INTEGRATING HIGH-THROUGHPUT COMPUTATIONS AND EXPERIMENTAL KNOWLEDGE TO ADVANCE DESIGN AND DISCOVERY OF NOVEL FUNCTIONAL MATERIALS

Vladan Stevanović, Colorado School of Mines & National Renewable Energy Laboratory
vstevano@mines.edu

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The ability of first-principles computational approaches to provide access to relevant properties of materials is critical for accelerating the pace at which materials design and discovery occurs. Yet, in many instances the complexity of the properties of interest renders direct, first-principles calculations difficult to attain within the required accuracy. A practical way of dealing with this challenge is the development of physically motivated proxies and/or semi-empirical models that combine first-principles based methods with experimental knowledge in order to achieve computationally tractable approaches that are able to guide identification of novel functional materials. In this talk, I will discuss recent work in developing and applying such computational approaches to predict materials properties that were traditionally problematic to assess solely from first-principles. These properties include: (1) enthalpies of formation and related problem of predicting the existence – i.e. stability with respect to decomposition – of new/unreported compounds[1], and (2) electric and thermal transport properties of materials to advance the search for new photovoltaic[2] and thermoelectric materials[3]. In both cases our recent developments provide quantitative predictions of relevant properties, which, in turn, enable high-throughput calculations and identification of new candidate materials. Results of these efforts are open and available via NRELMatDB (http://materials.nrel.gov) and TEDesignLab (http://tedesignlab.org).

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