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Coupled experimetal and theoretical study of photon absorption and charge transport in BiVO4 photoanodes for solar water splitting[1]
YUAN PING, California Institute of Technology, TAE WOO KIM, University of Wisconsin, Madison, GIULIA GALLI, University of Chicago, KYOUNG-SHIN CHOI, University of Wisconsin, Madison — Bismuth vanadate (BiVO4) has been identified as one of the most promising photoanode materials for water-splitting photoelectrochemical cells. The major limitations of BiVO4 are its relatively wide bandgap (2.5 eV) and low electron mobility (0.2 cm-2V-2S-1), which limit its solar-to-hydrogen conversion efficiency. In this talk we will present the results of a coupled experimental and ab initio theoretical study showing that nitrogen doping together with extra oxygen vacancies lead to both a reduction of BiVO4 band gap and to an increase of the majority carrier density and mobility. In turn these improvements lead to the applied bias photon-to-current efficiency over 2%, a record for a single oxide photon absorber, to the best of our knowledge[1]. The codoping method adopted in our work could also be applied to simultaneously enhance photon absorption and charge transport in other oxides, providing new possibilities for photocatalytic materials. [1] T. Kim, Y. Ping, G. Galli and K. Choi, Nature Communications, 6,8769, (2015).

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