Abstract Submitted
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Electronic and Optical Properties of Tungsten Oxide and Copper Tungstate for Water Oxidation[1] YUAN PING, Department of Chemistry, University of California, Davis, YAN LI, Computational Science Center, Brookhaven National Laboratory, JAMES C. HILL, Department of Chemistry, Purdue University, KYOUNG-SHIN CHOI, Department of Chemistry,University of Wisconsin-Madison,Madison, GIULIA GALLI, Department of Chemistry and department of Physics, University of California, Davis — We report first principles calculations of the electronic and optical properties of tungsten oxide clathrates [1,2] and copper tungstate solid solutions, which are considered to be promising materials for oxygen evolution in photo-electrochemical cells. In particular, we considered WO3 intercalated with rare gas atoms and small closed shell molecules, and CuW xMo1-xO4 solid solutions. Although relatively efficient photoanode materials, WO3 and CuWO4 are poor light absorbers, due to their band gap above 2.3 eV. In the case of WO3, we found that intercalation with Xe, N2 and CO may lead to a substantial decrease of the optical gap, mostly due to structural modifications of the oxide lattice. Our results for dinitrogen provided an interpretation of recent experiments [1]. In the case of CuWO4, we observed a 0.5-0.6 eV decrease of the gap when doping with Mo (50% to 75% concentration), in agreement with recent measurements. The gap decrease originates from a downward shift of the conduction band minimum. A detailed discussion of how intercalation and doping affect the electronic properties of tungsten oxide and copper tungstates will be presented. [1] Q. Mi et al, J. Am. Chem. Soc. 2012, DOI: 10.1021/ja3067622 [2] Y. Ping et al, Chem. Mat. 2012, DOI:10.1021/cm3032225

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