Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

First-principles calculation of electronic properties of SiC-based bilayer and trilayer heterostructures

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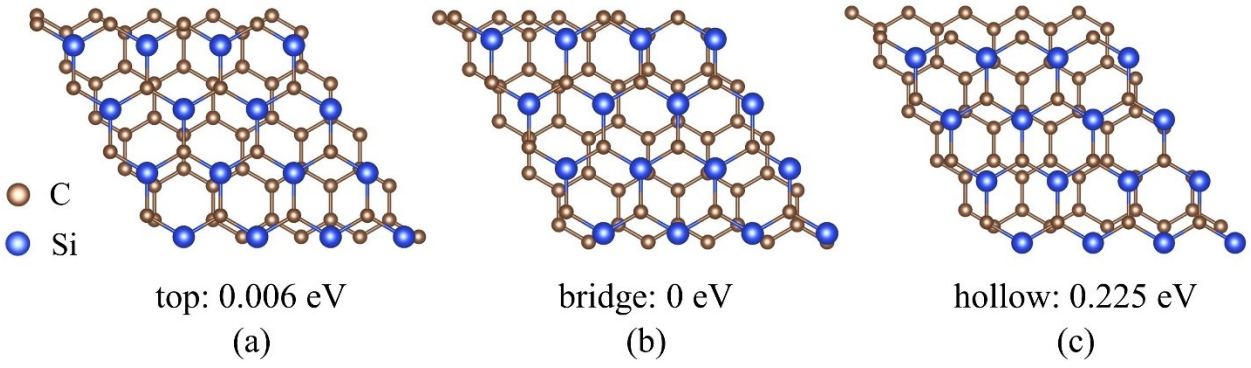

Figure S1. Top view of the three stacking configurations of SiC-4×4/Graphene-5×5 heterostructure. (a) top site; (b) bridge site; (c) hollow site. These configurations are categorized according to the relative position of carbon (graphene) and silicon (SiC) on the left-down corner. The relatively energy differences are shown below. The energy of bridge site configuration are set as reference.

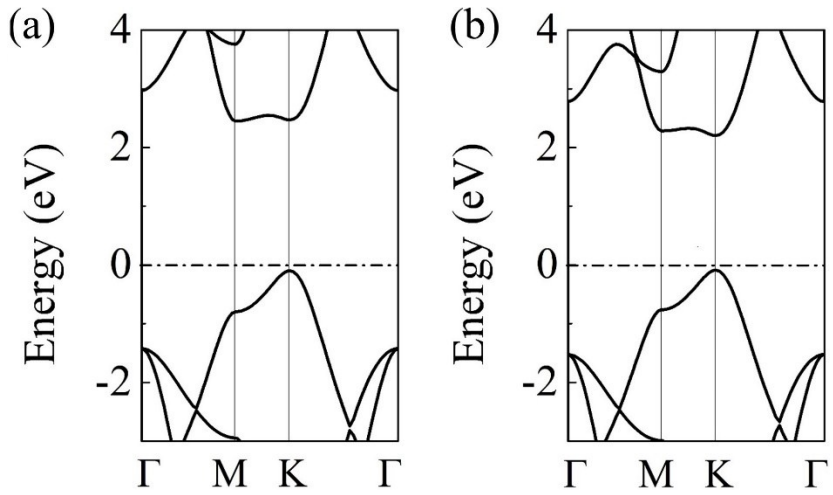

Figure S2. (a) The band structure of pristine SiC layer and (b) the band structure of SiC layer with 3% strain. The dash line denotes the Fermi level.

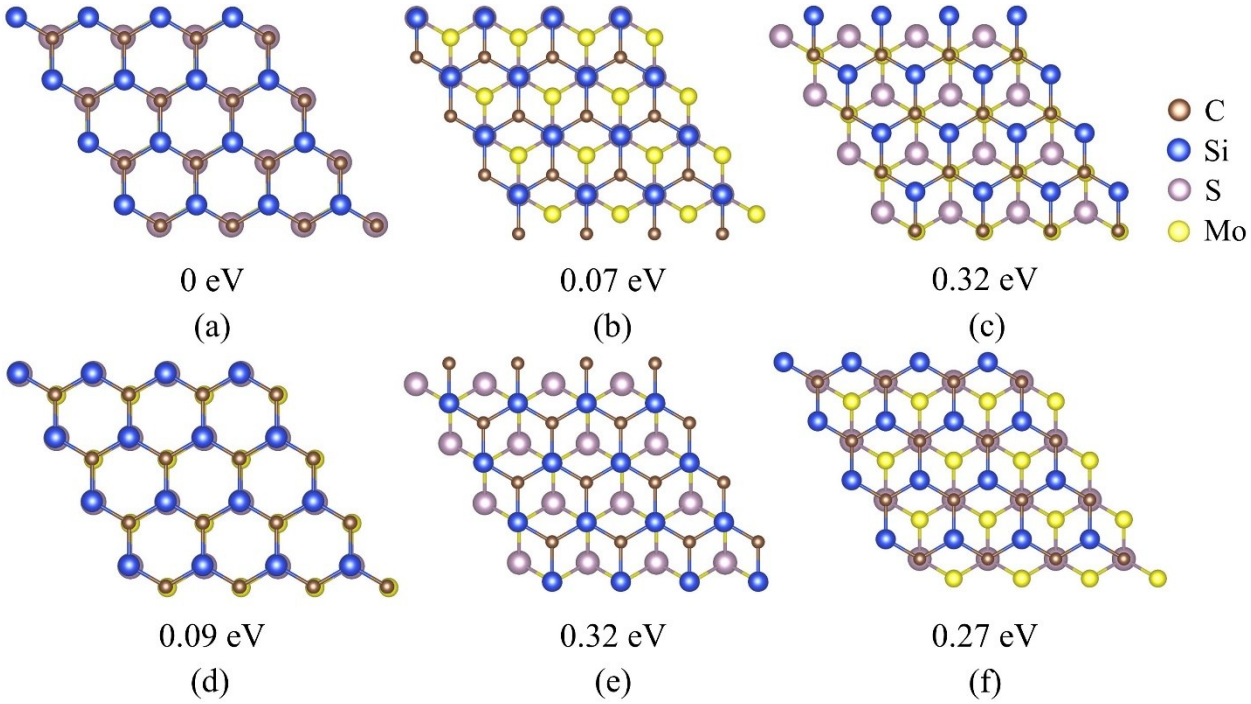

Figure S3. Top view of the six stacking configurations of SiC-4×4/MoS_2-4×4 heterostructures. The relatively energy differences are shown below. Configuration (a) has the lowest energy.