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Electronic properties of misoriented bilayer transition metal dichalcogenides[1] SUPENG GE, DARSHANA WICKRAMARATNE, MAHESH NEUPANE, SHANSHAN SU, ROGER LAKE, Univ of California - Riverside — Motivated by a growing interest in vertically stacked van-der-Waal heterostructures, we explore the effect of misorientation in bilayers of MoS2, MoSe2, WS2 and WSe2 on their electronic properties. Mechanical stacking of individual monolayers or chemical and epitaxial growth of this family of layered materials often leads to misoriented interfaces between individual monolayers. Isolated monolayers of MoS2, MoSe2, WS2 and WSe2 exhibit a direct band gap between 1 - 2 eV. The band gap transitions from direct to indirect when the film thickness increases from a monolayer to a bilayer. The question we address is "Does misorientation between semiconducting TMD bilayers electronically decouple them, as is observed in misoriented bilayers of graphene?" Using density-functional-theory we investigate the effect of different commensurate rotation angles, stacking order and displacements on the electronic structure of these materials. The effect of these atomic structural variations on the inter-layer coupling, band gaps and effective masses is presented and compared to the equivalent monolayer and bilayer properties for each material.

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