The quantitative energy strength of electrostatic energy, exchange repulsion energy and dispersion energy of the total binding energy between the two-dimensional bilayer stacked structures

Shuo Cao
Changcheng Xu, Shaofeng Wang, Jianjun Sun, Qing Wang
School of Physics, Liaoning University, Shenyang, P.R. China
E-mail: shuocao@lnu.edu.cn

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. The weak interaction is of great significance in heterojunctions. The quantitative analysis of the weak interaction force between stacked two-dimensional materials is less. Through energy decomposition analysis based on the force field (EDA-FF) method, 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, and 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, which is useful for understanding the stabilization and reliability of 2D stacked material heterojunctions for practical applications. by applying electric fields of different directions and sizes, the change of the average charge differential density before and after the formation of the 2D stacked material reflects the change of the weak interaction between the layers.

References

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Figures

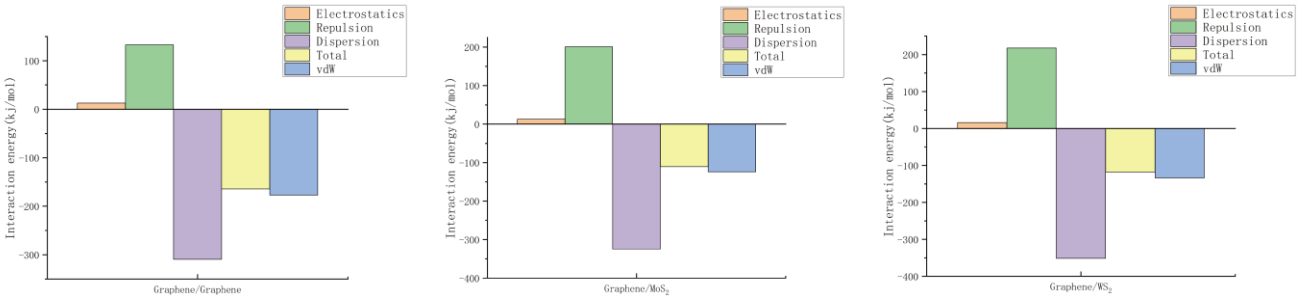

Figure 1: EDA-FF analysis result histograms: (a) bilayer graphene, (b) graphene/MoS_2, and (c) graphene/WS_2.

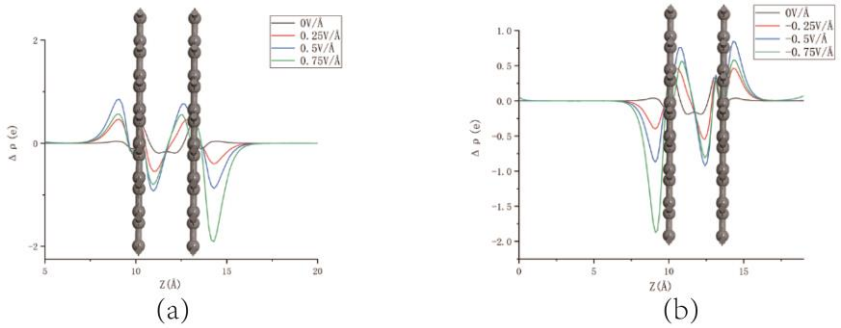

Figure 2: (a) The average differential charge density in the + Z direction under 0 ~ 0.75V/Å electric field, (b) The average differential charge density in the -Z direction under 0 ~ -0.75V/Å electric field.