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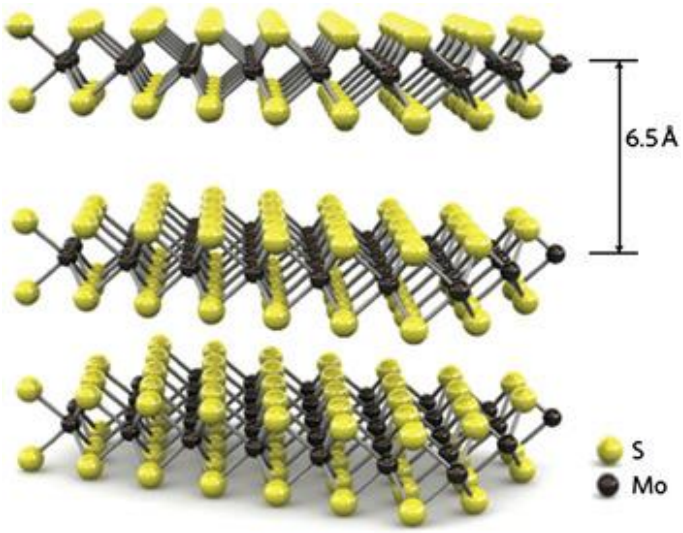

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Designing 2D-Layered Materials for Device Applications

Abstract

During the last decade, 2D layered materials have caused a paradigm-shift in our understanding of nanomaterials and opened up a new era of physics. The current family of 2D materials covers a vast variety of fundamental properties. The possibility of engineering 2D materials with strategic innovations through assembly, alloying and doping, provides many opportunities. However, it is impossible to explore the properties of such a huge material-domain experimentally. Discovery of novel 2D-material configurations with desired properties can be accelerated through predictive materials modeling. Such selective designing requires a deeper understanding of how structural configurations relate to their electronic and other physical properties. Based on the results from first principles density functional theory, we investigate the structural/electronic and vibrational properties of doped and alloyed 2D materials systems, and explore for their device applications. In this talk, I will overview the recent progress of our research group with three topics: (i) Structural modifications of Group IV-monochalcogenides that leads to an indirect-direct transition. (ii) Modeling optical properties to characterize large area grown MoS_2, and lastly (iii) Enhancing catalytic activity of doped-MoS_2 for CO_2 reduction.

2:00-3:00 p.m., Monday, April 30th, McLane Hall 258
Special time and place. All are welcome!