MAR17-2016-020195

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Discovery of new solar fuels photoanode materials with a combination of high-throughput theory and experiment[1]

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The discovery and design of new complex functional materials – and an understanding of their emergent phenomena and functional behavior in terms of their chemical composition and atomic-scale structure – is a grand challenge. In particular, the dearth of known low-band-gap photoelectrocatalytic materials poses roadblocks for the efficient generation of chemical fuels from sunlight. In this talk, I will describe a new pipeline that integrates high-throughput *ab initio* density functional theory calculations with high-throughput experiments. Our pipeline has led to the rapid identification of 12 ternary vanadate oxide photoelectrocatalysts for water oxidation, doubling the number of known photoanodes in the band gap range 1.2-2.8 eV, and establishing these vanadates as the most prolific class of photoanode materials for generation of chemical fuels from sunlight. Additionally, our calculations reveal new correlations between the VO_4 structure motif, d electron configuration, and electronic band edge character of these oxides. Accordingly, I will discuss how this work could initiate a 'genome' for photoanode materials and future applications of our high-throughput theory-experiment pipeline for materials discovery.

[1]This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231.