UNIVERSITY OF CALIFORNIA, IRVINE

Department of Materials Science and Engineering

First-Principles Studies of the Optoelectronic Properties of Materials

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Abstract: Low-cost and earth-abundant materials, such as wide bandgap semiconductors, chalcogenides, and organic molecules, are currently being pursued as integrated components within next-generation optoelectronics. The design and optimization of these materials requires understanding of their structural features and spectroscopic properties at the nanometer scale, i.e. how electronic excitations, charge transfer, and charge transport relate to their chemical structure and are influenced by solid-state morphology. Theory and computation provide important tools for predicting material properties on the atomic scale, and guiding synthesis and experimentation. In this talk, I will present our recent advances in applying state-of-the-art first-principles computational methods, based on the laws of quantum mechanics, to understand the excited-state electronic properties of next-generation materials. In particular, we explain the role that structural complexity, arising due to the presence of defects, interfaces, and phonons, plays on the electronic and optical excitations of bulk and low-dimensional semiconductors, and demonstrate that simple physical models can explain these phenomena. Collectively, our first-principles simulations provide a physical intuition of complex materials to understand and improve the performance of next-generation devices.

Bio: Dr. Sahar Sharifzadeh is an Assistant Professor at Boston University. She obtained her PhD from Princeton University, working under the guidance of Prof. Emily Carter, and subsequently joined the Molecular Foundry at Lawrence Berkeley National Laboratory as a postdoctoral fellow and project scientist in the group of Dr. Jeffrey Neaton. Prof. Sharifzadeh was awarded the Department of Energy Early Career Award in 2017, the National Science Foundation Early Career Award in 2019, and the Bost University College of Engineering Early Career Award in 2019. Her research focuses on first-principles computational modelling of materials.