MoS_2 Heterostructure with Tunable Phase Stability: Strain Induced Interlayer Covalent Bridge Formation

SUPPLEMENTARY INFORMATION

S1. Total energy for all heterostructure stacking sequences between MoS_2 and BML

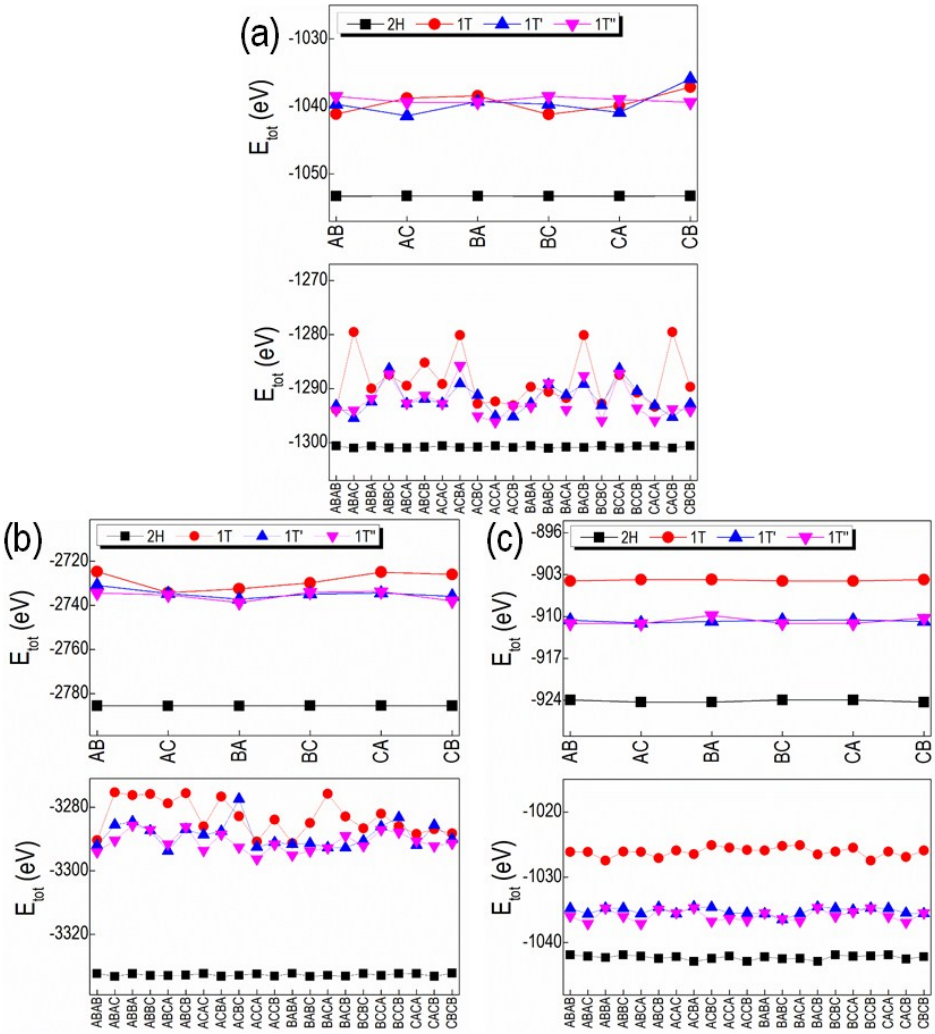

Fig. S 1 (Color Online) Calculated total energies for the three types of heterostructures. In each subfigure, the top and bottom panels correspond to the case of the MoS_2/BML bilayers and the BML/MoS_2/BML sandwiched structures. (a) MoS_2/Si, Si/MoS_2/Si; (b) MoS_2/Ge, Ge/MoS_2/Ge; (c) MoS_2/Sn, Sn/MoS_2/Sn.

S2. 3D energy surfaces as a function of strain

The energy surface of each phase under planar strain is demonstrated in Fig. S2. At each strain state, the phase with the lowest energy surface corresponds to the most stable one. The phase boundaries shown in Fig. 4 correspond to the cross lines of the two lowest energy surfaces.

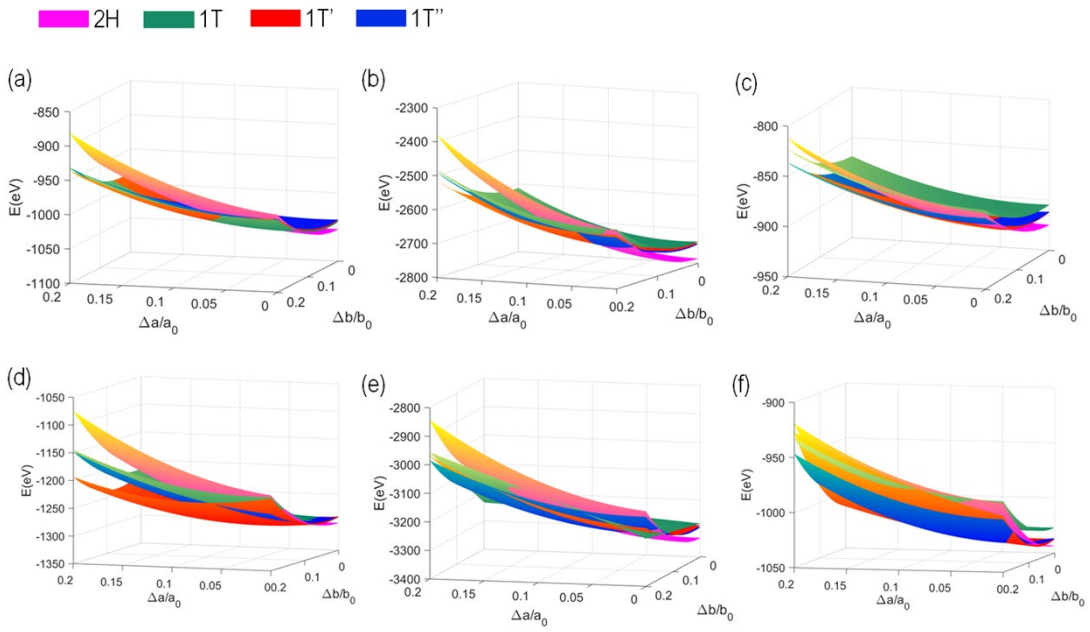

Fig. S 2 (Color Online) Calculated energy surface under planar strain for (a) MoS_2/Si; (b) MoS_2/Ge; (c) MoS_2/Sn; (d) Si/MoS_2/Si; (e) Ge/MoS_2/Ge; (f) Sn/MoS_2/Sn heterostructures.

S3. Electronic properties of the MoS_2/BML heterostructures:

The partial density of states (PDOS) of MoS_2 within all types of heterostructures have been calculated and demonstrated in Fig. S3 below:

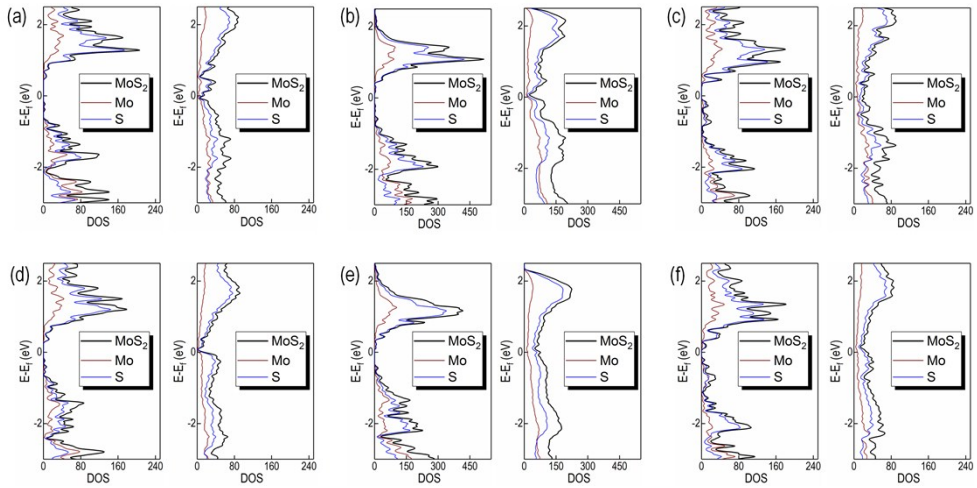

Fig. S 3 (Color Online) Partial density of state (PDOS) of MoS_2, Mo atoms, S atoms in (a) MoS_2/Si; (b) MoS_2/Ge; (c) MoS_2/Sn; (d) Si/MoS_2/Si; (e) Ge/MoS_2/Ge; (f) Sn/MoS_2/Sn. For each subfigure, the left one indicates the PDOS of 2H-MoS_2/BML with the lowest energy stacking while the right one indicates the PDOS of T-MoS_2/BML heterostructure with the lowest energy stacking