HydroGEN
Advanced Water Splitting Materials

Sandia Technical Seminar

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Room 903/1021-1022
and by WebEx live stream

Perovksite Materials Design for Solar-thermochemical Processes by Combining Experimental and Theoretical Thermodynamic Data

Abstract: Two-step solar thermochemical redox cycles have gained broad interest, as they allow the storage and utilization of solar energy. A key element in optimizing these cycles is the choice of suitable redox materials which serve as oxygen carriers. Perovskites are ideal candidate materials for this optimization, as their composition can be tuned versatilely through the formation of solid solutions. It is shown how $AMO_{3-\delta}$ perovskites with two different transition M metals and two different alkali, alkali earth, or lanthanide metals A can be designed to reach any redox enthalpy value between 0 and 400 kJ/mol O. A thermodynamic model is presented describing the redox enthalpy and entropy change as a function of the non-stoichiometry δ, which is based both on theoretical data and experimental data. The theoretical data consists of DFT calculations and has been gathered using the infrastructure of Materials Project, whereas the experimental data has been contributed by DLR through thermogravimetric scans using the van't Hoff method. Both datasets are combined in user-controlled interactive graphs on MP Contribs within the infrastructure of Materials Project. For any of the studied materials, graphs describing the chemical equilibrium as a function of the temperature, oxygen partial pressure, and/or δ can be created. Moreover, using a simplified generic process model, the energy demand per mole of oxygen, hydrogen, or carbon monoxide produced is calculated, and materials can be ranked based on the expected overall energy consumption for a set of over 10,000 different process parameters. By this means, materials for solar-thermochemical applications can be chosen according to the specific field of application and process parameters. This work is the result of a joint effort between the Lawrence Berkeley National Laboratory (LBNL) and the German Aerospace Center (DLR).

Biography: Josua Vieten is working on his dissertation at the Institute of Solar Research of the German Aerospace Center (DLR). His research is focused on the targeted design of perovskite redox materials for solar-thermochemical processes. In fall 2017, he worked as a visiting researcher at the Lawrence Berkeley National Laboratory (USA). He received a master's degree in Chemistry from the TU Munich in 2016 and a master's degree in Advanced Materials Science from a joint program of TU and LMU Munich and the University of Augsburg in 2015.

Registration: Email h2awsm@nrel.gov to request the WebEx link. Online attendance is limited to the first 200 registrants.

Organizer: Tony McDaniel, Sandia National Laboratories

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