Supplemental Material for

Piezoelectricity and valley polarization in a semilithiated 2H-$TiTe_2$ monolayer with near room-temperature ferromagnetism

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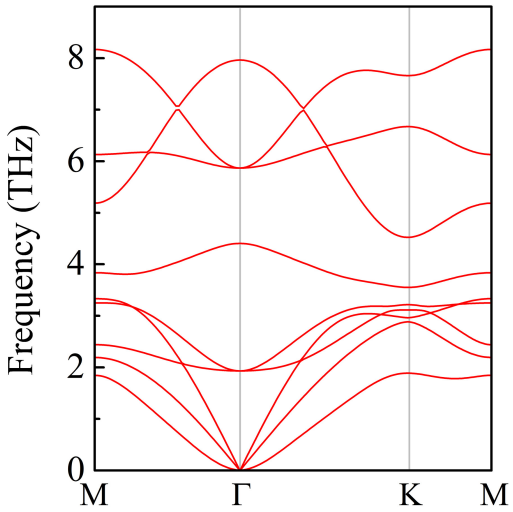

Figure S1: Phonon dispersion of the freestanding 2H-$TiTe_2$ monolayer with a $3 \times 3 \times 1$ supercell considered in the calculation. Absence of imaginary modes in the whole Brillouin zone confirms its kinetic stability.

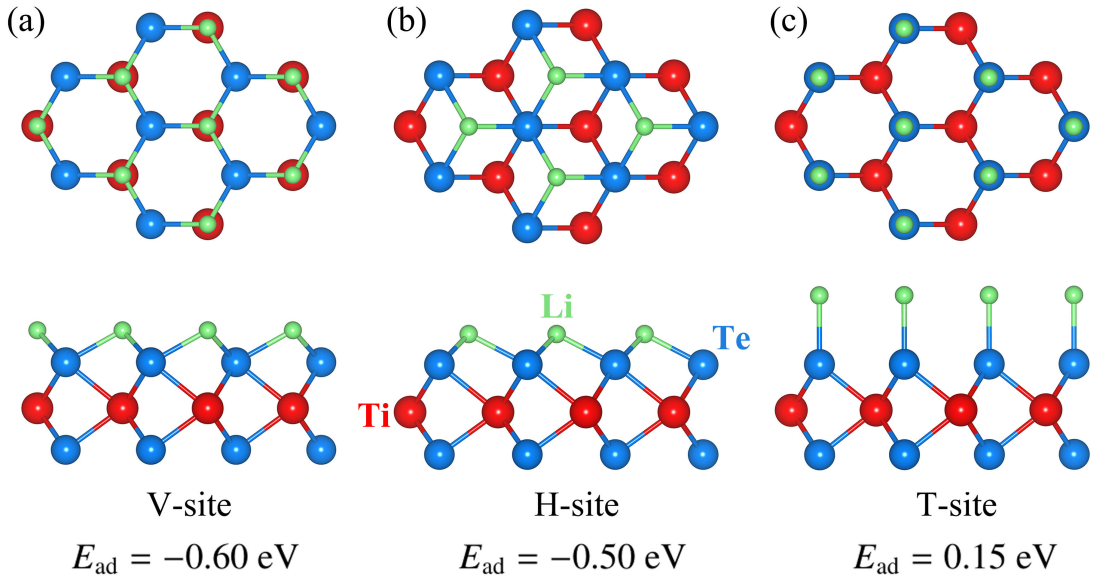

Figure S2: Top and side views of three possible Li-adsorption configurations for the semilithiated 2H-$TiTe_2$ monolayer. It is noted that after full structural relaxation, the Li atom spontaneously moves to the V-site when initially placed at the B-site (not shown). Also shown are the adsorption energies per Li atom.

Table S1: Adsorption energies (E_{ad}) per Li atom on the 2H-$TiTe_2$ surface at three possible adsorption sites.

Adsorption sites	V-site	H-site	T-site
E_{ad} (eV)	−0.60	−0.50	0.15

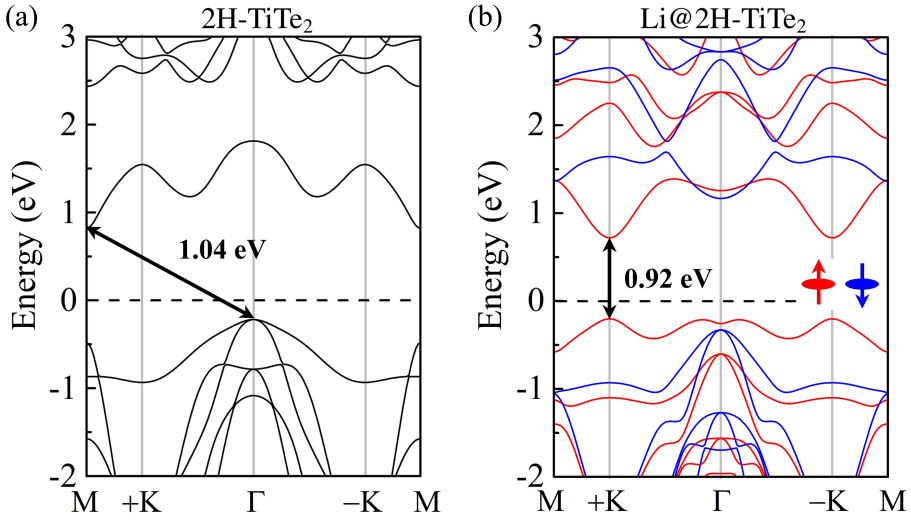

Figure S3: Band structures at the HSE06 level for the 2H-$TiTe_2$ and Li@2H-$TiTe_2$ monolayers in the absence of the SOC effect. The Fermi level is set to zero.

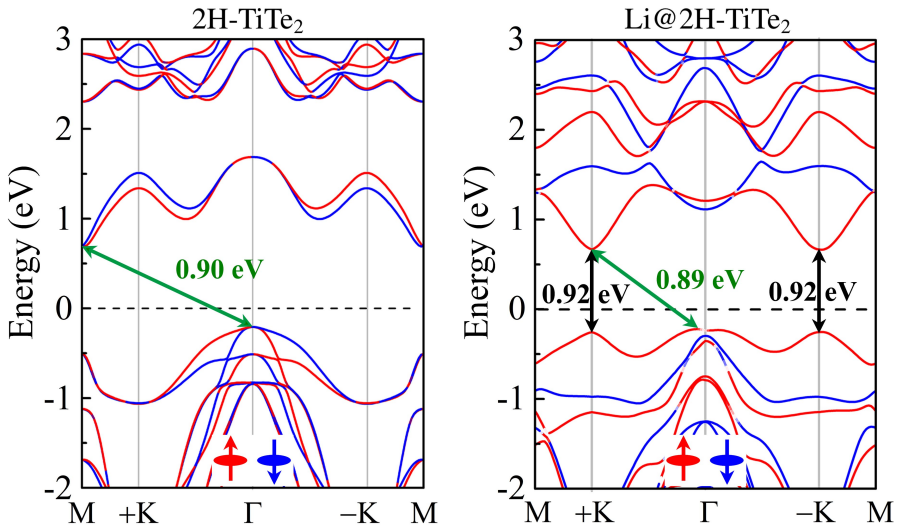

Figure S4: Band structures at the HSE06 level for the 2H-$TiTe_2$ and Li@2H-$TiTe_2$ monolayers in the presence of the SOC effect. The Fermi level is set to zero.

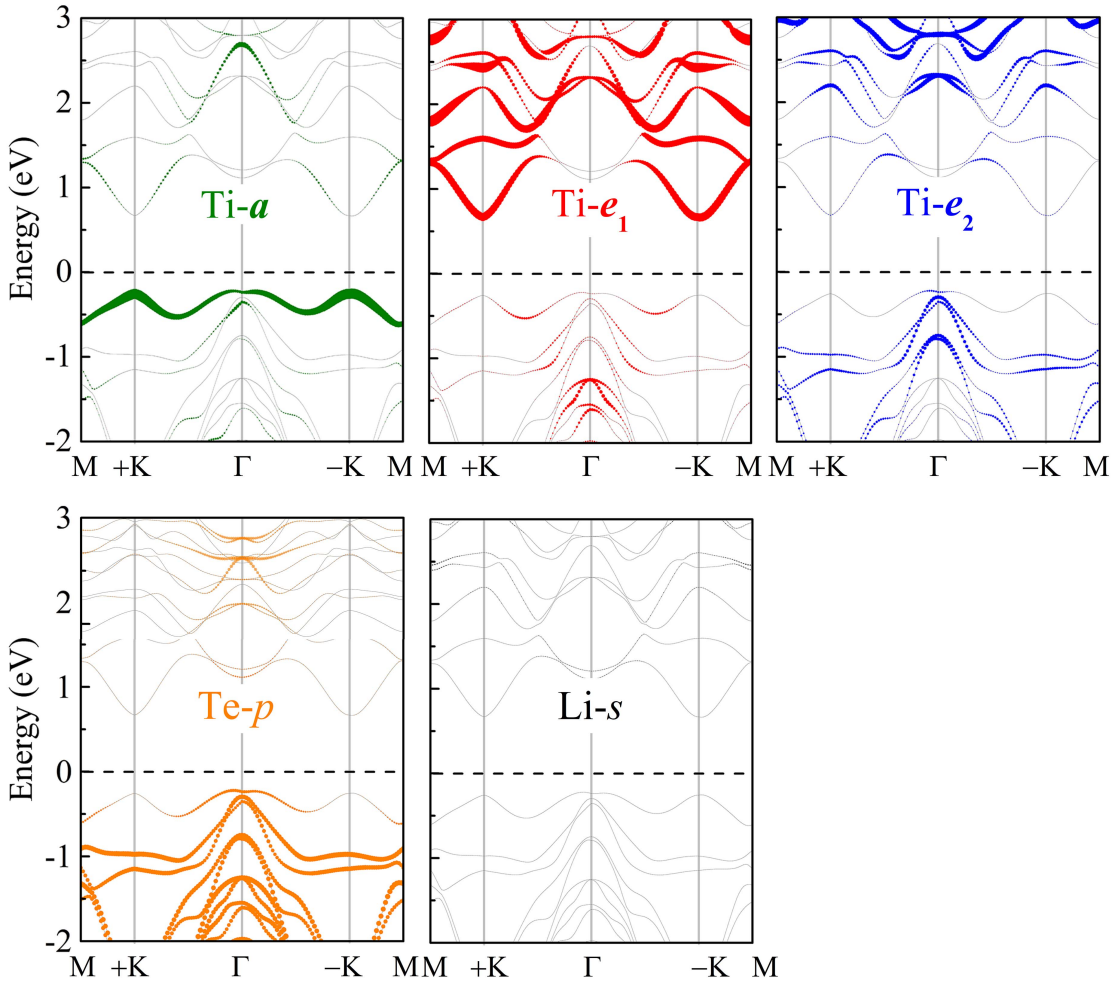

Figure S5: Orbital-resolved band structure at the HSE06 + SOC level for the Li@2H-$TiTe_2$ monolayer. The Fermi level is set to zero.

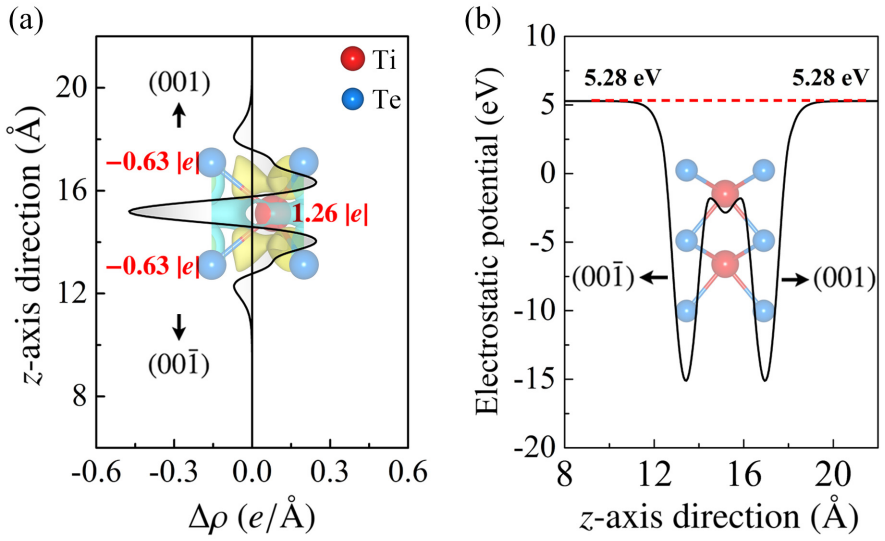

Figure S6: (a) Planar mean charge density of the 2H-$TiTe_2$ monolayer. Also covered are the 3D charge density difference and the amounts of transferred charges at different constituent atoms. Cyan and yellow regions stand respectively for charge accumulation and depletion with the isosurface value set to 0.005 e/Bohr^3. (b) Plane mean electrostatic potential of the 2H-$TiTe_2$ monolayer on the PBE level.