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Interlayer Hybridization in van der Waals Heterostructures. NAM LE, University of South Florida, Department of Physics, HUAN TRAN, University of Connecticut, Institute of Materials Science, LILIA WOODS, University of South Florida, Department of Physics — Van der Waals heterostructures composed of chemically inert dissimilar layers are of great interest for fundamental science and applications. The weak interplanar interactions and orbital overlap are expected to bring modifications to the constituent materials. By using first principles simulations, we investigate the properties of several heterostructures, including graphene/silicene, graphene/MoS2, and silicene/MoS2. The calculations reveal superlattice characteristic points in the Brillouin zone associated with the different stacking patterns. Band structures projected on each of the constituents show hybridization features related to specific orbital overlap for each heterostructure. Phonon dispersion spectra for the considered heterostructures are also investigated.

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