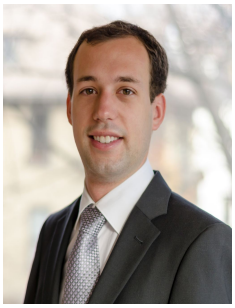
High-Throughput Computational Screening of Perovskites for Thermochemical Water Splitting Applications



Antoine Emery,

Northwestern University, Evanston, Illinois

Tuesday November 1, 14:00, Room MED 2 1522

Abstract: Among the several possible routes of hydrogen synthesis, thermochemical water splitting (TWS) cycles is a promising method for large scale production of hydrogen. The choice of metal oxide used in a TWS cycle is critical since it governs the rate and efficiency of the gas splitting process. In this work, we present a high-throughput density functional theory (HT-DFT) study of ABO_3 perovskite compounds to screen for thermodynamically favorable two-step thermochemical water splitting materials. We demonstrate the use of two screens, based on thermodynamic stability and oxygen vacancy formation energy, on 5,329 different compositions to predict 139 stable potential candidate materials for water splitting applications. Several of these compounds have not been experimentally explored yet and present promising avenues for further research. Additionally, the large dataset of compounds and stability in our possession allowed us to revisit the structural maps for perovskites. This study shows the benefit of using first-principles calculations to efficiently screen an exhaustively large number of compounds at once. It provides a baseline for further studies involving more detailed exploration of a restricted number of those compounds.

Short Bio: Antoine Emery is currently a fifth-year PhD candidate in the Wolverton group at Northwestern University. He earned his Bachelor's degree in materials science and engineering from the EPFL in 2009. After studying one semester at the ETHZ and completing his Master's thesis at Northwestern University, he obtained a Master's degree from EPFL in materials science and engineering in 2011. Antoine currently works on high-throughput density functional theory discovery of materials for thermochemical water splitting applications. In his thesis work, he uses the Open Quantum Materials Database (OQMD) to screen for thermodynamically favorable metal oxide to produce hydrogen in an environmentally friendly. He is a Hierarchical Materials Cluster Program Fellow.