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**Electronic Excitations in Light Absorbers for Photoelectrochemical Energy Conversion: First Principles Calculations Based on Many-Body Perturbation Theory<sup>1</sup>**

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The efficiency of photo-electrochemical cell for water splitting relies on the availability of Earth abundant, stable light absorbers with band gaps in the visible range, and band edges properly aligned with water redox potentials. We will present several ab initio calculations aimed at understanding and predicting the electronic properties of candidate photo-electrode materials [1]. Our calculations were carried out at different levels of theory, including density functional and many body perturbation theory (MBPT). We focused on  $\text{WO}_3$  and  $\text{CuW}_{1-x}\text{Mo}_x\text{O}_4$ , and on functionalized Si wires for the photo-anode and photo-cathode, respectively. In particular, we will discuss how to decrease the band gap of  $\text{WO}_3$  by small molecule and rare gas atom intercalation [2,3], and by forming copper tungstate solid solutions [4]; in addition we will discuss how to improve band alignments with water redox potentials by considering phases of  $\text{WO}_3$  stable at high temperature [5]. Finally we will present calculations of absorption spectra of  $\text{WO}_3$  and silicon wires obtained using MBPT, by solving the Bethe Salpeter Equation, and we will present comparisons with recent experiments.

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[5] Y. Ping and G. Galli, submitted, 2013.

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