On a Quest for Novel Functional Materials: Theory and Computation Guided Discovery and Design

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Abstract
Discovery and design of novel functional materials is of paramount importance for accelerating development of disruptive technologies needed to help secure a more sustainable future. However, searching for and designing new materials requires knowledge of a number of properties that are relevant applications and that are typically not available for a large number of systems. Hence, computational approaches, which are able to provide access to these properties with the required accuracy are instrumental in accelerating the pace at which materials discovery and design occurs. In this talk I will present our recent work, which draws on the solid-state and semiconductor theory to develop predictive, computationally tractable and experimentally validated approaches to search for novel functional materials. The application space covers photovoltaic, thermoelectric, as well as materials for transparent and power electronics. The main focus is on methods to predict transport properties of semiconductors including the charge carrier and heat transport as well as the tolerance to defects and the ability to be doped. In many of the application areas our recent developments offer quantitative predictions of relevant properties, which, in turn, allow large-scale calculations and identification of new candidate systems. I will present examples of our material searches and discuss experimental realization of the computationally identified material systems.

Short Biography
Vladan Stevanović is a theoretical solid-state physicist with multidisciplinary research background in applied computational physics and materials science. He currently holds a joint Assistant Professor position at the Department of Metallurgy and Materials Engineering, Colorado School of Mines, and National Renewable Energy Laboratory (NREL). In pursuit for novel energy materials Vladan’s research stands at the intersection between solid-state physics, materials science, large-scale (high-throughput) computations and big data. With the focus on photovoltaic, thermoelectric and materials for transparent and power electronics, it combines development and application of predictive methods to model relevant properties of real materials. Topics of interest include materials thermochemistry and the problem of predicting the existence of new (previously unreported) compounds, predictive methods for modeling optoelectronic and transport properties, and screening of large chemical spaces in searching for, and designing novel functional materials.