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Interlayer coupling in few-layers transition metal dichalcogenides

BOXIAO CAO, TIANSHU LI, George Washington Univ — The vertically heterostructured transition metal dichalcogenides (TMD) few-layers may display a wide range of lattice registry. By density functional theory and numerical structural analysis, we examined both the atomic and electronic structures of arbitrarily stacked TMD few-layers. It is shown [1] that the variation of indirect band gap in MoS_2 bilayers is mainly attributed to the interlayer sulfur-sulfur (S-S) interaction. We developed a structural model that allows understanding such interaction under an arbitrary stacking sequence. It is shown the arbitrarily stacked MoS_2 bilayers should exhibit a weak twist angle dependence on the magnitude of its indirect band gap, except for those special twist angles that recover high symmetry stacking sequences. Our analysis provides a thorough theoretical explanation to the recently measured photoluminescence spectroscopy and can form the basis for understanding the coupling in other vertically heterostructured TMD few-layers. For example, through a close experimental collaboration, we have recently identified the electronic origin for the metallization of WS_2 under high hydrostatic pressure (up to 35 GPa) [2].

1. B. Cao and T. Li, J. Phys. Chem. C 119, 1247 (2015)
2. A. Nayak, *et. al.*, ACS Nano 9, 9117 (2015)

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