Abstract Submitted
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The role of dispersion interactions in the formation of near-surface oxygen defects in CeO_2(111): Comparing DFT+U with HF/DFT hybrid functionals using plane-waves as a basis set[1] JOACHIM PAIER, CHRISTOPHER PENSCHKE, JOACHIM SAUER, Humboldt-University, Unter den Linden 6, 10099 Berlin, Germany — Cerium oxide is of paramount importance in the field of heterogeneous catalysis and in solid oxide fuel cells. Its ability to easily release and store oxygen goes together with the distinct facility to form and heal oxygen vacancies. Upon its formation, the electrons left need to localize, but conventional semilocal density functionals (LDA, GGA) are known to fail here. Viable solutions to this problem are the DFT+U approach and hybrid Hartree-Fock/DFT functionals being computationally more demanding [1]. However, common implementations of aforementioned approaches do not incorporate long-range dispersion interactions. Given that relaxation effects upon defect formation lead to more open structures and given the relatively high polarizability of Ce-atoms, dispersion interactions are supposed to be none-neglible. We apply Grimme's dispersion correction [2] and carefully cross-check results. Furthermore, we will give thorough estimates on dynamic effects and try to shed some light on the effects induced by the defect concentration. [1] M. V. Ganduglia-Pirovano, J. L. F. Da Silva, and J. Sauer, Phys. Rev. Lett. **102**, 026101 (2009). [2] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).

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