Role of van der Waals Interactions in Alleviating Epitaxial Strain in WS$_2$/WSe$_2$ Lateral Heterojunctions

LIJIE TU, KA UN LAO, SAIEN XIE, JUNTENG JIA, Cornell University, ALVARO VAZQUEZ-MAYAGOITIA, Argonne National Laboratories, JIWOONG PARK, ROBERT A. DISTASIO JR., Cornell University — Novel 2D transition metal dichalcogenides (TMD) materials are emerging as promising candidates for high-performance mechanical, electrical, optical, and magnetic devices with tunable parameters. In this work, we will consider a WS$_2$/WSe$_2$ (4% lattice mismatch) lateral heterostructure that was grown with epitaxial interfaces on an SiO$_2$ substrate and showed periodic ripples in the WSe$_2$ monolayer. To explain these experimental findings, we have investigated the subtle energetic balance between epitaxial strain and van der Waals (vdW) interactions with the underlying substrate in this system. To obtain a quantitative theoretical estimate of the bending and stretching energy components of the WSe$_2$ monolayer, we extended current bulk continuum mechanical theory to atomically-thin nanofilms. For the vdW interactions, we considered different first-principles based approaches that account for both pairwise-additive dispersion interactions and the many-body dispersion (MBD) expansion of the long-range correlation energy. We will also briefly discuss our computational strategy, which utilizes novel algorithmic developments with high-performance computing resources, to explore the flat-rippled phase space in this realistic 2D material containing $\approx$150,000 atoms.

Lijie Tu
Cornell University

Date submitted: 11 Nov 2016
Electronic form version 1.4