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

Supporting Information

Temperature-dependent mechanical properties of 2D $Ti_{n+1}C_nO_2$ (n = 1, 2) MXene monolayers

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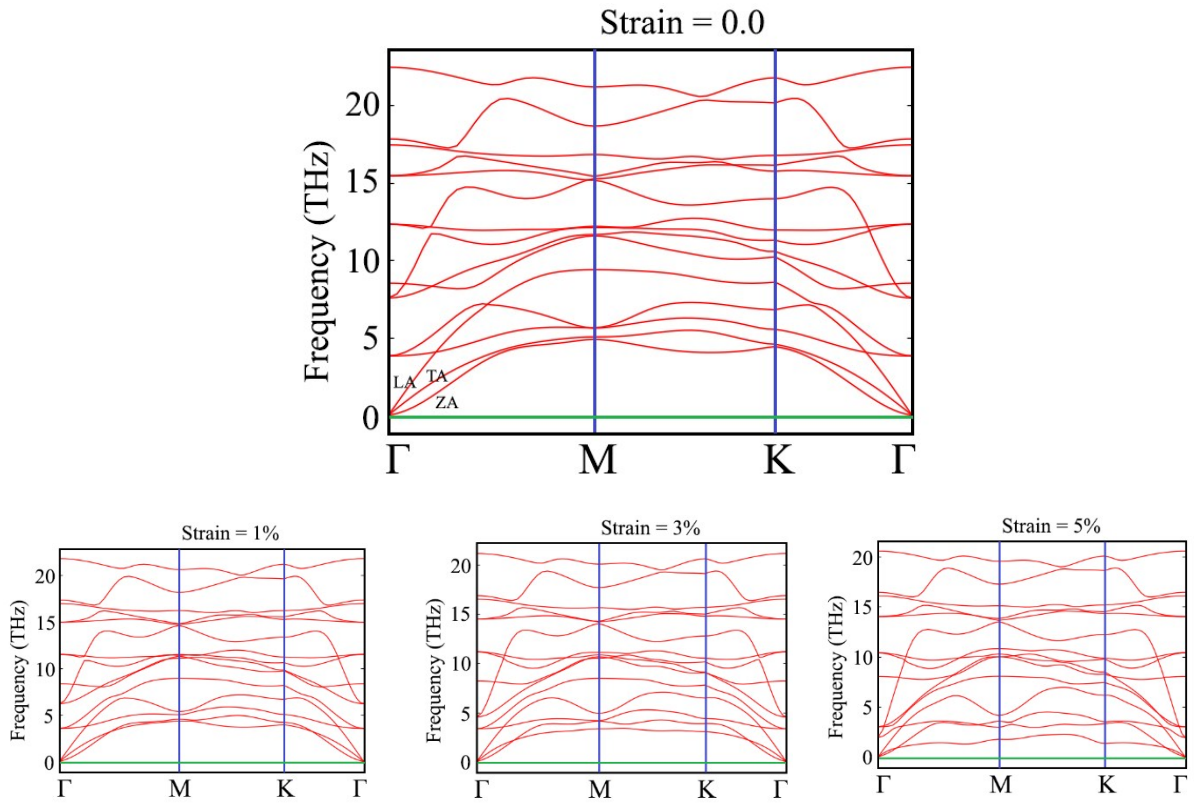
Dynamical stability

The phonon spectra of 2D $Ti_{n+1}C_nO_2$ (n = 1, 2) at state-free state and biaxial tensile and compressive strain of 1%, 3%, and 5% in the basal plane are shown in **Figs. S1** and **S2**, which passes several high symmetry directions ($\Gamma_{(0,0,0)} \rightarrow M_{(1/2,0,0)} \rightarrow K_{(1/3,1/3,0)} \rightarrow \Gamma_{(0,0,0)}$).



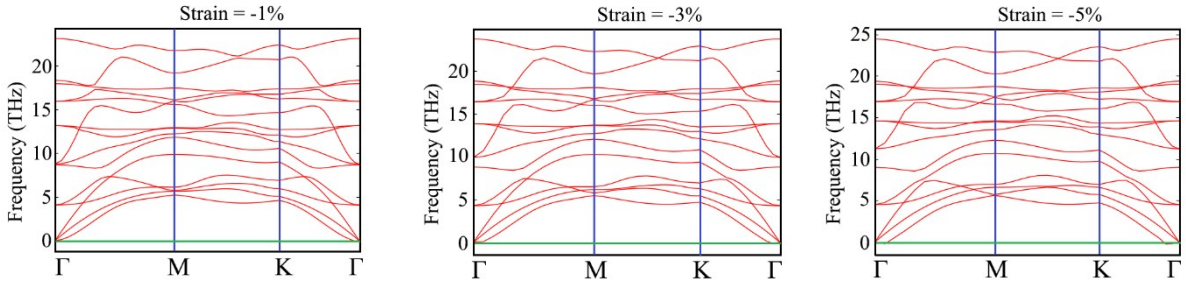


Figure S1. Phonon dispersion curves for Ti_2CO_2 at state-free state and biaxial tensile and compressive strain of 1%, 3%, and 5% in the basal plane.

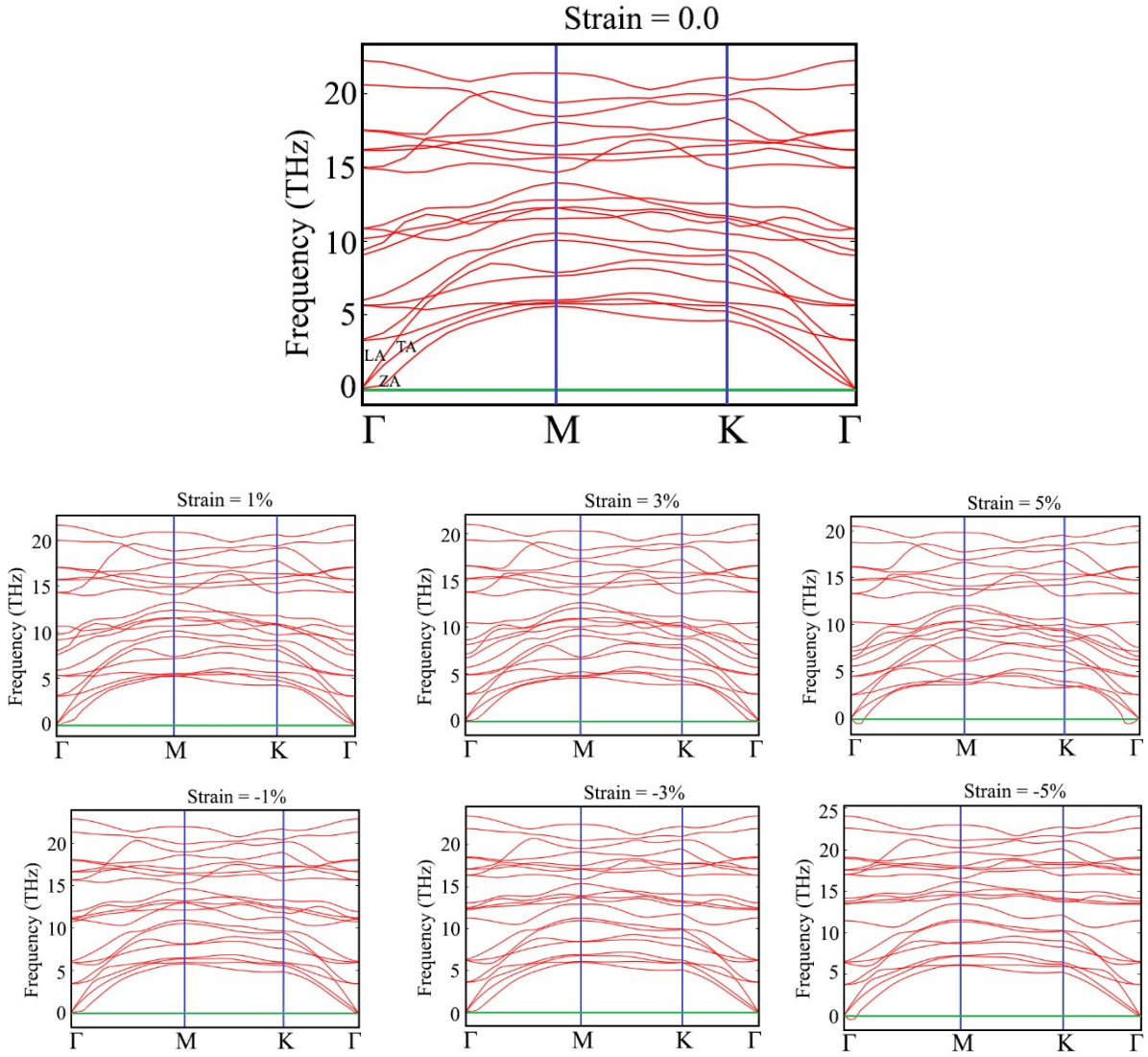


Figure S2. Phonon dispersion curves for $Ti_3C_2O_2$ at the state-free state and biaxial tensile and compressive strain of 1%, 3%, and 5% in the basal plane.

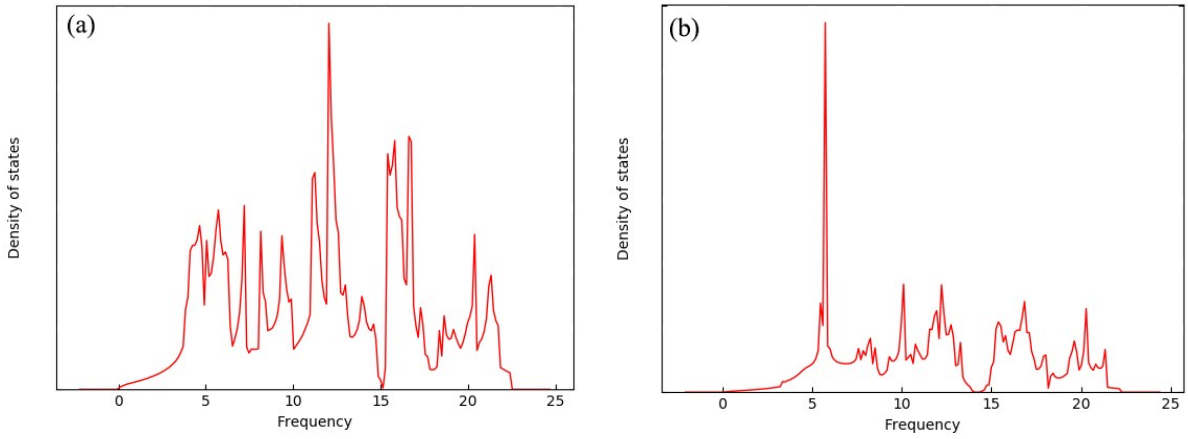


Figure S3. Calculated phonon DOS of (a) Ti_2CO_2 and (b) $Ti_3C_2O_2$ monolayers at the state-free state.