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Electronic Structure Modeling for 2D Layered Material Stacks[1]
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— The van der Waals heterostructures have promising electronic applications and offer access to two-dimensional theoretical physics. It is crucial to have efficient approaches to model these heterostructures with desired properties by harnessing different flavors of the layered materials and the twist angle in between. In our work, we construct the ab-initio tight binding models by employing Wannier transformation of density functional theory calculation for both intra- and inter-layer couplings. Our models are further applied to the comparison with magneto-transport experiments, incommensurate stacking crystals and the strain effects.

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