Computational Discovery of Novel 2D Materials for Optoelectronic Device and Energy Technologies

The rapid rise of novel single-layer materials, presents the exciting opportunity for materials science to explore an entirely new class of materials. This comes at the time when mature computational methods provide the predictive capability to enable the computational discovery, characterization, and design of single-layer materials and provide the needed input and guidance to experimental studies. I will present our data-mining and evolutionary algorithm approaches to identify novel 2D materials with low formation energies and show how unexpected structures emerge when a material is reduced to sub-nanometers in thickness. We discovered several 2D materials in the families of group III-V compounds and group-II oxides with promising properties for electronic devices and identify suitable metal substrates that can stabilize several of these as-yet hypothetical materials. In the families of group-III monochalcogenides and transition metal dichalcogenides we identify several 2D materials that are suitable for photocatalytic water splitting. For several transition-metal chalcogenide compounds we find that ferromagnetic order emerges at temperatures accessible to experiments. This opens the opportunity to investigate the interplay of magnetic order and reduced dimensionality and may provide materials for spintronics applications. Our results provide guidance for experimental synthesis efforts and future searches of materials suitable for applications in energy technologies and optoelectronic devices.