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Interlayer coupling in WS_2-MoS_2 heterostructure with different stacking angles: A first- principles study

Two-dimensional transition metal dichalcogenides (TMDCs) such as WS_2 and MoS_2 have been considered as potential platforms for next generation electronic devices. Monolayer TMDCs have direct band gap, and its lack of inversion center allows the access to the valley degree of freedom for potential valleytronic devices [1]. However, for multilayer TMDCs, it is known that their physical properties are significantly modified by the interlayer coupling at the interface [2,3]. The interlayer coupling is a function of stacking angles as well as the layer materials, allowing more options in engineering the optical and electronic properties of stacked 2D TMDCs [4,5]. In this work, we investigate the possibility to tune interlayer coupling in WS_2-MoS_2 bilayer heterostructure using various stacking angles by first-principle density of states calculations and compare this with the interlayer coupling in WS_2 bilayer and MoS_2 bilayer.

References

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Figures

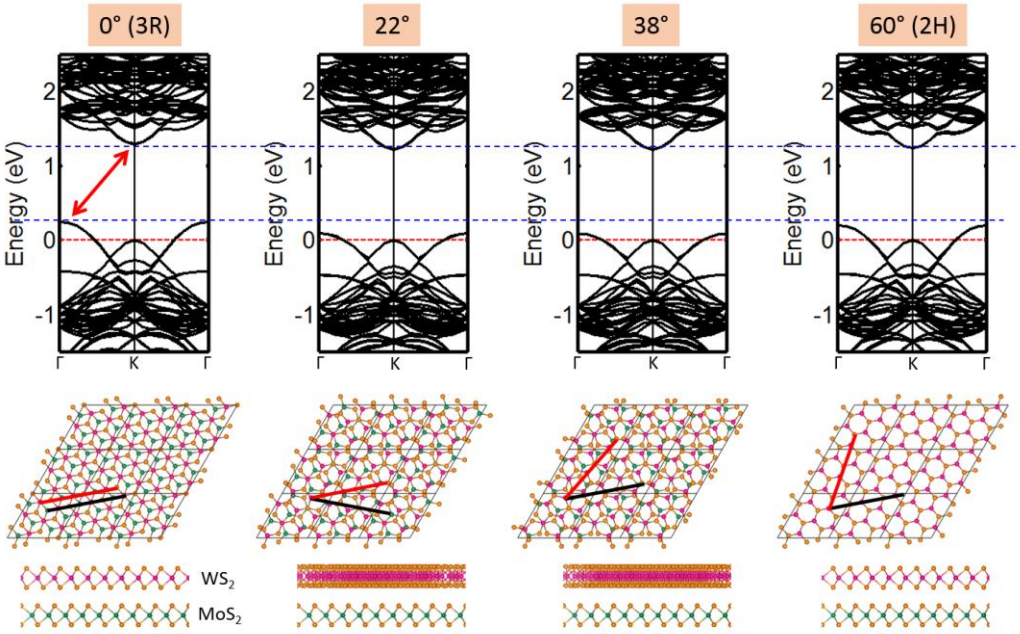

Figure 1: Calculated band structure and atomic structure of WS_2-MoS_2 heterostructure with 0°, 22°, 38°, and 60° stacking angle, respectively.