Abstract Submitted
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Band gap engineering and optical properties of tungsten trioxide[1]
YUAN PING, Department of Chemistry, University of California, Davis, YAN LI, Computational Science Center, Brookhaven National Laboratory, DARIO ROCCA, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — Tungsten trioxide (WO3) is a good photoanode material for water oxidation but it is not an efficient absorber of sunlight because of its large band gap (2.6 eV). Recently, stable clathrates of WO3 with interstitial N2 molecules were synthesized [1], which are isostructural to monoclinic WO3 but have a substantially smaller bang gap, 1.8 eV. We have studied the structural, electronic, an vibrational properties of N2-WO3 clathrates using ab-initio calculations and analyzed the physical origin of their gap reduction. We also studied the effect of atomic dopants, in particular rare gases. Substantial band gap reduction has been observed, especially in the case of doping with Xe, due to both electronic and structural effects. Absorption spectra have been computed by solving the Bethe-Salpeter Equation [2] to gain a thourough insight into the optical properties of pure and doped tungsten trioxide. [1] Q. Mi, Y. Ping, Y. Li., B.S. Brunschwig, G. Galli, H B. Gray, N S. Lewis (preprint) [2]D. Rocca, D. Lu and G. Galli, J. Chem. Phys. 133, 164109 (2010)

[1]NSF-Chem CALTECH 68D-1086057 and DOE-BES DE-FG02- 06ER46262

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