FROM DEFECTS TO ALLOYS: COMPUTATIONAL DESIGN OF NON-STOICHIOMETRIC MATERIALS

Stephan Lany, National Renewable Energy Laboratory, Golden, CO 80401
Stephan.Lany@NREL.gov

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Non-stoichiometry provides an important route to materials by design. Using an extensive toolset of first principles computations, we predict the evolution of materials properties with changes of the composition. These approaches span the range from isolated point defects, to highly doped materials with dopant-defect interactions, to alloy systems. Highlighted examples include: (a) Doping and defect phase diagram in Ga_2O_3, an ultra-wide band gap material receiving high current interest. (b) Heterostructural MnO-ZnO alloys, where the composition induced rock-salt to wurtzite transformation enables photo-electrochemical water splitting applications [1]. (c) Disorder and extended anti-site defects in the photovoltaic Cu chalcogenides Cu_2SnS_3 and Cu_2ZnSnS_4 [2,3].

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