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

Supporting Information

Metal-Semiconductor Transition of Two-Dimensional Mg_2C Monolayer Induced by Biaxial Tensile Strain

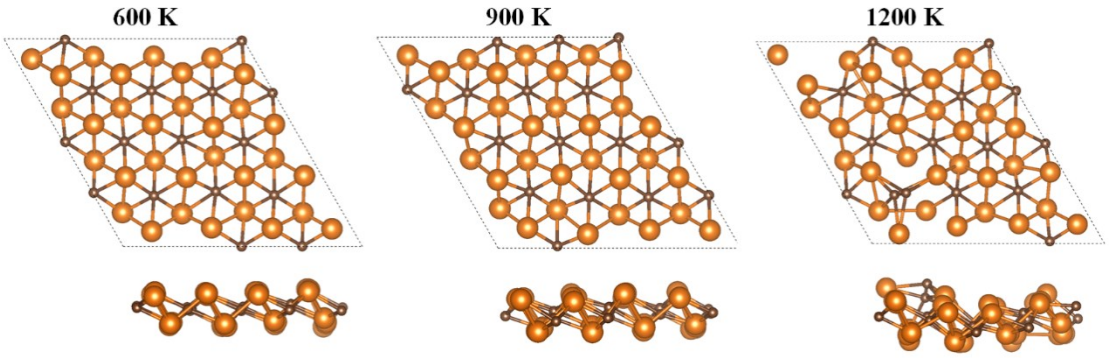

Figure S1. Snapshots of the final frame of each molecular dynamics simulation of the Mg_2C monolayer from 600, 900, and 1200 K (top and side views). Magnesium atoms are yellow, and carbon gray. Bonds to atoms outside this 4 × 4 section exist but are not shown.

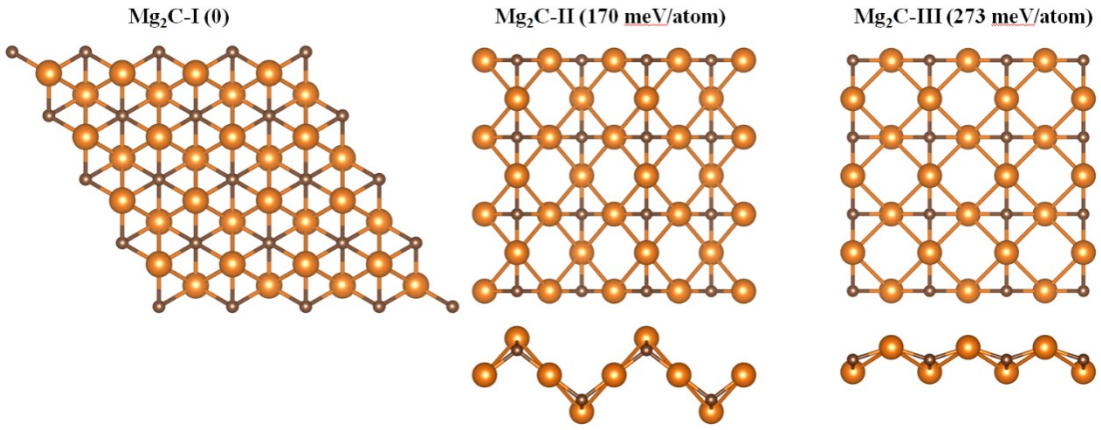

Figure S2. Low lying isomers and relative energies of the Mg_2C monolayer in 2D space found by particle swarm search. Bonds to atoms outside of these sections exist but are not shown. Mg_2C-I corresponds to the structure discussed in the text.

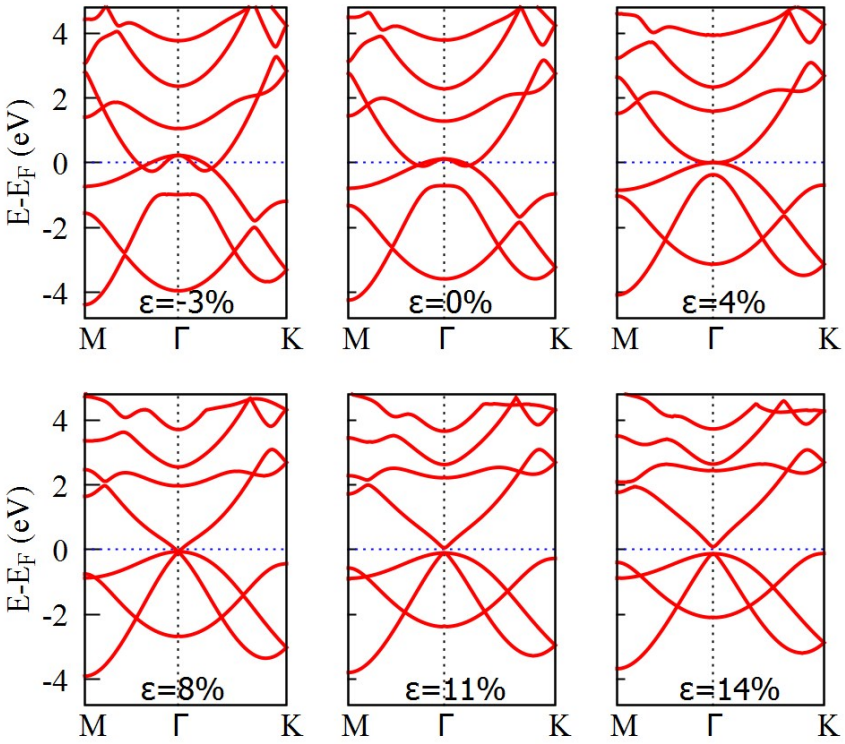

Figure S3. Electronic band structures of the Mg_2C monolayer under in-plane homogeneous biaxial strains calculated by PBE functional.

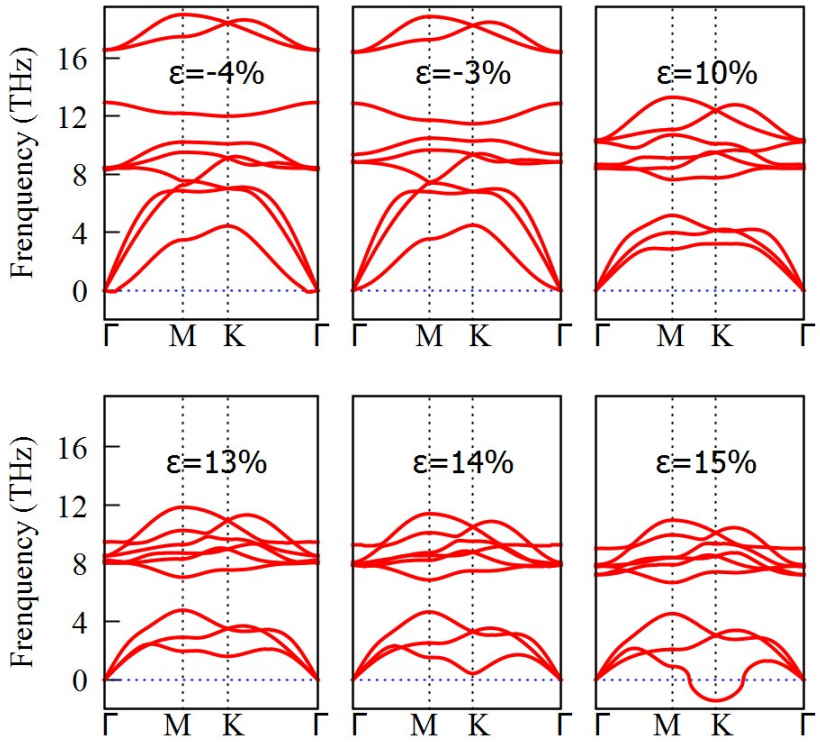

Figure S4. Phonon dispersion of the Mg_2C monolayer under six representative biaxial strains.