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

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Discovery and design of novel functional materials is critical to a broad range of important applications. However, searching for and designing new materials requires knowledge of a number of relevant properties that are typically not available from experiments for a large number of systems. Hence, computational approaches, which are able to provide access to these properties with the required accuracy can be 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, and materials for transparent and power electronics. The main focus is on methods to predict charge carrier and heat transport in semiconductors including the defect chemistry and doping tendencies. 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.