Supplementary Information (SI) for Physical Chemistry Chemical Physics.

First-Principles Investigation of a Two-Dimensional Magnesium Carbide Monolayer: Tunable Bandgap, Light Carriers, and Strain-Induced Topological and Semiconductor-to-Metal Transitions

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(Supplementary)

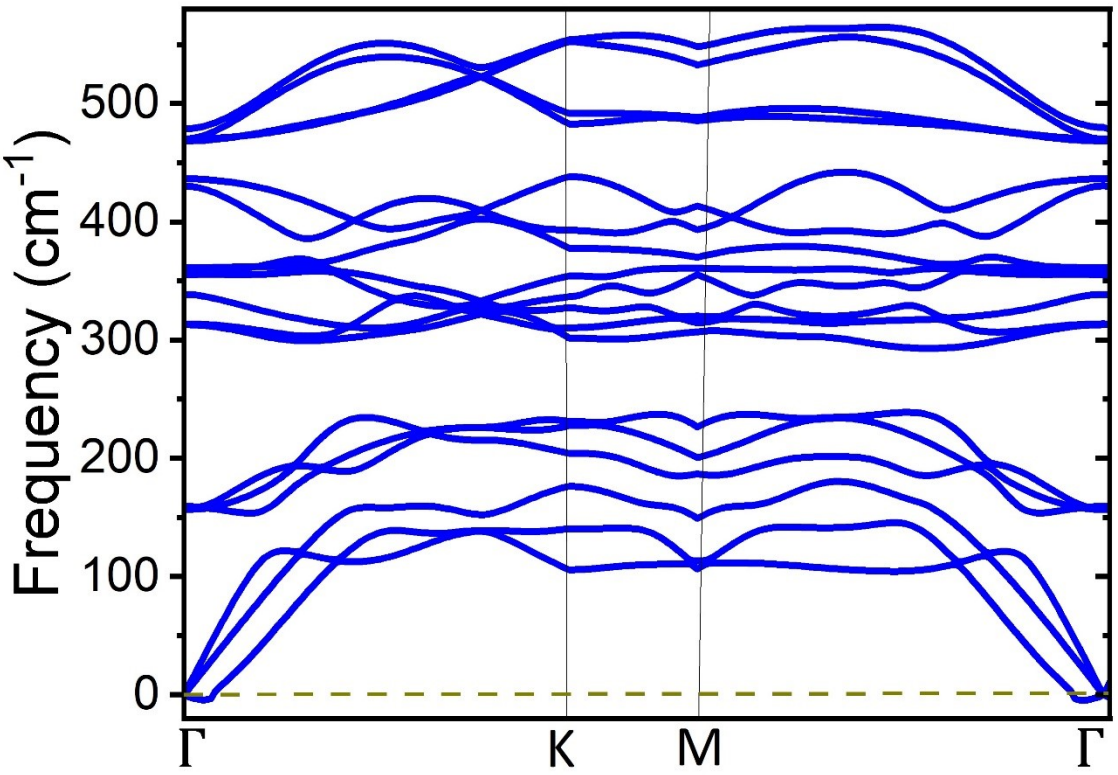

Figure S1: Phonon dispersion curve of the 2D Mg_2C monolayer along the high-symmetry points (Γ-K-M-Γ) in the Brillouin zone. The absence of imaginary frequencies confirms the dynamical stability of the monolayer structure.

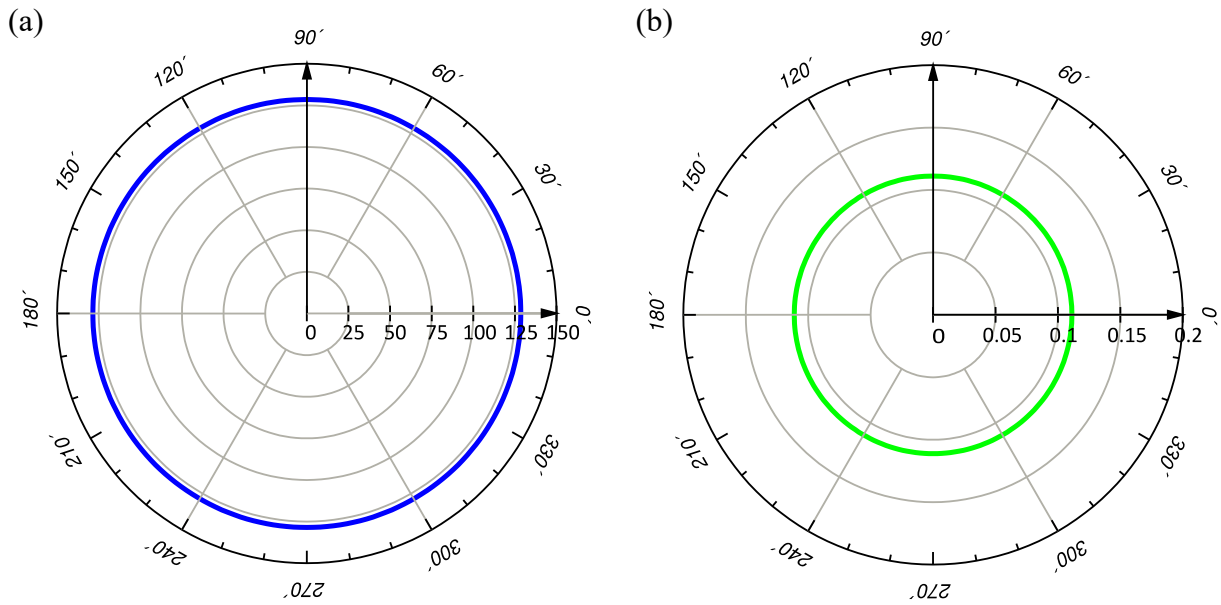

Figure S2. Polar plots illustrating the orientation-dependent (left) Young's modulus E(θ) (blue line) and (right) Poisson's ratio ν(θ) (green line) for the 2D Mg_2C monolayer. The circular shape of both plots indicates in-plane isotropy for both Young's modulus and Poisson's ratio, signifying uniform mechanical properties in all directions within the monolayer plane.