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

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Abstract: 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.

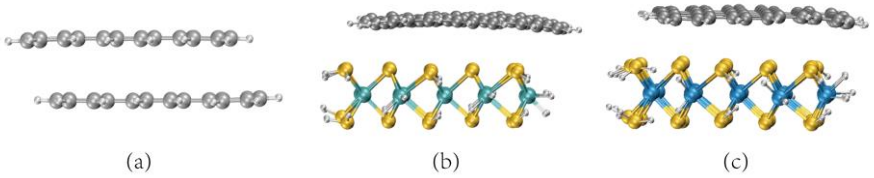

Figure 1, Stable configurations of the three 2D bilayer stacked structures: (a) bilayer graphene, (b) graphene/MoS_2 heterostructure, and (c) graphene/WS_2 heterostructure.

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.

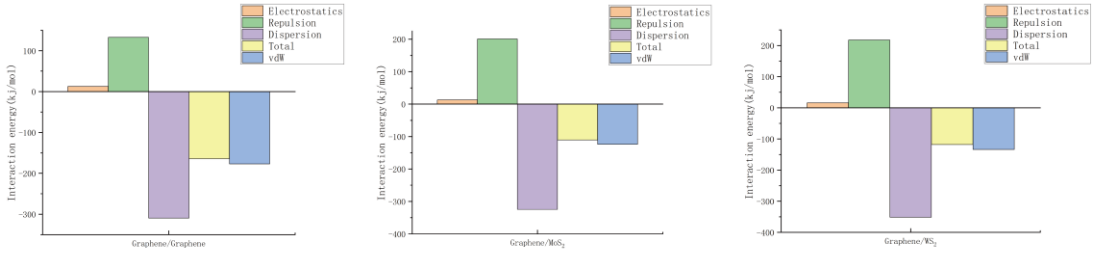

Figure 2, EDA-FF analysis result histograms: (a) bilayer graphene, (b) graphene/MoS_2, and (c) graphene/WS_2.

The two heterostructures of the graphene/MoS_2 and graphene/WS_2 have strong absorption peaks in the visible region, and the charge transfer forms at the strong absorption peak can be determined according to the charge transfer diagram, shown in Figure 3.

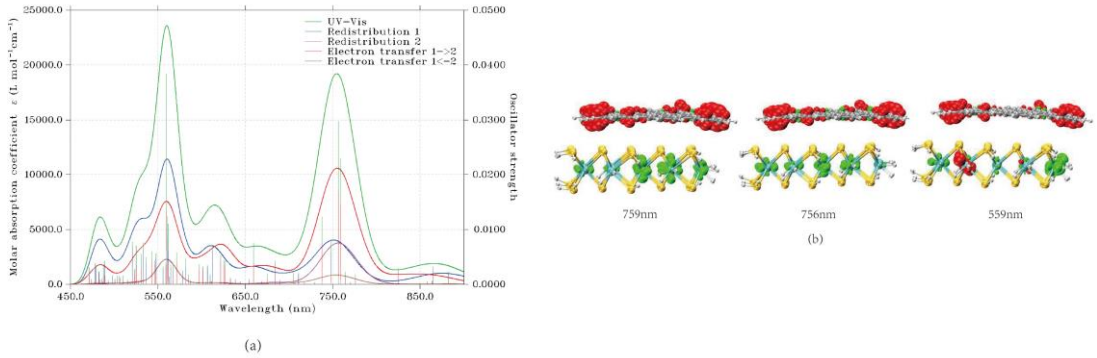

Figure 3, (a) Absorption spectrum of the graphene/MoS_2 heterostructure and (b) charge difference densities of the three excited states, where green and red represent holes and electrons, respectively.

References:

[1] Ki Seok Kim, Doyoon Lee, Celesta S. Chang, Seunghwan Seo, Yaoqiao Hu, Soonyoung Cha, Hyunseok Kim, Jiho Shin, Ju-Hee Lee, Sangho Lee, Justin S. Kim, Ki Hyun Kim, Jun Min Suh, Yuan Meng, Bo-In Park, Jung-Hoon Lee, Hyung-Sang Park, Hyun S. Kum, Moon-Ho Jo, Geun Young Yeom, Kyeongjae Cho, Jin-Hong Park, Sang-Hoon Bae & Jeehwan Kim, Nature 614, 88 (2023).
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