Abstract Submitted
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Optimizing photoabsorbers for water splitting: ab initio calculation of defective WO_3[1] MATTEO GEROSA, University of Chicago, Chicago, IL 60637, USA, FRANCOIS GYGI, University of California, Davis, CA 95616, USA, GIULIA GALLI, University of Chicago, Chicago, IL 60637, USA — Tungsten trioxide (WO_3) is a promising photoabsorber for water splitting [1], widely studied in the last decade. By means of ab initio simulations with dielectric-dependent hybrid functionals [2], we investigated a realistic model of the most stable surface of WO_3, which presents a high concentration of oxygen vacancies. We found multiple, stable local minima of the WO_3 surface, that may be attained depending on the type of lattice distortions occurring close to defects at finite temperature. Our results showed that the potential energy surface of the defective WO_3 surface is highly corrugated, with singlet and triplet states close in energy, and associated frontier orbitals with different localization properties. We gained insight on the effect on transport properties and of charge localization at the surface by using first principles molecular dynamics. [1] Q.X. Mi, Y. Ping, Y. Li, B.F. Cao, B.S. Brunschwig, P.G. Khalifah, G. Galli, H.B. Gray, and N.S. Lewis, J. Am. Chem. Soc. 134, 18318 (2012) [2] J.H. Skone, M. Govoni, and G. Galli, Phys. Rev. B 89, 195112 (2014)

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