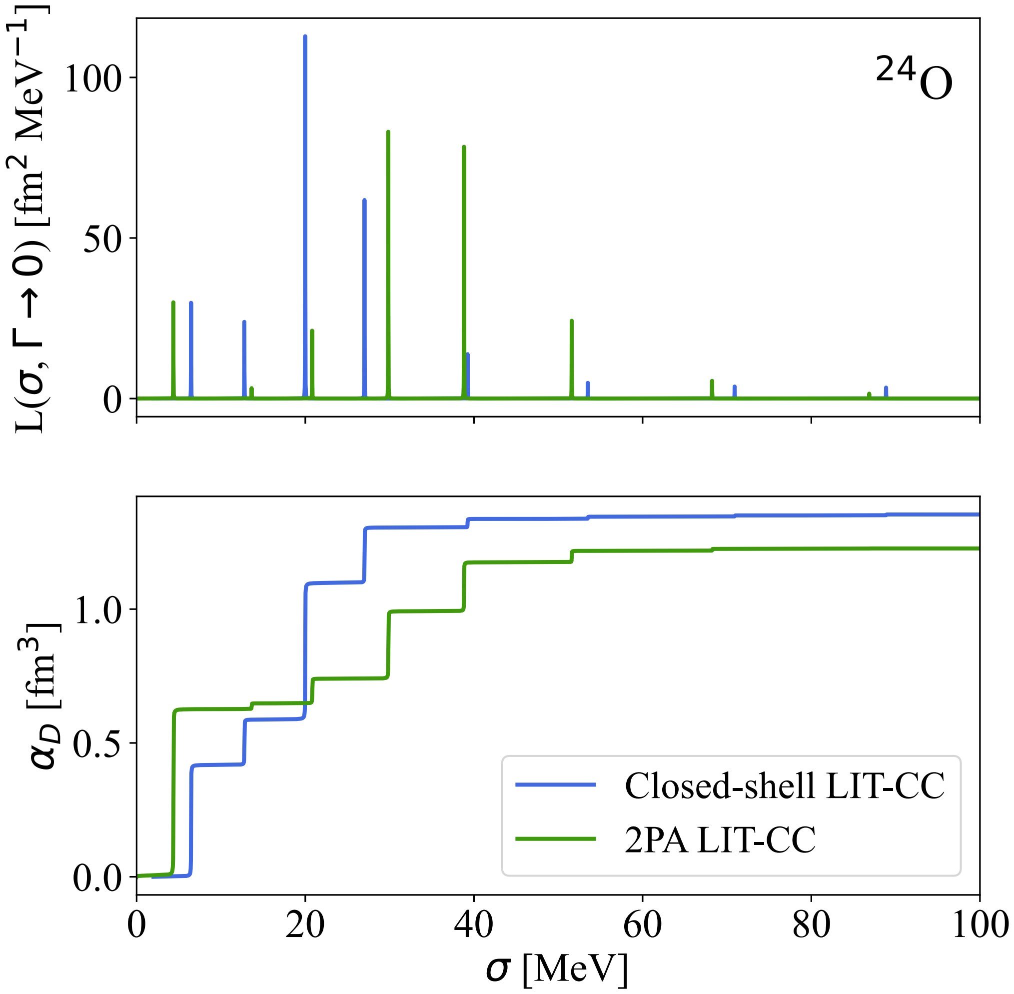
FB et al., arXiv:2405.05608 [nucl-th]

Electric dipole polarizability of ^{24}O



FB et al., arXiv:2405.05608 [nucl-th]

Electric dipole polarizability of ^{24}O



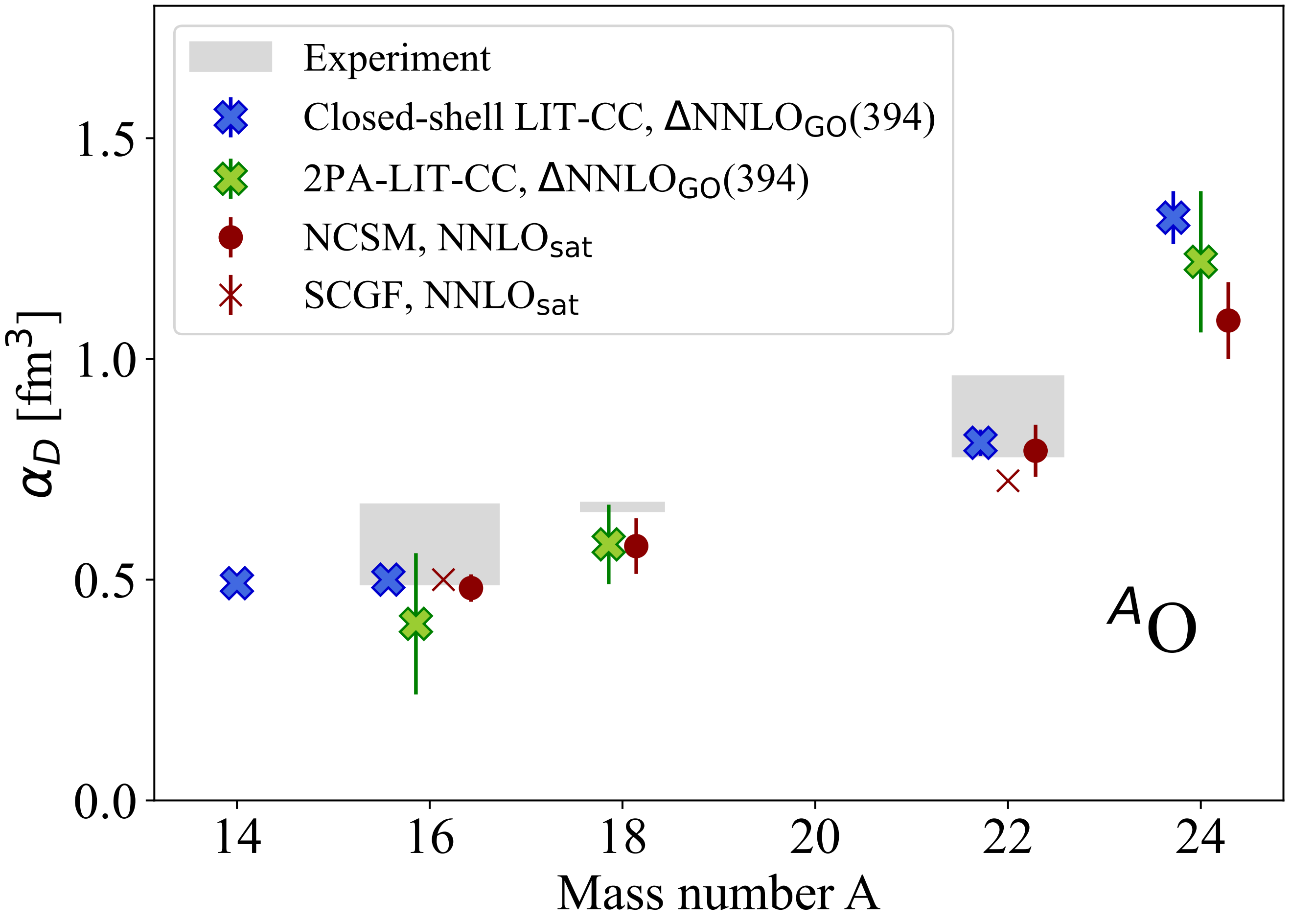
Can be useful to look at the **wavefunction's share** in **2p-0h configurations**

Ground state	First 1^- state
90%	88%

but rapidly decreases for **higher-energy states!**

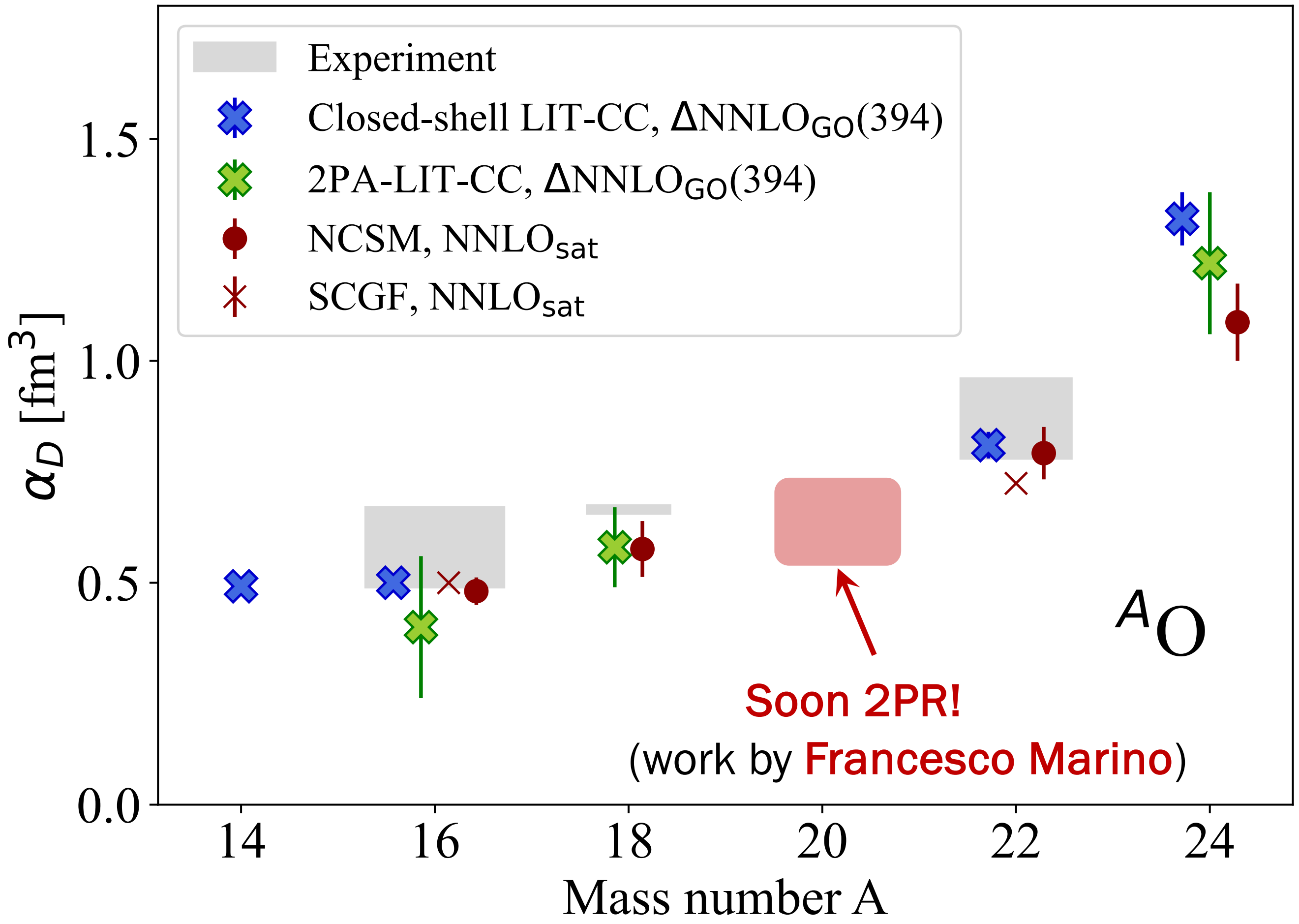
FB et al., arXiv:2405.05608 [nucl-th]

α_D along the oxygen chain



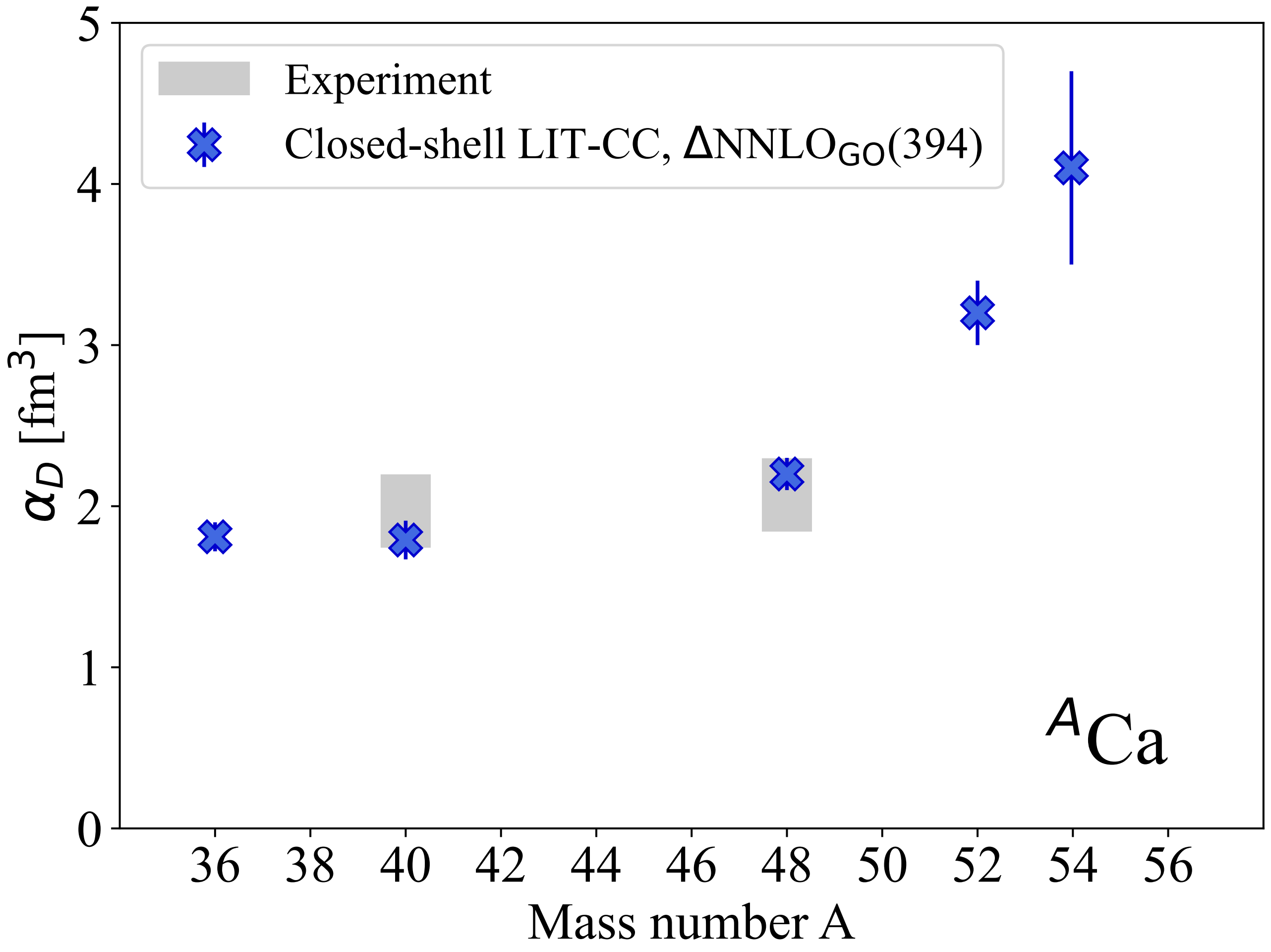
FB et al., arXiv:2405.05608 [nucl-th]

α_D along the oxygen chain



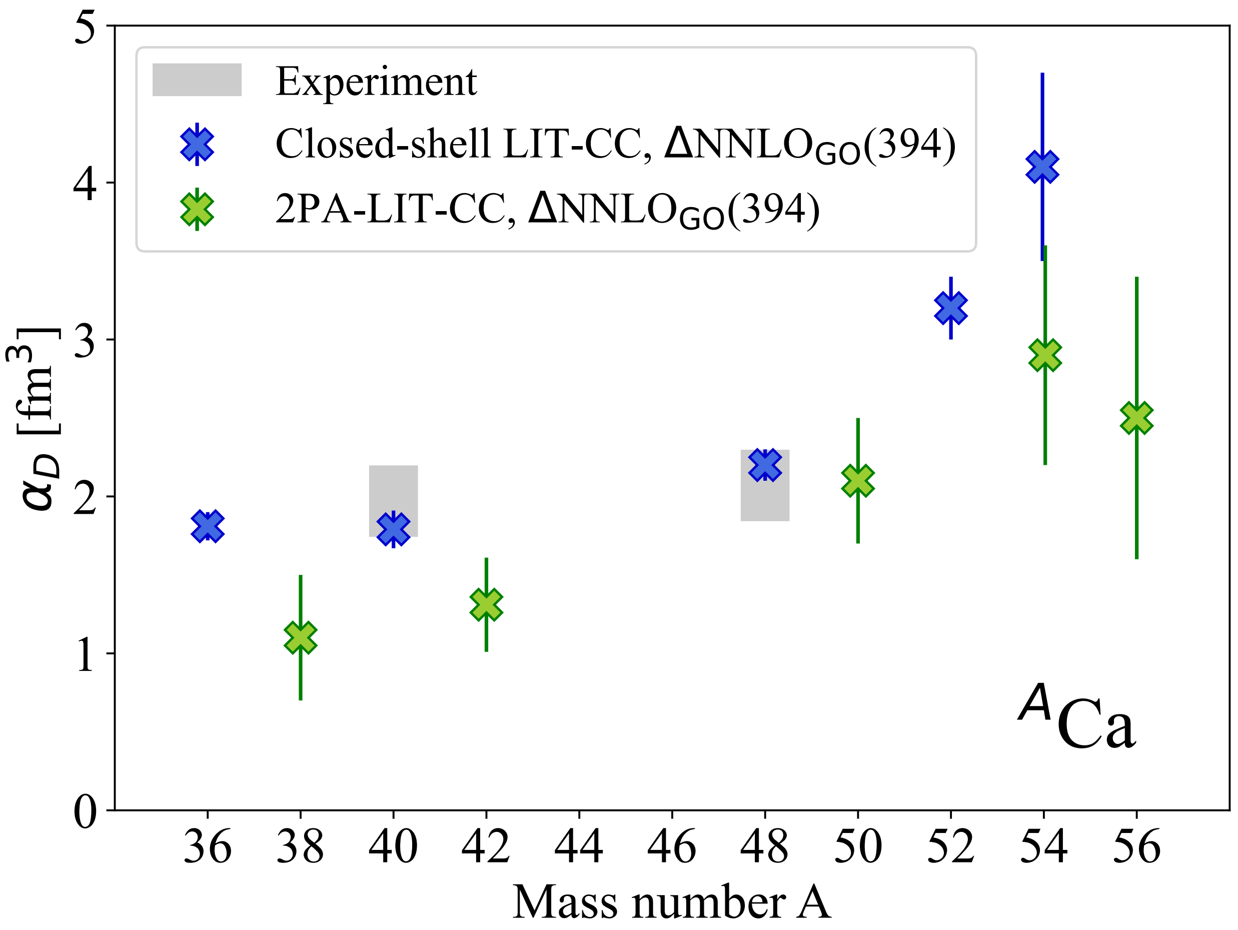
FB et al., arXiv:2405.05608 [nucl-th]

α_D along the calcium chain



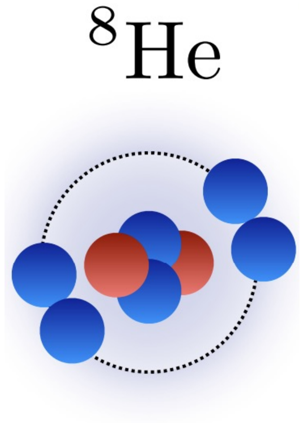
FB et al., arXiv:2405.05608 [nucl-th]

α_D along the calcium chain

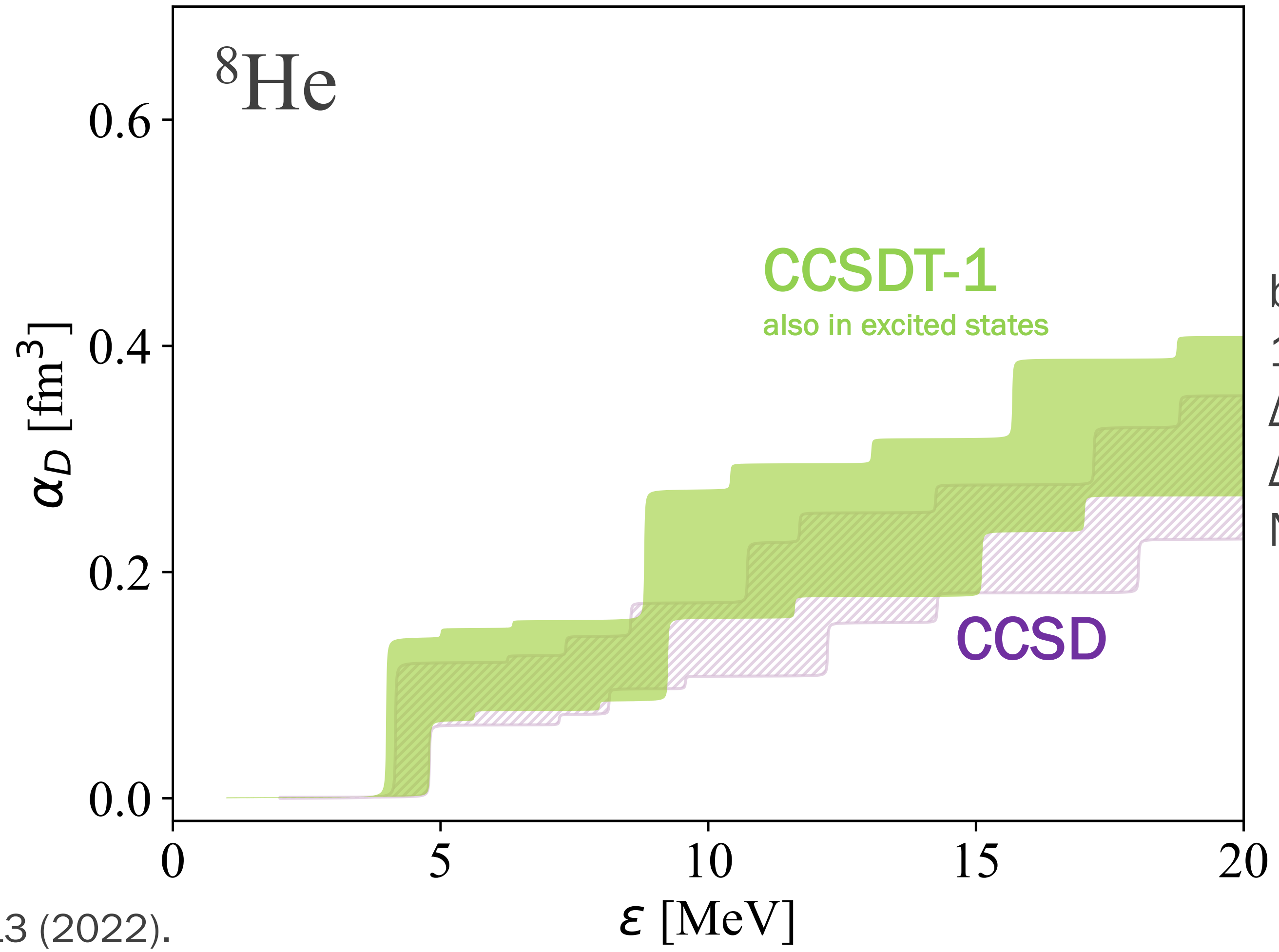


FB et al., arXiv:2405.05608 [nucl-th]

Second case study: halo nuclei



Theory…

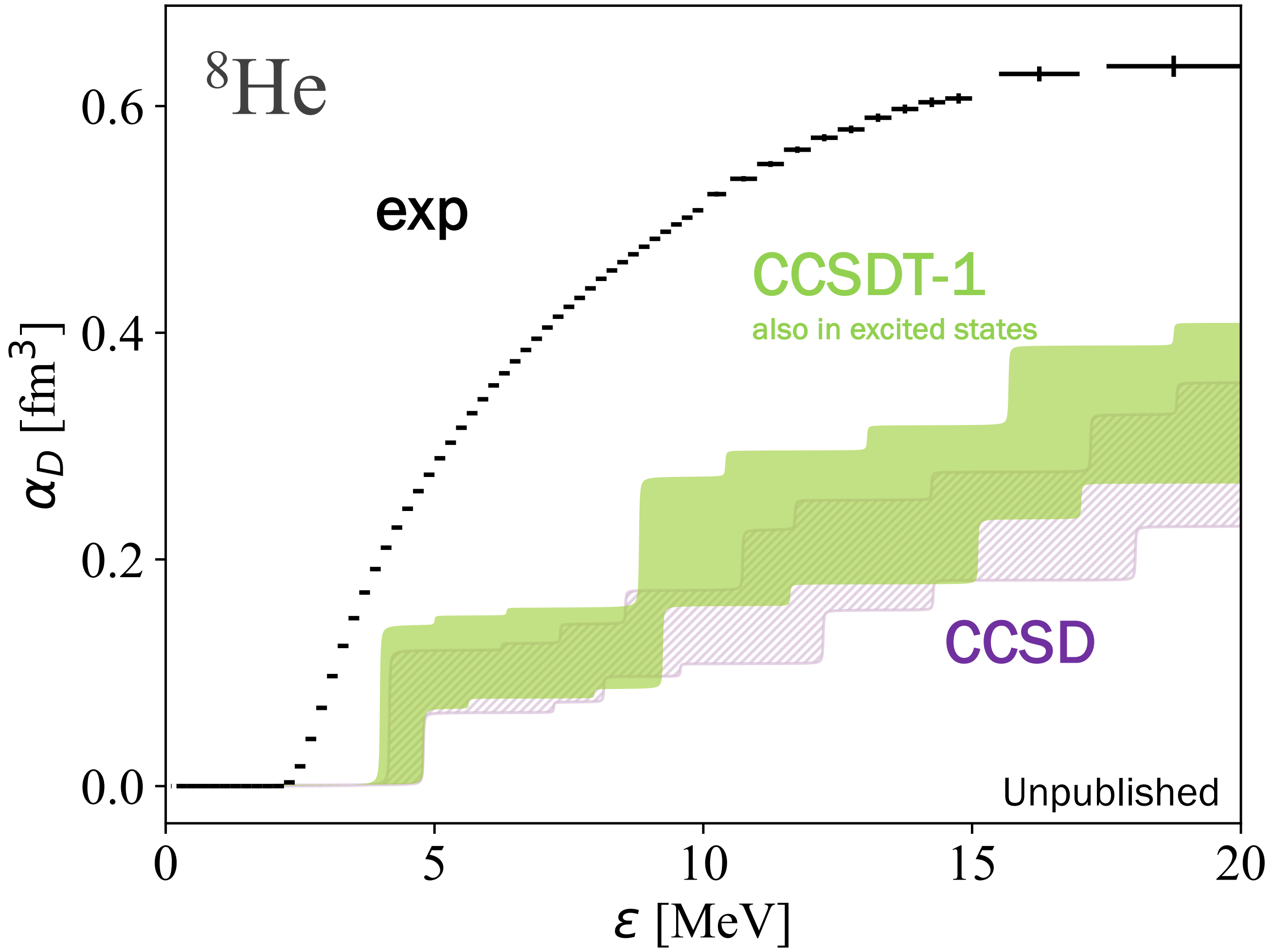


band spanning
1.8/2.0 (EM)
ΔNNLO$_{GO}$(394)
ΔNNLO$_{GO}$(450)
NNLO$_{sat}$

FB et al., PRC 105, 034313 (2022).
FB et al., FBS 65, 54 (2024).

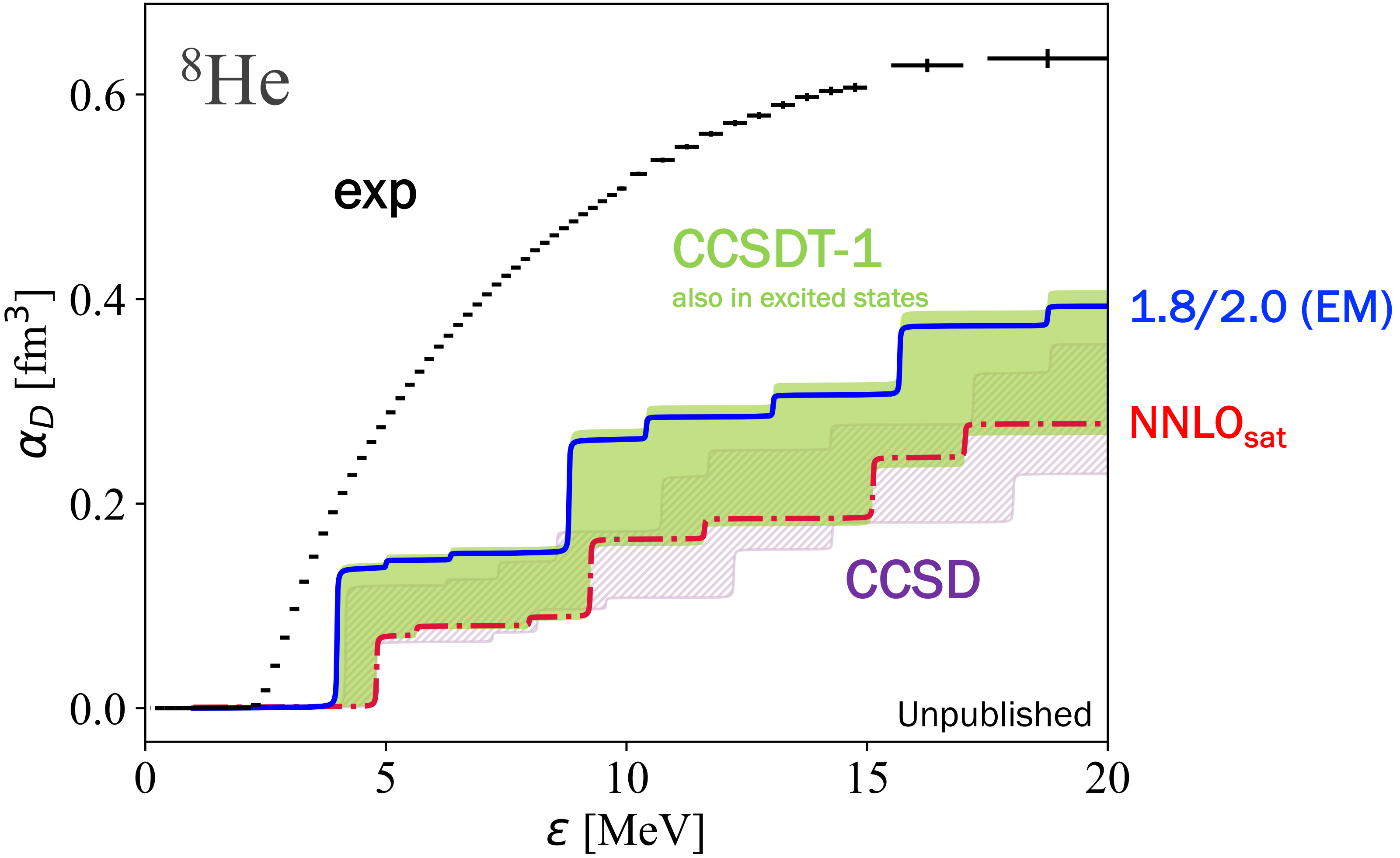
… and experiment

Exp data: C. Lehr (TU Darmstadt PhD thesis)&SAMURAI collab.



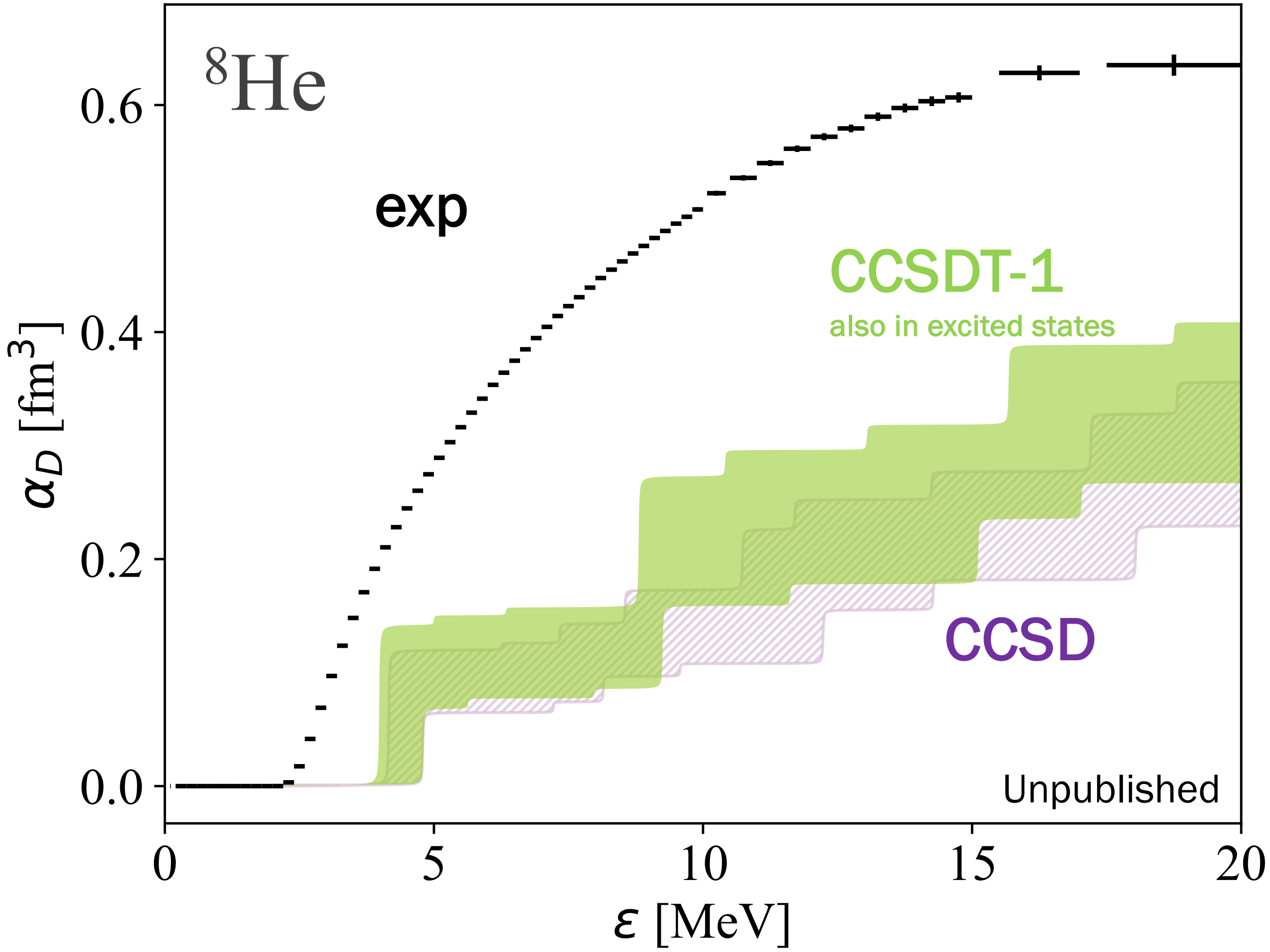
Strong dependence on the Hamiltonian

Exp data: C. Lehr (TU Darmstadt PhD thesis)&SAMURAI collab.



Missing higher order correlations?

Exp data: C. Lehr (TU Darmstadt PhD thesis)&SAMURAI collab.



For NNLO$_{sat}$, NCSM value available

C. Stumpf, PhD thesis, TU Darmstadt, 2017

$$\alpha_D = 0.4454(19)\ \text{fm}^3$$

compared to CC

$$\alpha_D = 0.37(3)\ \text{fm}^3.$$

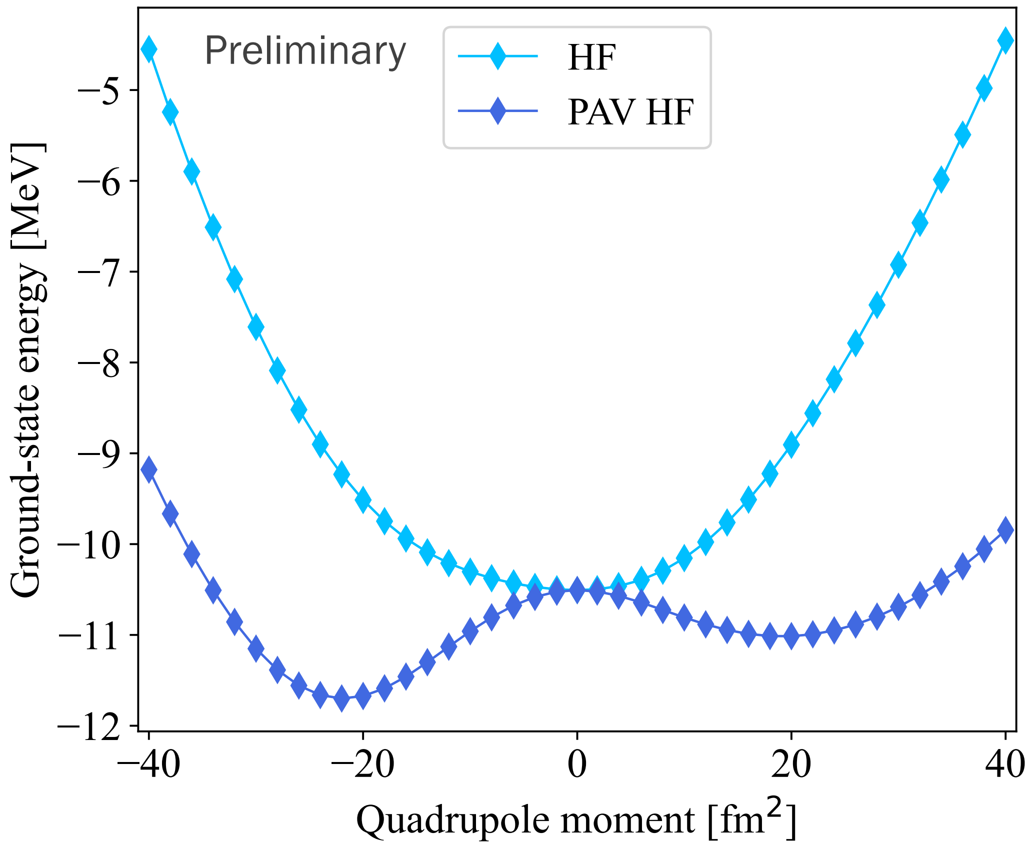
Indication of the impact of 4p-4h correlations?

Deformation in ^{8}He?

We start from **Hartree-Fock calculations** where:

- ❑ only axial symmetry is assumed,
- ❑ we minimize the energy under the constraint of a **fixed expectation value for the quadrupole moment**.

We then perform an **angular momentum projection** after variation (PAV) of the E_{gs} vs Q curve.

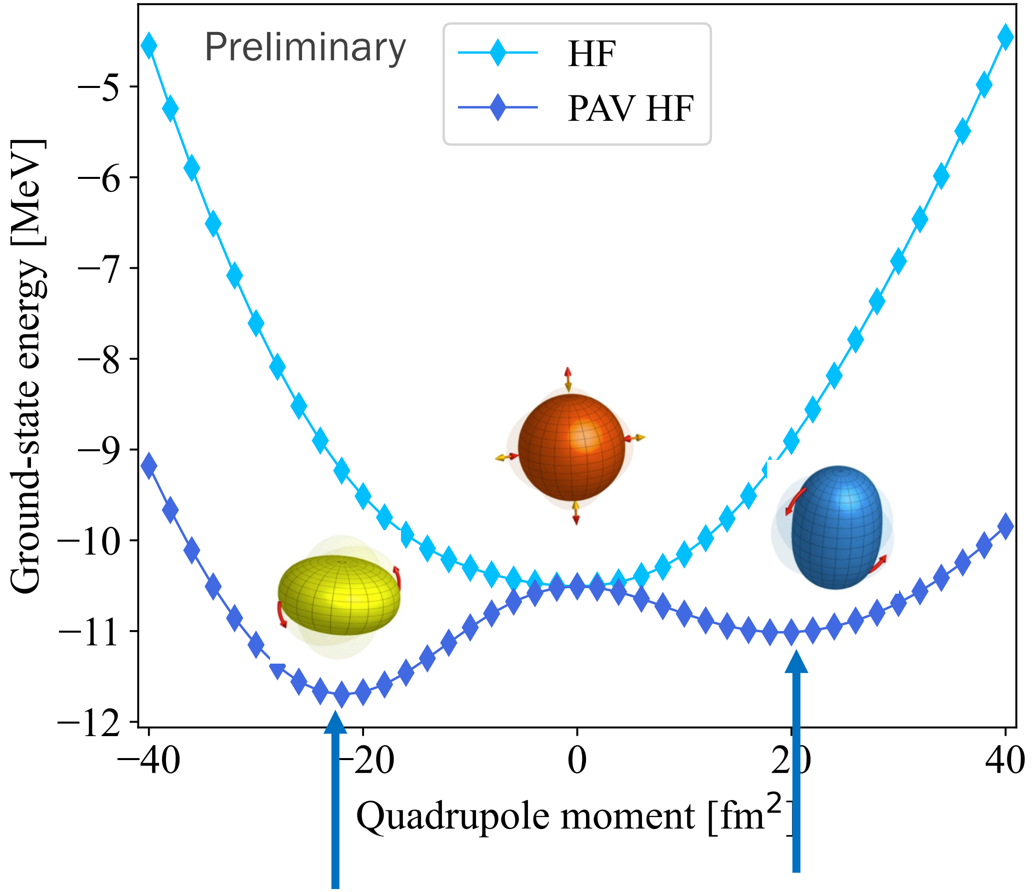


Deformation in ^{8}He?

We start from **Hartree-Fock calculations** where:

- only axial symmetry is assumed,
- we minimize the energy under the constraint of a **fixed expectation value for the quadrupole moment**.

We then perform an **angular momentum projection** after variation (PAV) of the E_{gs} vs Q curve.



two minima away from the spherical point!

Food for discussion

- In some cases, we can get more info on chiral EFT convergence with respect to many-body convergence

LO ⟶ NLO ⟶ N²LO ⟶ N³LO

versus

IMSRG(2) → IMSRG(3) → IMSRG(4)

2p-0h → 3p-1h → 4p-2h

from Alex's talk

- Is expert assessment the only way to get to many-body uncertainties? Can "metrics" as e.g. partial norms help us in developing a more rigorous strategy?

- In the presence of clustering or deformation phenomena, our estimate of the many-body uncertainty is not always reliable. Comparison with Halo/Cluster EFTs/virtually exact methods?

Thank you for your attention!