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

Supporting Information

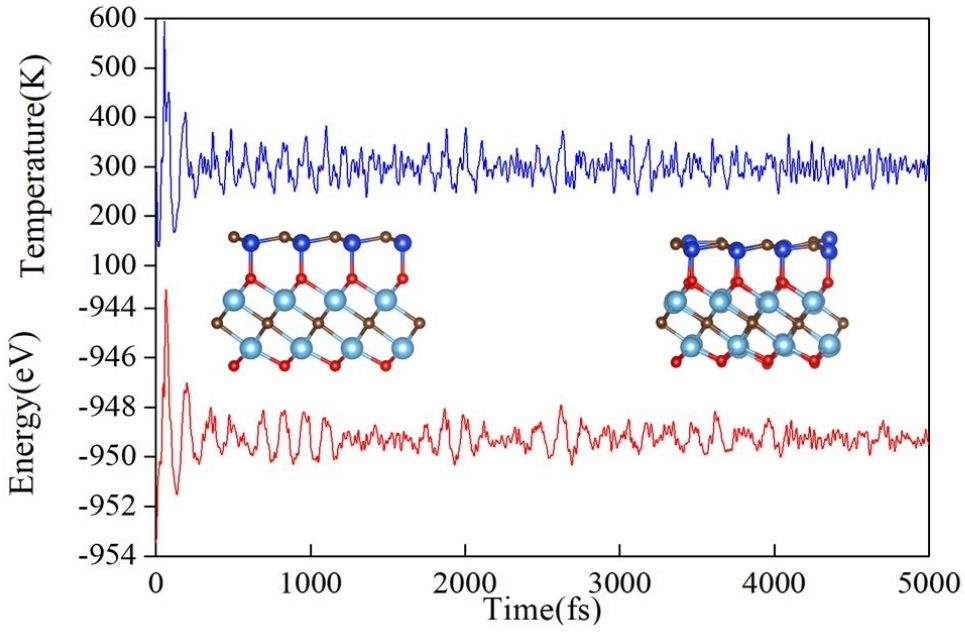

Fig. S1 The result of AI configuration molecular dynamics simulation with time, the structure has sightly deformation after heating

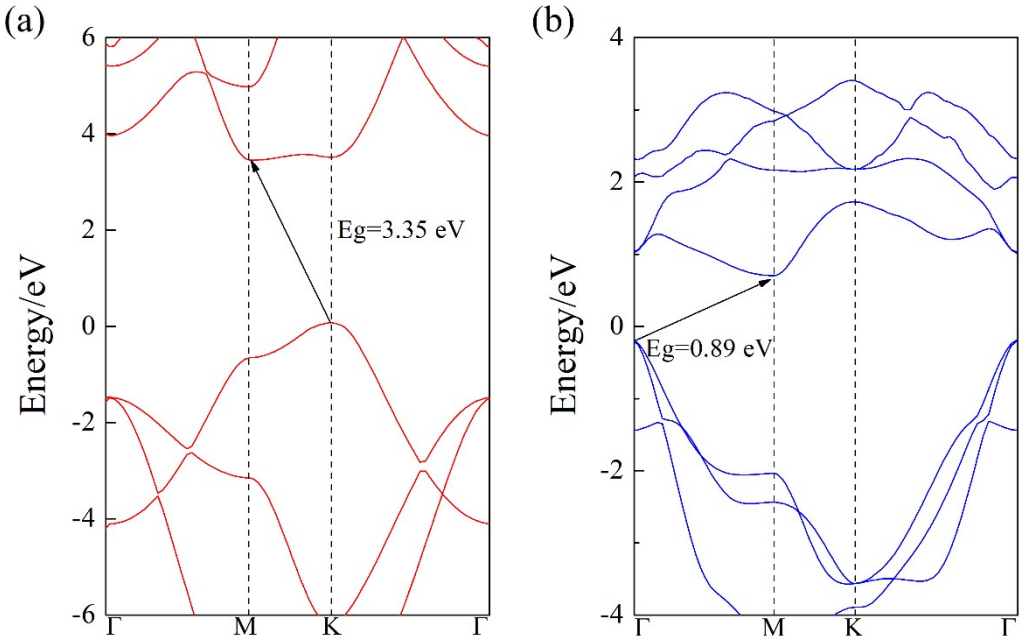

Fig. S2 The projected band structures of SiC (a) and Ti_2CO_2 (b) monolayers

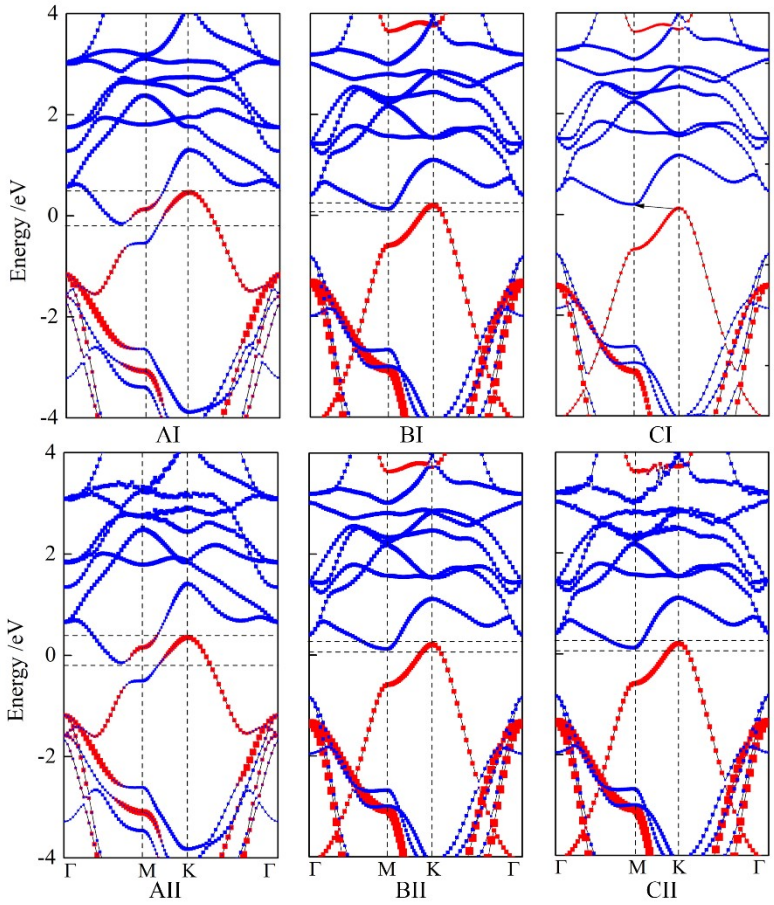

Fig. S3 The projected band structures of SiC/Ti_2CO_2 heterojunction under different configuration, in which SiC is the red line and Ti_2CO_2 is the blue line.

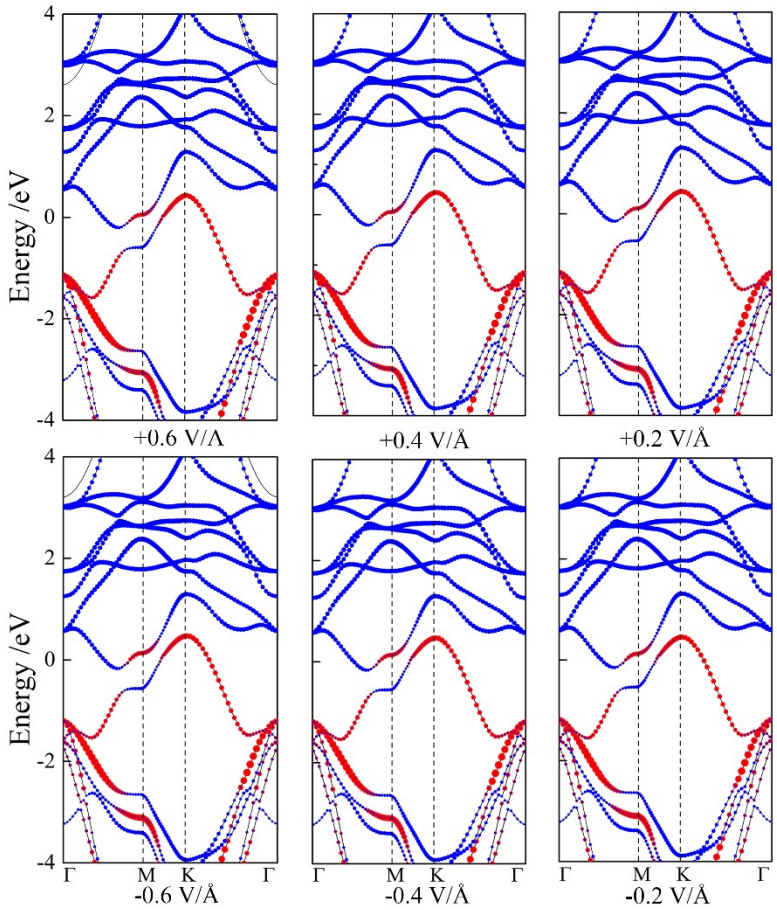

Fig. S4 The projected band structures of SiC/Ti_2CO_2 heterojunction under external electric field, in which SiC is the red line and Ti_2CO_2 is the blue line.

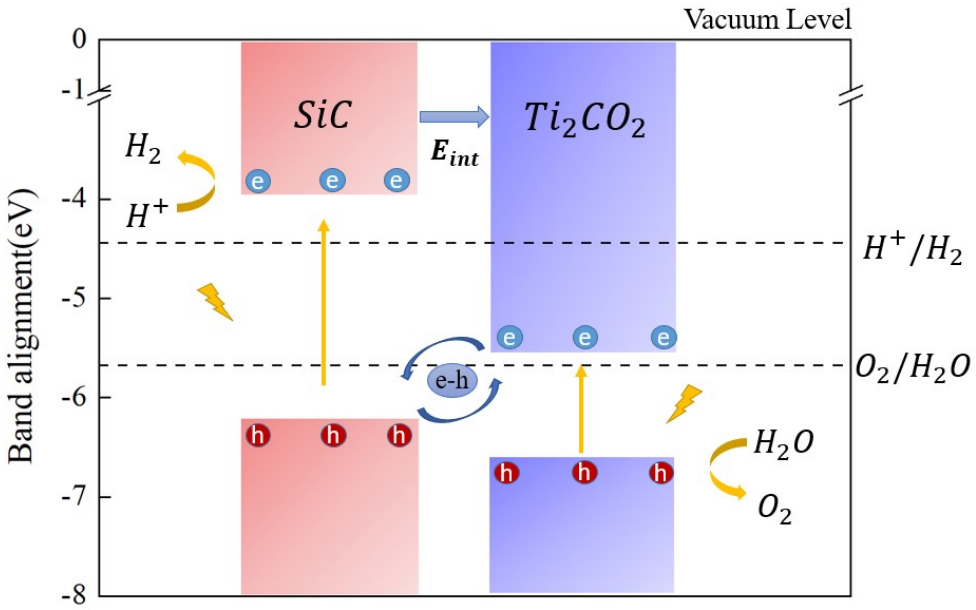

Fig. S5 The type-II band alignment of SiC/Ti_2CO_2 heterojunction under the strain of 3% to 6%

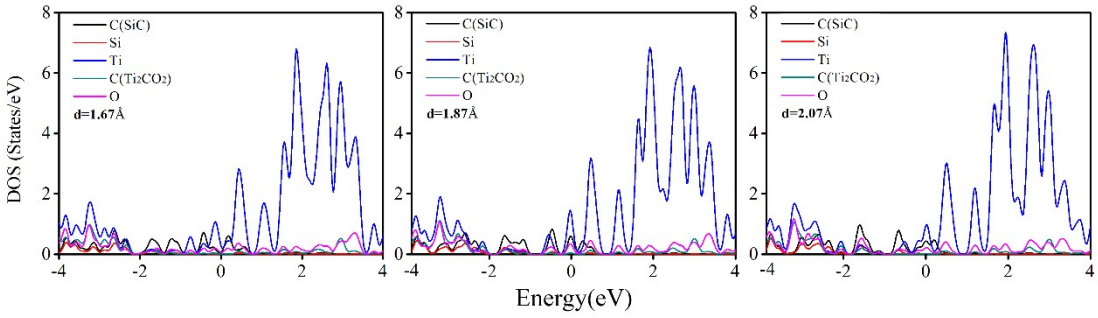

Fig. S6 The density of states (DOS) of SiC/Ti_2CO_2 heterojunction under the interlayer spacing (d) from 1.67 to 2.07 Å

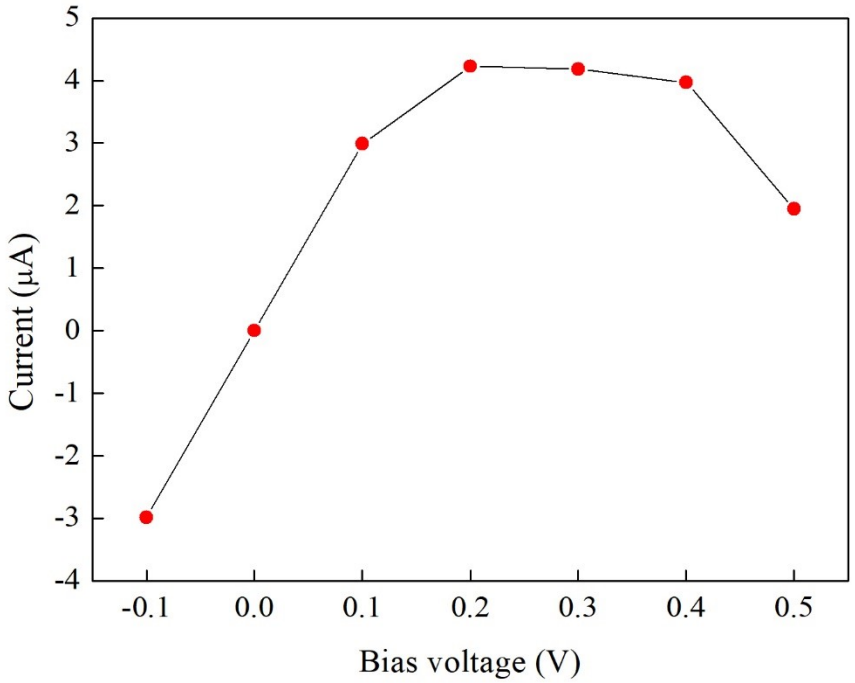

Fig. S7 The I-V curve for the SiC/Ti_2CO_2 heterojunction at an interlayer distance of 3.37 Å