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The Hubbard- and van der Waals-corrections on the DFT calculations of epsilon-zeta transition pressure in solid oxygen

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In this study, we consider the treatments of short-range and long-range interactions in solid oxygen at the epsilon-zeta phase transition using the Hubbard U and van der Waals dispersion, respectively. We show that the London dispersion may correctly capture the nonlocal interactions in solid oxygen instead of the Hartree-Fock exchange [1]. The nonlocal effect is expected to be dominant at below 20 GPa. A correct treatment of the local and nonlocal interactions on an equal footing is, thus, important to study the solid oxygen. A comparison of a direct van der Waals correction vdW-D and nonlocal two-body correlation functionals vdW-DF with the nonlocal Hartree-Fock exchange in hybrid functionals [2] will be presented.

References

- [1] Le The Anh, Phys. Chem. Chem. Phys. 25, 25654 (2023).
- [2] A. J. Ochoa-Calle, Chem. Theory Comput. 11, 3 (2015).

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