

**Supporting Information for**  
**Controllable Schottky Barriers and Contact Types of BN Intercalation Layer in**  
**Graphene/MoSi<sub>2</sub>As<sub>4</sub> vdW Heterostructures via Applying External Electrical**  
**Field**

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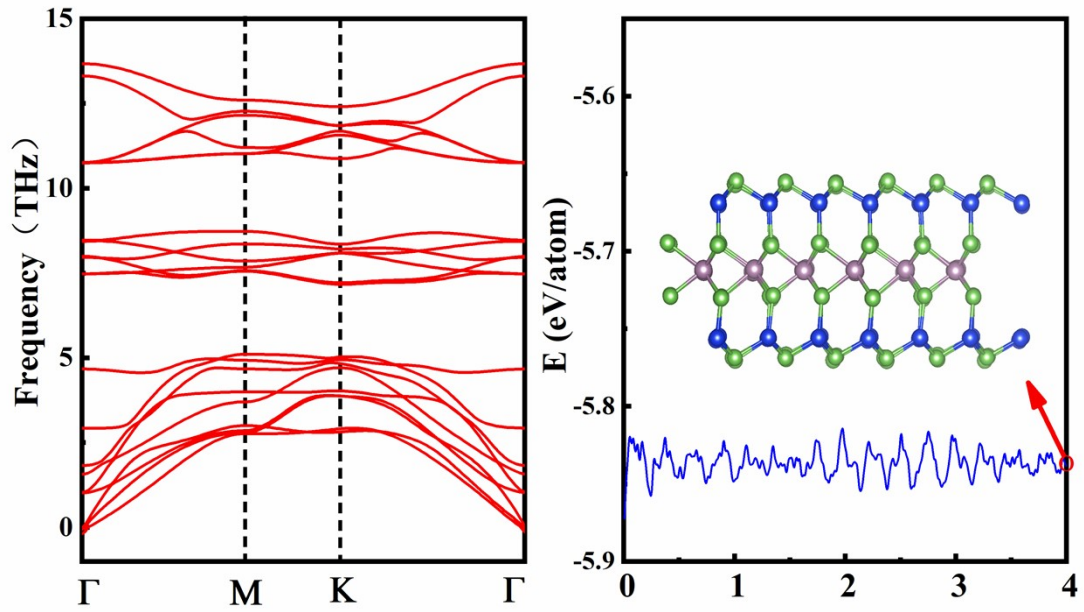


Fig S1. The calculated phonon dispersion curves (left) and ab initio molecular dynamics (AIMD) simulations (right) of MoSi<sub>2</sub>As<sub>4</sub> monolayer.

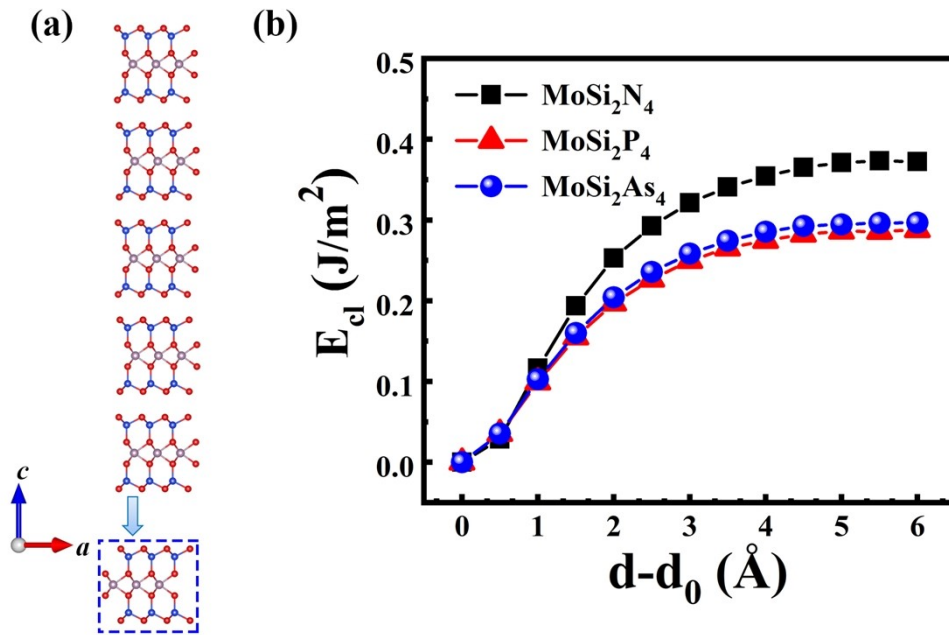


Fig S2. (a)The exfoliation of a layer from the surface of a bulk material. (b) Monolayer exfoliation energies for MoSi<sub>2</sub>Z<sub>4</sub> (Z=N, P, As), where the black, red and blue dots-lines represent for MoSi<sub>2</sub>N<sub>4</sub>, MoSi<sub>2</sub>P<sub>4</sub> and MoSi<sub>2</sub>As<sub>4</sub>, respectively.

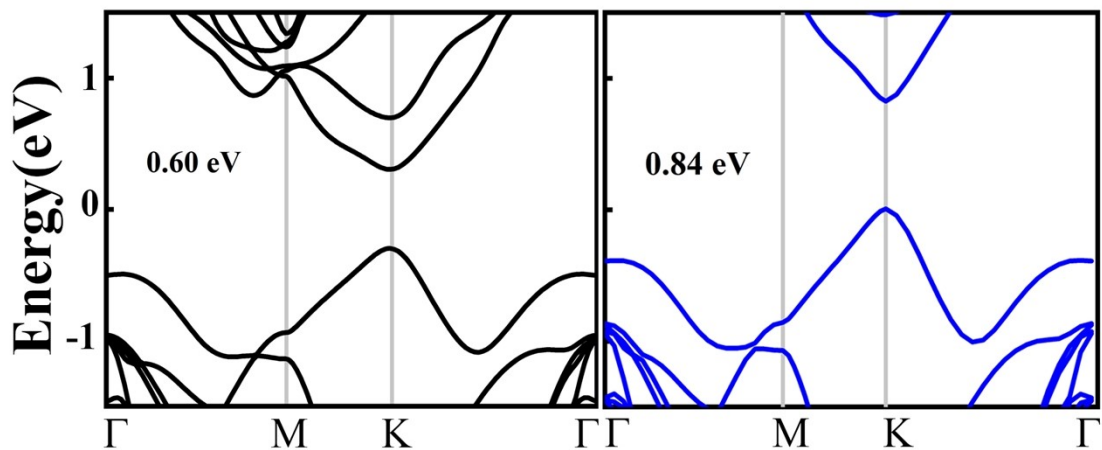


Fig S3. The calculated band structures by PBE (left) and HSE06 (right) methods for MoSi<sub>2</sub>As<sub>4</sub> monolayer.

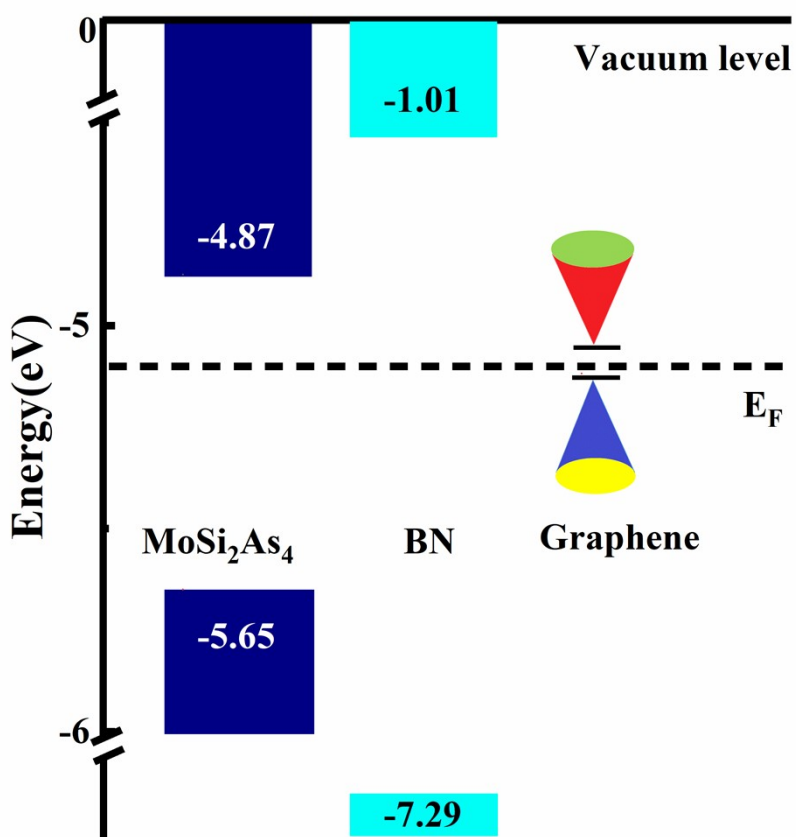


Fig S4. The band alignment of Graphene/BN/MoSi<sub>2</sub>As<sub>4</sub> heterostructure calculated by HSE06 functional.