Electronic band structure of Gr/MS_2 (M=Mo, W) and WX_2/MoX_2 (X=S, Se) van der Waals heterostructures

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Van der Waals heterostructures (vdWh) are vertically stacked two-dimensional materials with remarkable properties. Superconductivity of twisted bilayer graphene at the magic angle, interlayer excitons in transition metal dichalcogenide (TMD) heterostructures, and optoelectronic properties of TMD/graphene heterostructures, are examples, among others, where vdWh significantly differ from their monolayer constituents. Ab-initio electronic structure calculations for vdWh and their interpretation are challenging as different crystal lattices combine into a single material (Fig. 1a,b) and large simulation cells are required. We have developed a methodology for unfolding and analyzing the electronic band structure of vdWh in a way that a clear comparison with the electronic bands of each monolayer can be made (Fig. 1c,d). Our results show that composition of monolayers, twist angles, and stress in the heterostructures have a strong influence on their observable optoelectronic properties. The effect of band hybridization occurring from the coupling of the monolayers is identified and discussed. TMD/TMD heterostructures are type II semiconductors when the band hybridization does not change the valence band maximum from K to Γ.

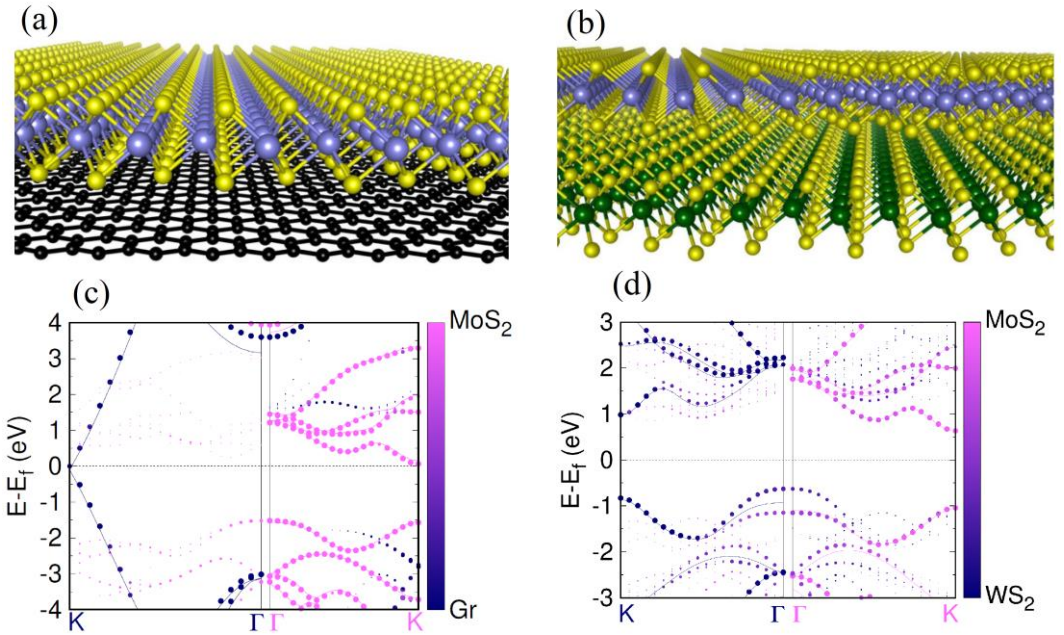

Figure 1: Van der Waals heterostructures, Gr/MoS_2 (a) and WS_2/MoS_2 (b). The unfolded band structures on the 1st Brillouin Zones of the bottom monolayer (dark blue K and Γ) and top monolayer (magenta K and Γ) for Gr/MoS_2 (c) and WS_2/MoS_2 (d), where the solid lines represent the band structures of the isolated monolayers and the points depict the unfolded electronic states of the heterostructure.

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