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

Supporting Information (SI)

Tunability of the electronic properties and electrical contact in Graphene/SiH heterostructure

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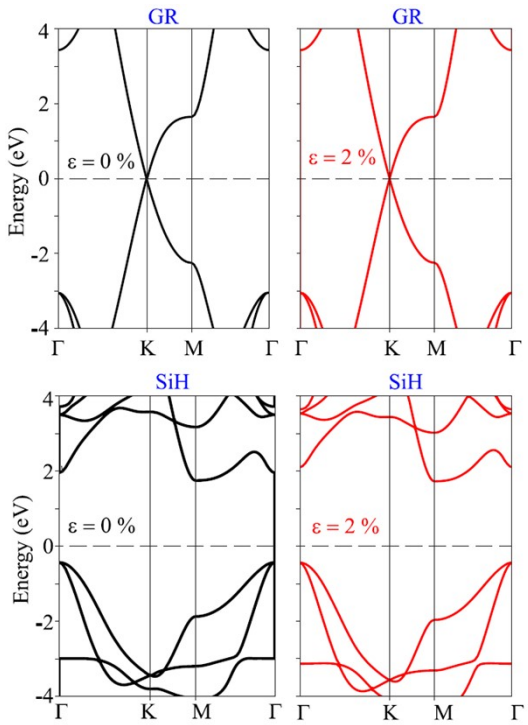

Fig. S1. Calculated band structures of GR and SiH monolayers under small biaxial strain of 2 %.

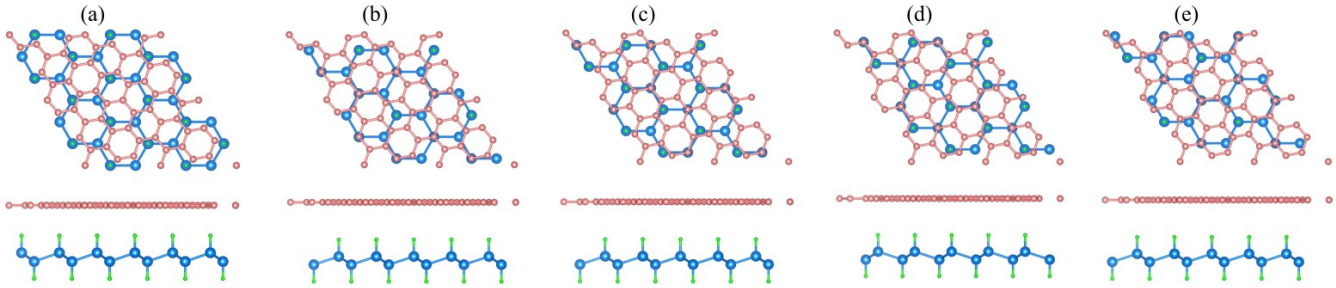

Fig. S2. Different stacking configurations and calculated binding energy of GR/SiH heterostructures for (a) stacking I, (b) stacking II, (c) stacking III and (d) stacking IV and (e) stacking V.

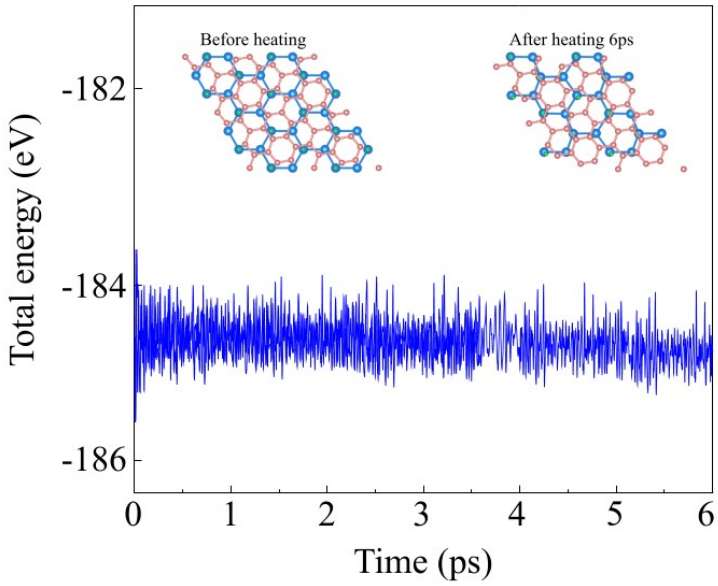

Fig. S3. The fluctuation of total energy as a function of time steps by performing ab initio molecular dynamics (AIMD) simulation at 300 K. The snapshots represent the atomic structures of Gr/SiH for the most stable stacking configuration before and after heating 6 ps.