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Coherently stacked MoS_2/WSe_2 heterostructures: Moiré pattern and its effect on interlayer couplings CHENDONG ZHANG, UT at Austin, MING-YANG LI, Academia Sinica; KAUST, CHIH-PIAO CHUU, Academia Sinica, MEI-YIN CHOU, Academia Sinica; Georgia Institute of Technology;NTU, Taiwan, LAIN-JONG LI, KAUST, CHIH-KANG SHIH, UT at Austin — Vertically stacked heterojunctions (HJs) of transition metal dichalcogenides (TMDs) have been proposed as fundamental building blocks for several novel electronic and photonic devices. Although such HJs can be easily achieved by sequential transferring of different TMDs, this approach is not scalable, and the orientation relationship between the layers is difficult to control. A much more desirable approach is to directly grow one kind of TMD on top of the other. In addition to being a scalable platform, the epitaxial approach also results in a well-defined orientation relationship. A very important question to ask is "What is the role of the interlayer coupling on the electronic structures of such a bilayer stack?" By using scanning tunneling microscopy/spectroscopy (STM/S) and first-principles calculations, we investigate the MoS_2/WSe_2 vertical heterojunctions formed by direct epitaxial growth. The different lateral lattice constants between MoS_2 and WSe_2 lead to the formation of a well-ordered Moire pattern with a superlattice constant of ˜8.5 nm. This superlattice reflects the variation of the lateral alignment between the MoS_2 and WSe_2 lattices. STS shows very large variations of interlayer coupling, as a function of the lateral alignment. More interestingly, depending on the location in the BZ, the interlayer coupling has very different consequences on the electronic structures.

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