Electronic Supplementary Information: Gate-tunable superconductivity and charge-density wave in monolayer 1T′-$MoTe_2$ and 1T′-WTe_2

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VALIDATION OF THE 2×5 CDW AGAINST THE 2×8 CDW

In order to find the **q**-point at which the lowest phonon frequency of the acoustic phonon mode for a given n_{2D} manifests, we computed phonon frequencies of $MoTe_2$ in the vicinity of $\mathbf{q} = \frac{4}{5}$XM with a fine **q**-grid at $n_{2D} = 1.80 \times 10^{14}$e/cm^2 using the jellium model doping. We confirmed that $\mathbf{q} = \frac{4}{5}$XM has lower frequency than $\mathbf{q} = \frac{3}{4}$XM as shown in Fig. S1.

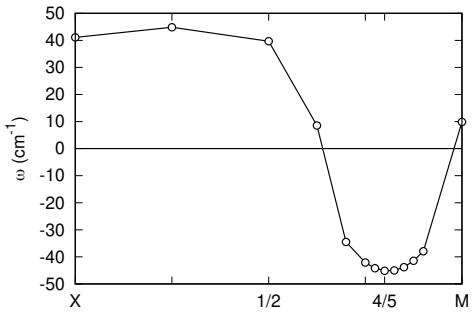

Figure S1. Acoustic phonon mode of $MoTe_2$ at $n_{2D} = 1.80 \times 10^{14}$e/cm^2 along XM line. Phonon frequencies are computed by density functional perturbation theory at each open circle.

Figure S2 shows relative energy gain by the formation of the 2×5 and 2×8 CDW phases. In the jellium model doping, as additional charges do not break inversion symmetry of the system, a CDW phase with inversion symmetry is possible. We found that 2×5 CDW phase with inversion symmetry is ~ 10 meV per 1×1 unitcell more stable than the 2×8 CDW phase which corresponds to the $\mathbf{q} = \frac{3}{4}$XM. These results support that the lowest phonon frequency occurs at $\mathbf{q} = \frac{4}{5}$XM in an intermediate doping region.

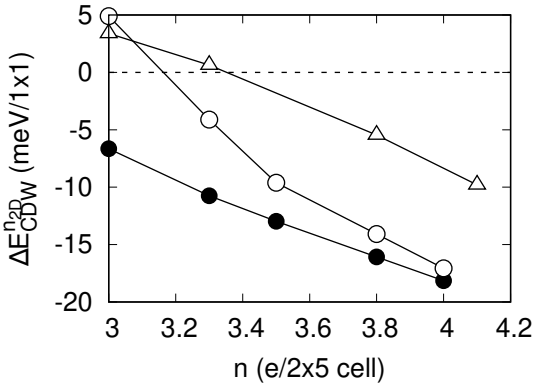

Figure S2. Energy gain by the CDW formation. Filled (open) circles represent 2×5 CDW phases with (without) inversion symmetry while open triangles represent 2×8 CDW phase.

PROJECTED BAND STRUCTURE OF 2×5 CDW

We plot projected band structure of the 2×5 CDW phase and find that band inversion is clearly shown ,which leads to a two-dimensional topological insulator.

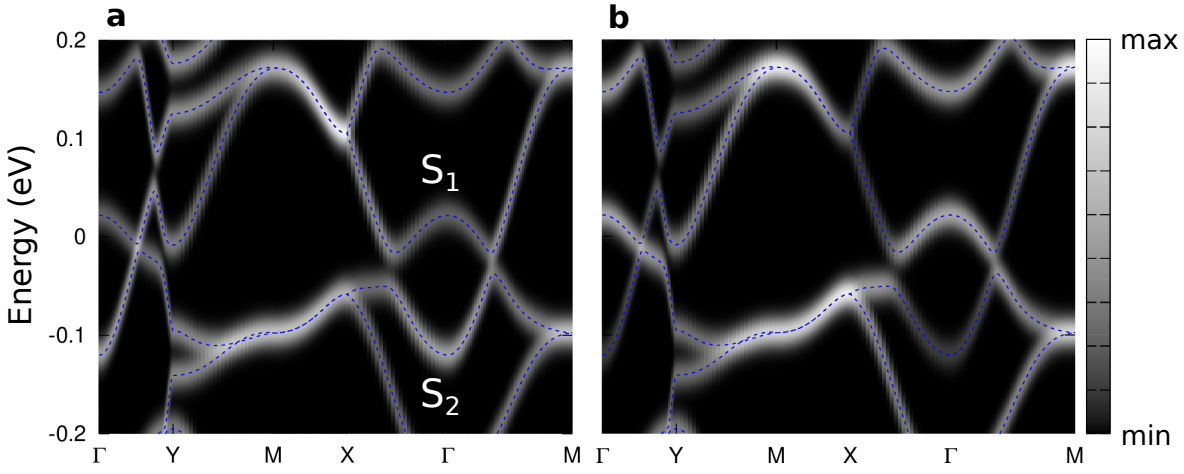

Figure S3. Band structures of the 2×5 CDW phase of $MoTe_2$ with 0.5% tensile strain along y-direction projecting (a) Mo and (b) Te contributions without SOC. S_1 and S_2 bands manifest distinct orbital character. Energy in zero is set to Fermi level. n_{2D} is set to 1.81×10^{14}e/cm^2.

ELECTRONIC STRUCTURE CHANGE UPON TENSILE STRAIN

We applied tensile strain along the y-direction and computed band structures as shown in Fig. S4. We confirm that a band gap forms while preserving inverted band character (Fig. S4(a)-

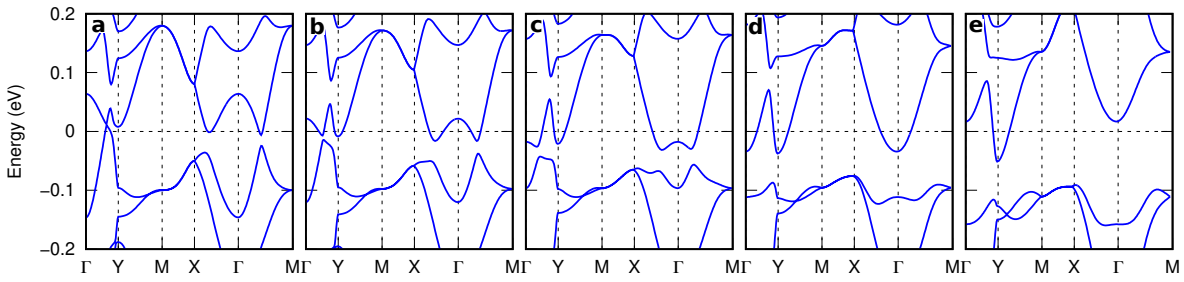

Figure S4. Band structures of the 2×5 CDW phase of $MoTe_2$ with respect to tensile strain along y-direction without SOC (a) pristine, (b) 0.5%, (c) 1.0%, (d) 2.0%, and (e) 3.0%. Energy in zero is set to Fermi level. SOC is not included. n_{2D} is set to 1.81×10^{14}e/cm^2.

(c)). As we increase the strain more than 2%, the inverted band character disappears as shown in Fig. S4(d) and (e).