Abstract Submitted
for the SES21 Meeting of
The American Physical Society

High-Throughput Screening of Semiconductors for Artificial Photosynthesis with Data-Mining and First Principles Calculations SEAN STAFFORD, Department of Physics, College of Arts and Science, Florida State University, ALEXANDER ADUENKO, Moscow Institute of Physics and Technology, JOSE MENDOZA-CORTES, Department of Chemical Engineering and Materials Science, Michigan State University — We propose an algorithm for efficient design of semiconductor structures with a selected set of physical properties. We deploy our algorithm to produce semiconductor candidates for artificial photosynthesis, i.e. photocatalytic water splitting. Our candidate structures are composed of earth-abundant elements, capable of trapping sunlight, suitable for H_2 and/or O_2 production, and stable to reduction and oxidation in aqueous media. First, we predict thousands of undiscovered semiconductors compositions using an ionic translation model trained on a large experimental database. Then, we screen the predicted semiconductors compositions for redox stability under HER or OER conditions. Finally, we generate thermodynamically stable crystal structures and calculate accurate band gap values for these compounds. Ultimately we produce dozens of promising semiconductor candidates with ideal properties for artificial photosynthesis.

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Date submitted: 07 Oct 2021 Electronic form version 1.4