Identifying novel perovskite materials for water splitting applications by high through-put density functional theory calculations

Ximeng Wang[1], Anuj Goyal[2], Stephan Lany[2] and Simon Phillpot[1]

[1] Materials Science and Engineering Department, University of Florida, Gainesville, FL 32601, USA

[2] Materials Science Center, National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO 80401, United States of America

Traditional energy sources generate serious environmental problems including air pollution and greenhouse gases. A promising green energy source is the solar thermochemical process that can be used to produce hydrogen via water splitting. Current solar thermochemical reactors utilize CeO2-x in a two-step redox process. However, the high reaction temperature required for the use of CeO2 and the large temperature difference between the reduction and oxidation steps drives the search for other materials. Perovskite materials are promising candidates for such water splitting applications. The perovskite ABO3 formula yields multiple combinations of potential interest, with various A elements (lanthanides) and B elements (Ti, Mo, Fe, Mn, Cr and Co). Substitutions of Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba for A and Mg, Zn, Al, Ga, In for B broadens the number of possible compositions. Here, we apply high through-put DFT calculations to select candidates from different A-sites substituted and B-sites substituted ABO3. Thermodynamic stability and oxygen vacancy formation energy (2.5 eV-5.0 eV) are used as criteria to select potential candidates. Several candidates are identified through our study.

Keywords: perovskite, water splitting, vacancy formation energy, thermodynamic stability, DFT