Computation-Informed Search for p-type Transparent Semiconductors

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Friday August 23rd, 14:00, Room MED 2 1124 (CoViz2)

Abstract: Discovery of a high performance p-type transparent conductor (TC) is critical to advancing photovoltaic technologies, e.g. as transparent contacts and window layers. Combined high-throughput computationand combinatorial experiments offer a promising pathway to achieve such materials, yet properties comparable to n-type ITO have not yet been found due to low hole mobilities and dopability. Non-oxide semiconductors (e.g. chalcogenides, pnictides) offer advantages to oxides due to lower ionization potentials and potential p-type dopability. My research uses a materials discovery pipeline to search for new non-oxide p-type TCs with the following steps: evaluating computational descriptors, performing computational screenings and analysis, identifying promising synthesizable compounds, synthesizing and characterizing thin film candidates, and incorporating them into devices. In this talk I will first provide an integrated computational and experimental evaluation of these descriptors by posing the question: can we use a high throughput screening methodology to accurately identify previously synthesized TCs? I then use this understanding to evaluate whether known materials emerge from the screening, and to motivate an updated, rational selection criterion for future screenings of p-type TCs. Second, I will explore wide-gap non-oxide ternary semiconductors that we have predicted computationally as p-type TCs, with a focus on the role of cation chemistry, hole dopability, and stability. Third, case studies will be presented of combinatorial sputtering to synthesize such compounds, investigate chemical phase space, and characterize structural and optoelectronic properties within a combinatorial framework. Lastly I will discuss progress in implementing these

materials as contacts in photovoltaic devices, in particular my work at EPFL on silicon heterojunction solar cells, to complete the computationally-guided materials discovery framework.

Bio: Rachel is a Ph.D. student at UC Berkeley, researching high-throughput computation, synthesis, and characterization of p-type transparent electrode materials for solar energy under Prof. Kristin Persson. As a UC Chancellor's Fellow and an NSF Graduate Research Fellow, she is conducting a joint thesis project at Berkeley Lab, NREL, and SLAC, and is currently on a ThinkSwiss research internship at EPFL PV-lab. She is the co-founder of Cycle for Science, a science education outreach organization, and spends her free time teaching science, exploring the outdoors, and envisioning a renewable-energy-powered future.