# Supporting Information

# First-principles Study for MXene Terahertz Detector

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# Computational Details

**Electronic Structures and Optical Properties:** For the DFT calculations of the electronic band structures and optical properties of MXene and graphene, generalized-gradient approximation with Perdew–Burke–Ernzerhof exchange–correlation functional was employed considering spin-polarization and spin-orbit coupling. The structures of the systems were relaxed with a variable cell size until the maximum force reduced below 0.05 eV $Å^{-1}$. The density mesh cutoff energy was set to be 150 hartree.

The size of the optimized hexagonal cell was 6.31 Å × 6.31 Å × 30 Å in the monolayer $Ti_3C_2$ while it was 6.31 Å × 6.31 Å × 9.87 Å in the stacked $Ti_3C_2$. The Monkhorst-Pack grid of k-point sampling was set to be 5×5×1 and 5×5×3 in the geometric optimization of monolayer $Ti_3C_2$ and stacked $Ti_3C_2$, respectively, while it was taken as 15×15×1 and 15×15×9 in the calculations of the electronic band structure and optical properties.

Meanwhile, the size of the optimized hexagonal cell was 2.46 Å × 2.46 Å × 30 Å in the monolayer graphene while it was 2.46 Å × 2.46 Å × 6.71 Å in the stacked graphene. The Monkhorst-Pack of k-point sampling was set to be 13×13×1 and 13×13×5 in the geometric optimization of monolayer graphene and stacked graphene, respectively, while it was taken as 39×39×1 and 39×39×15 in the calculations of the electronic band structure and optical properties.

**Thermoelectric Properties:** In the analysis of thermoelectric figure of merit (ZT) of stacked $Ti_3C_2$ flakes, the phonon transmission spectrum was obtained using a molecular mechanics based on the reactive force field with the k-mesh of 71×23 and solving the dynamic matrix of the supercell of 9×3×1, while the electron transmission spectrum was calculated using a density-functional tight-binding approach based on the Slater-Koster method with the k-mesh of 27×9. The mesh of $k_z$ in the electrodes was 100.

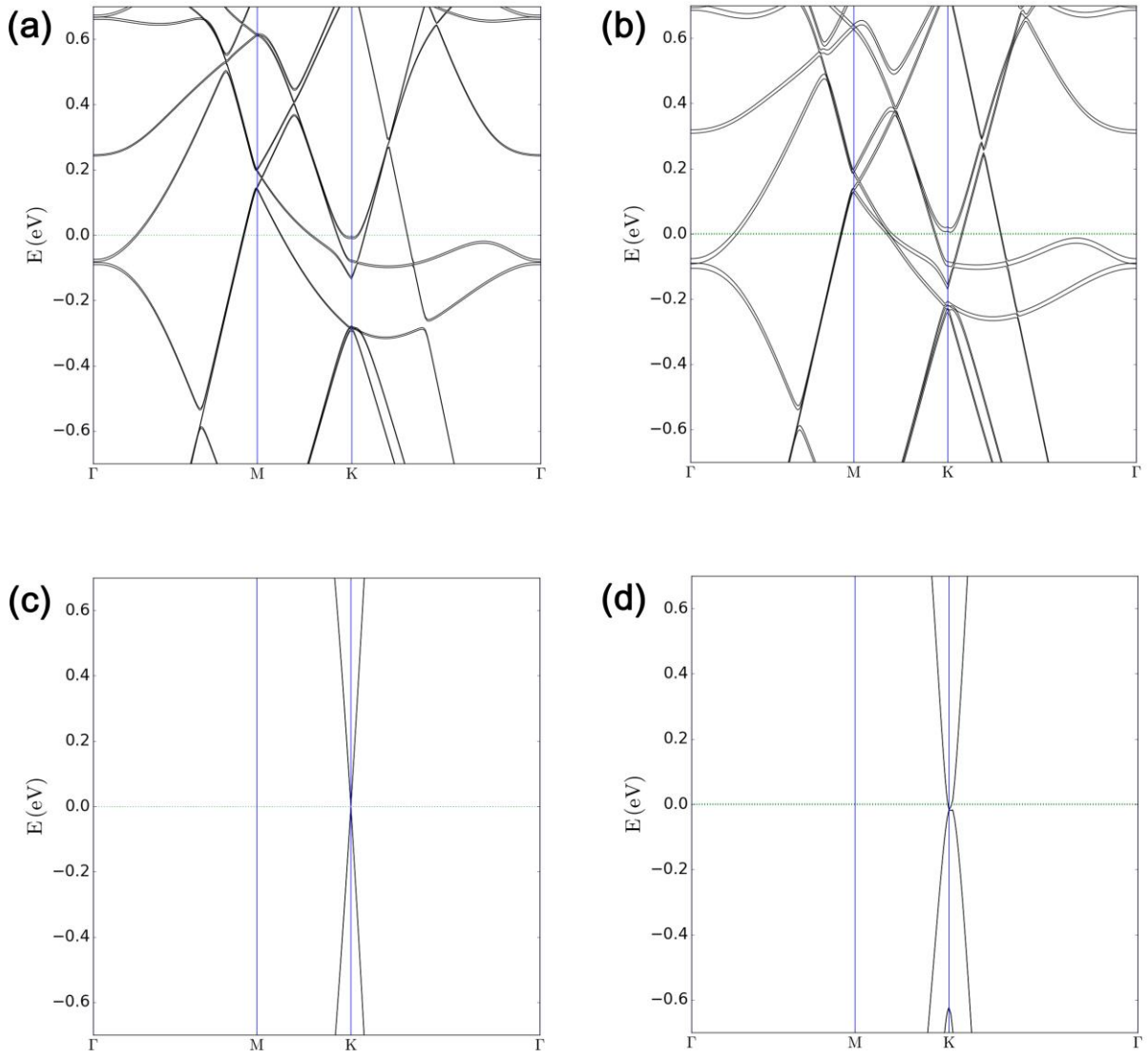


**Figure S1.** The electronic band structures of (a) monolayer $Ti_3C_2$, (b) stacked $Ti_3C_2$, (c) monolayer graphene, and (d) stacked graphene.

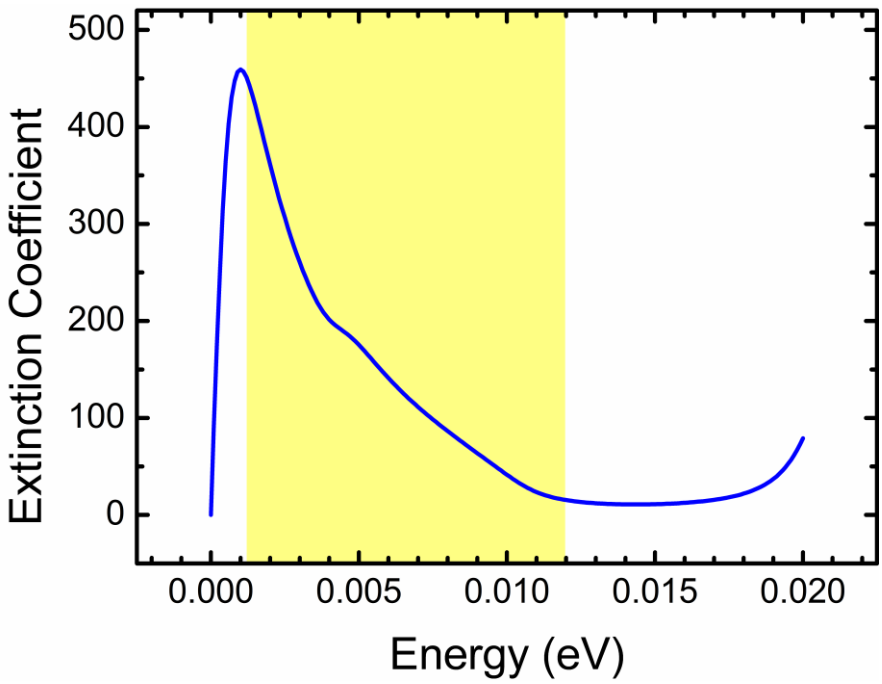


**Figure S2.** The extinction coefficient spectrum of monolayer $Ti_3C_2$ in the THz range. The shaded region indicates the THz range.

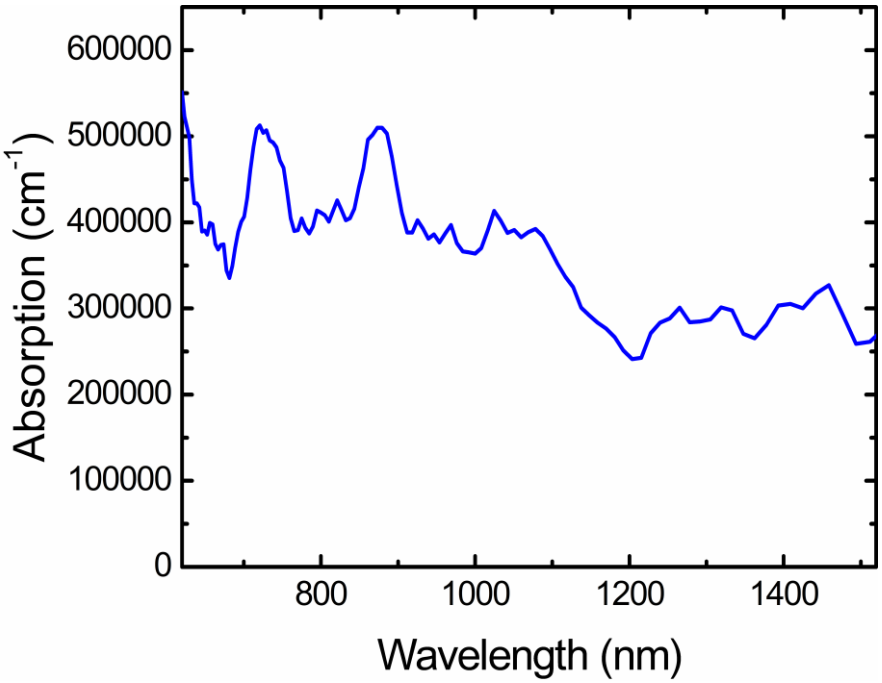


**Figure S3.** The visible to near-infrared optical absorption spectrum of stacked $Ti_3C_2$.

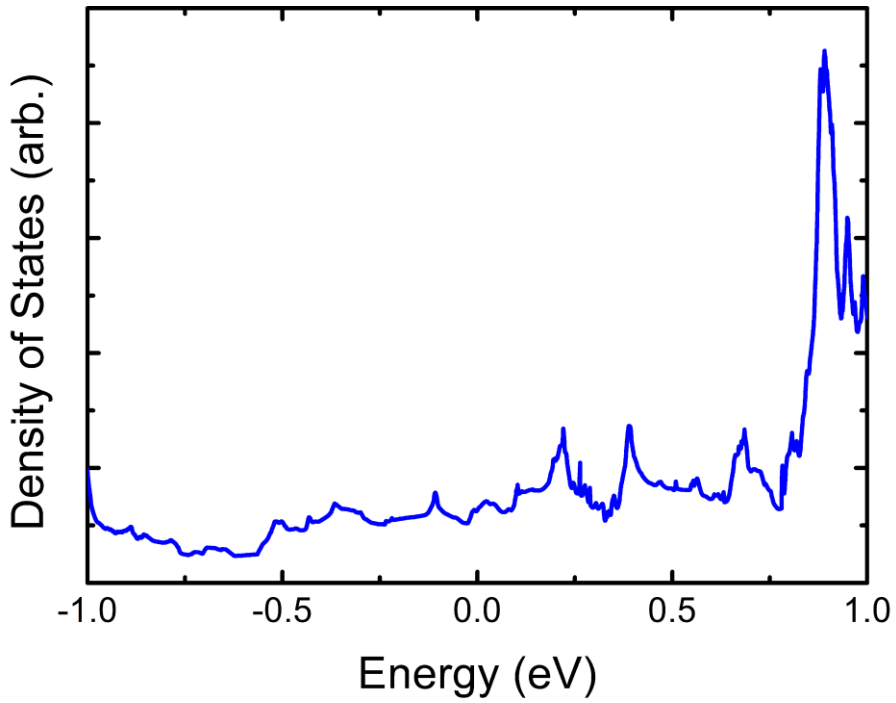


**Figure S4.** The electronic density of states of stacked $Ti_3C_2$ with interlayer water molecules.