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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 ≈150,000 atoms.

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