The dispersion energy strength of van der Waals interaction of the two-dimensional stacked structures

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Stacking different two-dimensional (2D) materials together to form van der Waals (vdW) heterojunctions can effectively improve the performance of low-dimensional optoelectronic devices[1,2]. The stability of the vdW interaction is a key factor and challenge for practical application of 2D stacked material photoelectric devices, but the quantitative analysis of the weak interaction force between stacked 2D materials is less. Through energy decomposition analysis based on the force field (EDA-FF) method[3], we obtained the quantitative energy strength of the three components — electrostatic energy, exchange repulsion energy and dispersion energy of the total binding energy between bilayer graphene, graphene/MoS$_2$ and graphene/WS$_2$, shown in Figure 1.
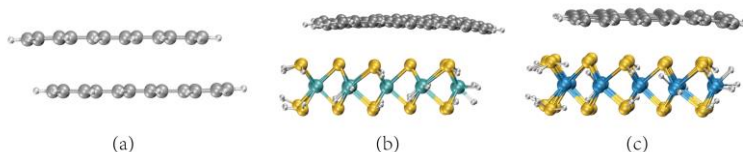

(a)   (b)   (c)

Figure 1, Stable configurations of the three 2D bilayer stacked structures: (a) bilayer graphene, (b) graphene/MoS$_2$ heterostructure, and (c) graphene/WS$_2$ heterostructure.

The dispersion energy of the vdW interaction accounts for more than 60% of the binding energy of the weak interaction between the 2D bilayer stacked structures, shown in Figure 2, which is useful for understanding the stabilization and reliability of 2D stacked material heterojunctions for practical applications.
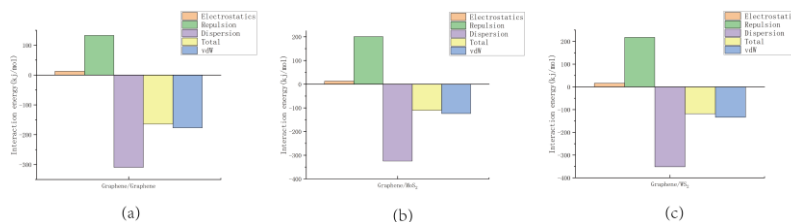

(a)   (b)   (c)

Figure 2, EDA-FF analysis result histograms: (a) bilayer graphene, (b) graphene/MoS$_2$, and (c) graphene/WS$_2$.

The vdW potential of the three single-layer materials is further analysed, shown in Figure 3. The dispersion attraction potential in the blue region can promote the combination of two of these 2D monolayer structures in the stacking process, which is the key factor in the stable formation of the 2D stacked bilayer structures.
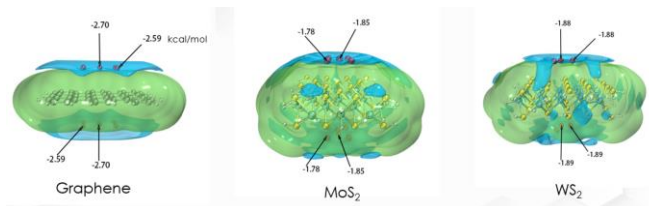

Figure 3, Isosurface plots of the vdW potential of the three monolayer structures.

Acknowledgement

References

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