Electronic Supplementary Information

Germanium Telluride Monolayer: A Two Dimensional Semiconductor with High Carrier Mobility for Photocatalytic Water Splitting

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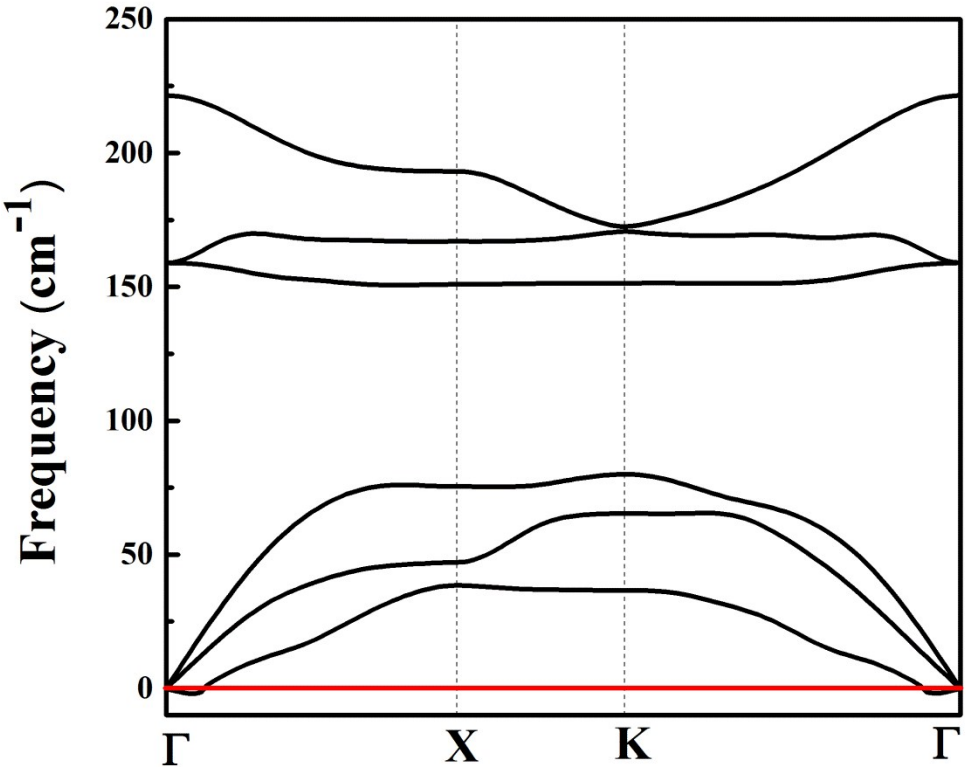

Fig. S1. Phonon spectrum of GeTe monolayer. Only tine imaginary phonon mode (−1.8 cm^{-}) is observed neat the Γ point. This could be fictitious instability due to the numerical error since the frequency of ZA mode approaches zero quadratically. Actually, this kind of tiny dip of imaginary frequency in the transverse acoustical phonon branch is similar to that of the honeycomb Ge monolayer[1] and borophene,[2] which has been experimentally realized on the surface of metal substrate.[2-4]

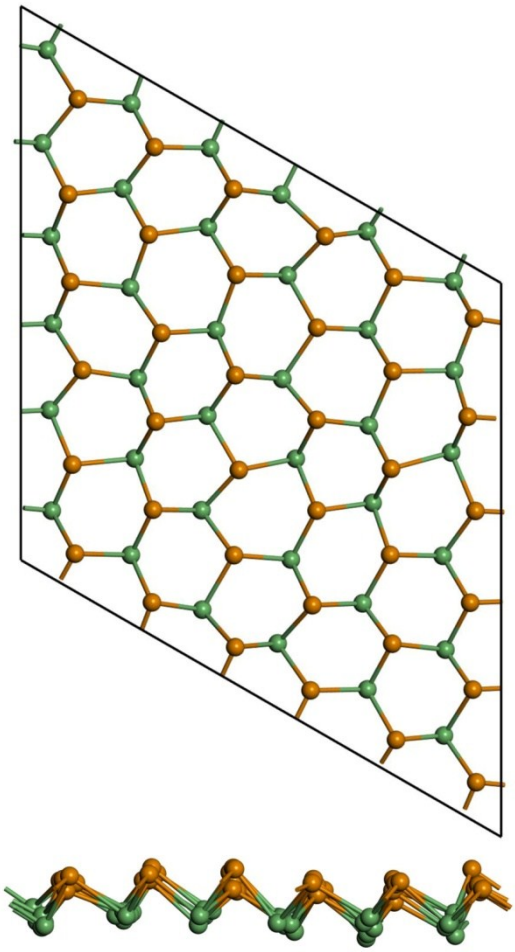

Fig. S2 Snapshots of the equilibrium structure of GeTe monolayer at 500 K at the end of 10 ps ab initio molecular dynamic (AIMD) simulations.

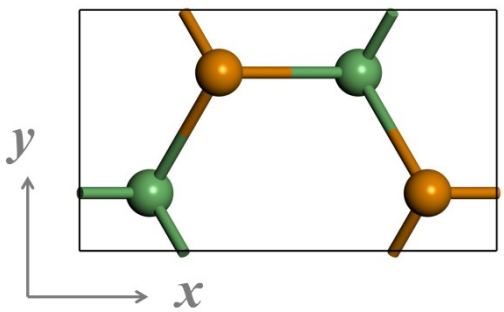

Fig. S3 Geometric structure of rectangle supercell of GeTe monolayer

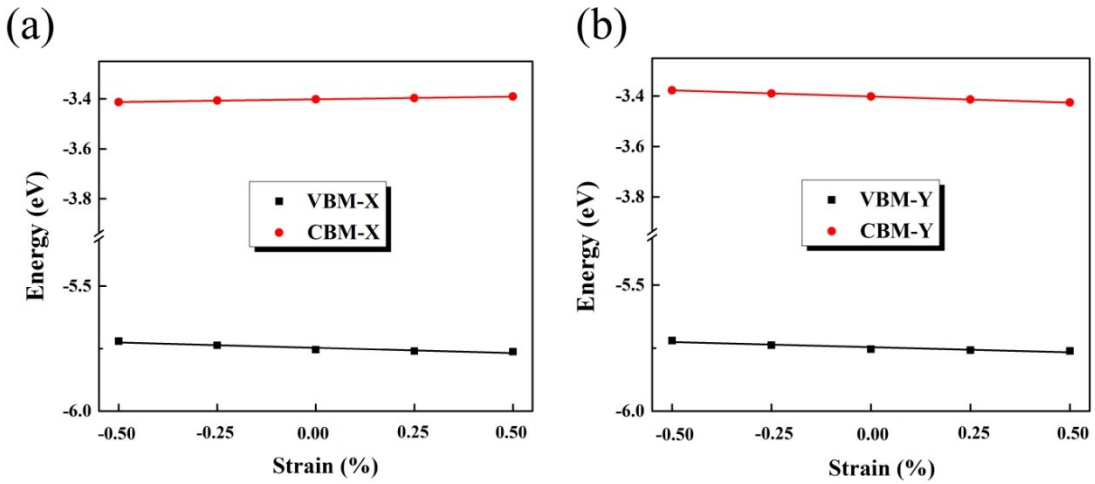

Fig. S4 Shifts of VBM and CBM of GeTe under uniaxial strain along *x* (a) and *y* (b) directions. Note that the energy positions of VBM and CBM have been corrected by taking account of the vacuum level.

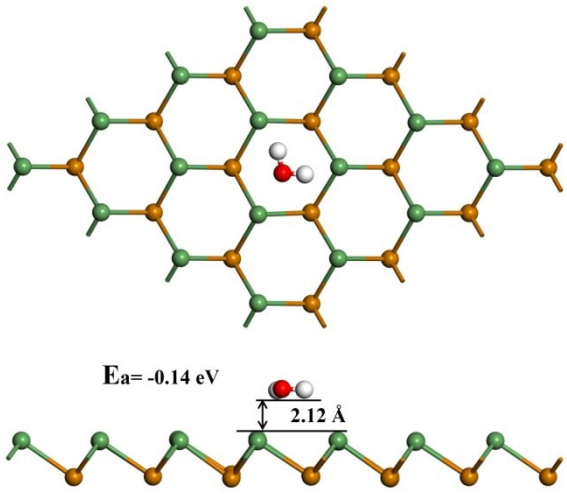

Fig. S5 Top and side views of the most stable structure of H_2O adsorption on the surface of GeTe monolayer. The adsorption energy of H_2O (E_a) is defined as: $E_a = E_{GeTe\text{-}H2O} - E_{GeTe} - E_{H2O}$, where $E_{GeTe\text{-}H2O}$, E_{GeTe}, and E_{H2O} stand for the total energy of the H_2O adsorbed GeTe monolayer, the pristine GeTe monolayer, and the H_2O molecule, respectively.

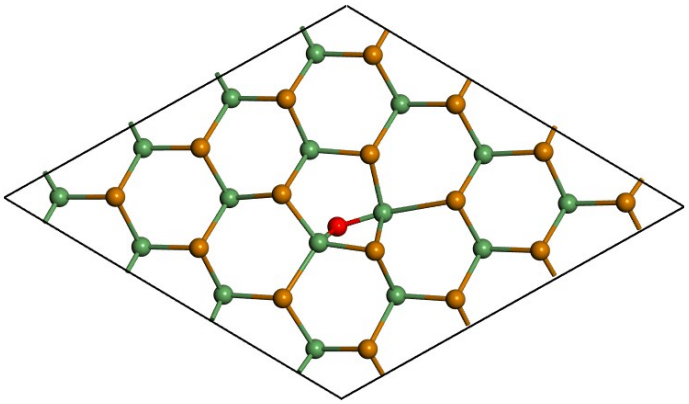

Fig. S6 Top view of the most stable structure of O adsorption on the surface of GeTe monolayer. The binding energy of O (E_O) is defined as: $E_O = E_{GeTe\text{-}O} - E_{GeTe} - \mu_O$, where $E_{GeTe\text{-}O}$ and E_{GeTe} stand for the total energy of the O adsorbed GeTe monolayer and the pristine GeTe monolayer, respectively, while μ_O is the chemical potential of O and is taken as the half binding energy of O_2 molecule.

References

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