Bottom-up Design of 2D Material Functionalities from First Principles

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Two-dimensional materials have many promising applications for next generation flexible devices. Rational bottom-up design of these functional materials rests on the ability to predict from first principles physical properties that are fundamental to the proposed functionalities. In this talk, we present insights from recent first principles calculations that map the atomic and electronic structure of 2D materials to important macroscopic observables, such as piezoelectricity, the valley Zeeman effect[1], optical properties[1-3], and the emergence of flat bands[3]. Coupled with high throughput calculations, we identify 2D materials with excellent piezoelectric properties and discuss how to optimize the piezoelectric properties and spontaneous ferroelectric polarization in these materials. Our predictions are confirmed with experiments. We also present a first principles approach for predicting the Landau levels and single-band g-factors in monolayer H-phase transition metal dichalcogenides. These predictions pave the way for controlling the magnetic-field response of 2D valleytronic materials by bottom-up design. Finally, time permitting, we discuss the bottom-up control of optical properties in quantum-confined 2D metals[2], and the emergence of flat bands and physics of multiple dimensions in 2D covalent organic framework materials[3].

[1] Physical Review Research, 2, 033256 (2020)

[2] Advanced Functional Materials, 2005977 (2020)

[3] Nanoscale, 12, 20279 (2020)