Supporting Information

Metal-Metal Transition of Two-Dimensional Mg$_2$C Monolayer Induced by Biaxial Tensile Strain

**Figure S1.** Snapshots of the final frame of each molecular dynamics simulation of the Mg$_2$C 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$_2$C monolayer in 2D space found by particle swarm search. Bonds to atoms outside of these sections exist but are not shown. Mg$_2$C-I corresponds to the structure discussed in the text.
Figure S3. Electronic band structures of the Mg$_2$C monolayer under in-plane homogeneous biaxial strains calculated by PBE functional.
Figure S4. Phonon dispersion of the MgC monolayer under six representative biaxial strains.