Supporting Information for

Strong Modulation of Electronic Properties in Monolayer $MoTe_2$ Using a Ferroelectric $LiNbO_3$(0001) Substrate

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Table S1 Total energy (eV) of five stacking configurations of $MoTe_2$/LNO(0001). Stacks Nos. 1-5 represent the configurations of different relative displacements of $MoTe_2$ monolayer relative to LNO, which are (0, 0), (1/4, 0), (1/4, 1/4), (1/2, 0), and (1/2, 1/2).

Stacks	No. 1	No. 2	No. 3	No. 4	No. 5
LNO Z-	-1232.907	-1232.917	-1232.918	-1232.916	-1232.918
LNO Z+	-1375.683	-1375.700	-1375.700	-1375.683	-1375.683

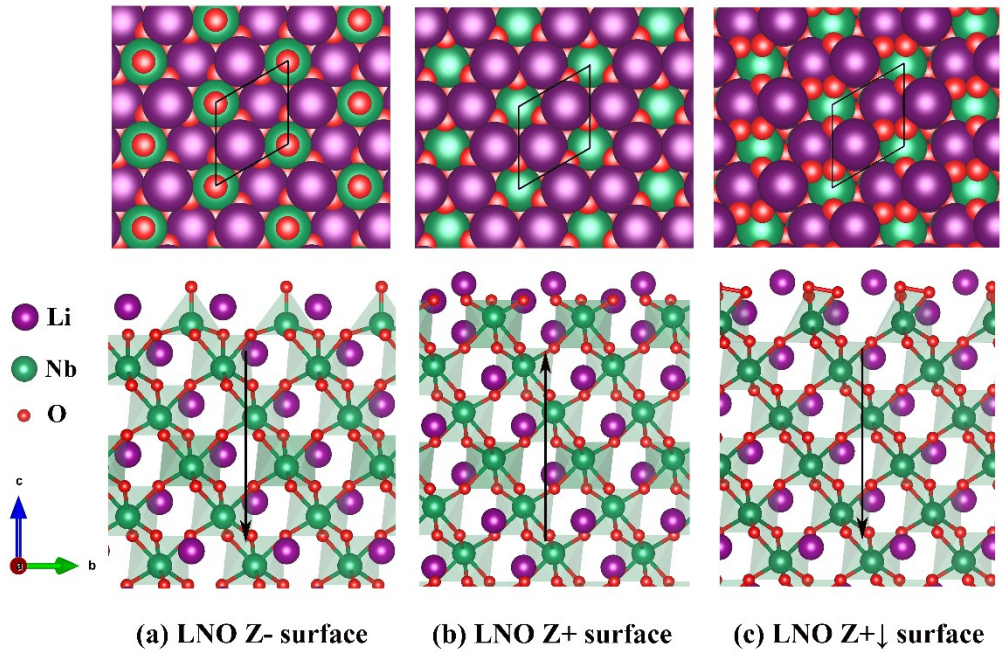

Fig. S1 Surface slab model of ferroelectric LNO(0001) stabilized (a) negative and (b) positive surface and (c) the polarization-reversed LNO Z+ surface. The upper layer is space-filling models, and the lower layer is side view. The black arrow represents the direction of ferroelectric polarization. The thermodynamic preferred surface terminations of LNO Z- and Z+ are -Li-O terminated and -Nb-O_3-Li_2 terminated, which are consistent with the surface terminations described in references 1 and 2. On the other hand, the LNO slabs uses six Nb-O_3-Li trilayers plus surface termination, fixes the lowest three atomic layers and optimizes only the outermost three Nb-O_3-Li trilayers plus stable surface termination.

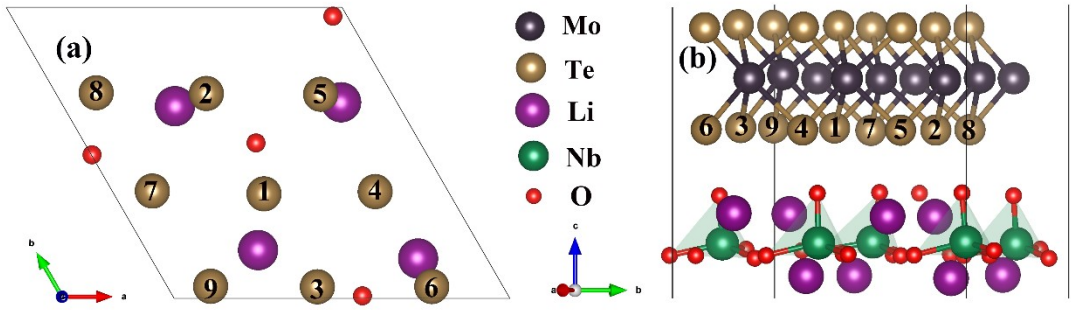

Fig. S2 To inspect the local chemical environment between the $MoTe_2$ monolayer and the LNO Z- surface, we draw the local atomic structure diagram. (a) Is the top view (-Li-O surface termination plus the lowest Mo atom layer in $MoTe_2$). (b) Is a side view with the c-axis of 0.38-0.62 in fractional coordinates. Note that Te atoms are labeled with numbers 1-9.

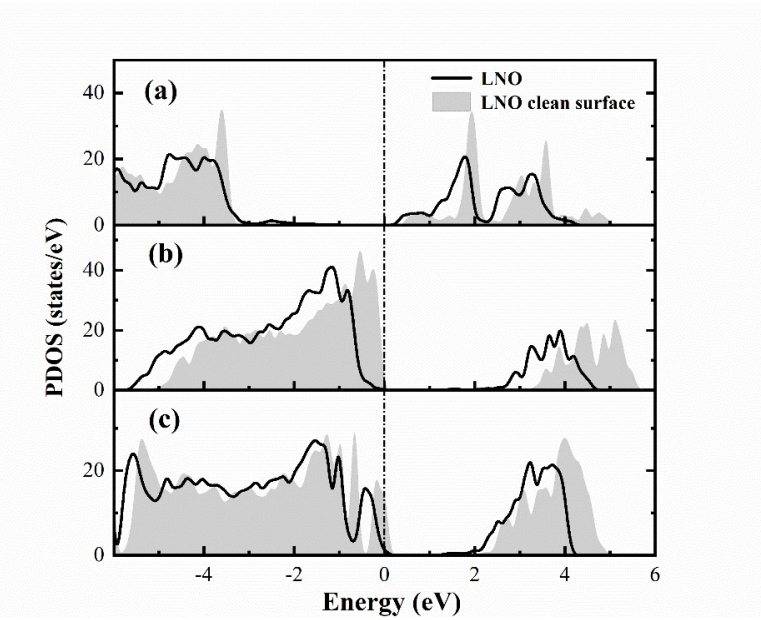

Fig. S3 Projected DOS on the LNO surface (one Nb−O_3−Li trilayer plus the surface termination) for $MoTe_2$/LNO(0001) heterogeneous systems. (a), (b) and (c) are $MoTe_2$/LNO Z-, $MoTe_2$/LNO Z+, and $MoTe_2$/LNO Z+↓ systems, respectively. The gray shaded area is the DOS of the corresponding LNO(0001) clean surface. The Fermi level is set to 0 eV.

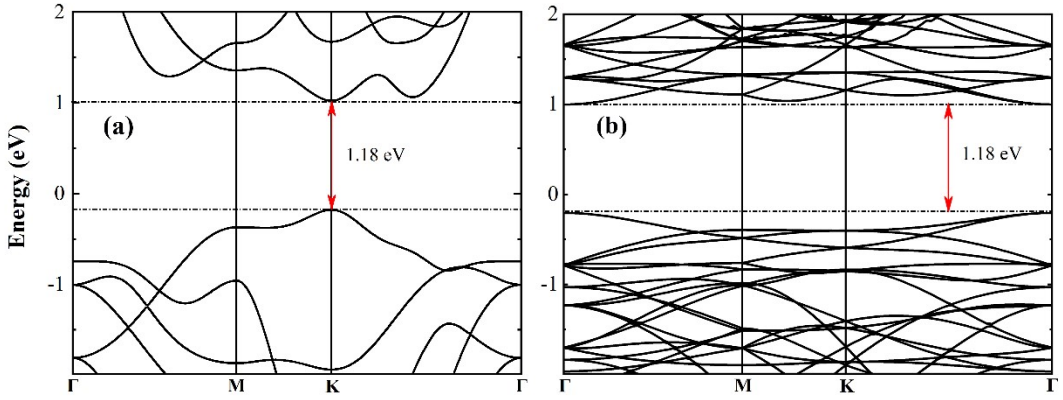

Fig. S4 Band structure for (a) the primitive cell and (b) 3×3 supercell of $MoTe_2$ monolayer. The red arrow indicates the optimal transition route of electrons, i.e., the k-point position corresponding to the conduction band minimum (CBM) and the valence band maximum (VBM). And the Fermi level is set to 0 eV.

1 S. Sanna and W. G. Schmidt, Lithium niobate X-cut, Y-cut, and Z-cut surfaces from ab initio theory, Phys. Rev. B 81 (2010) 214116.

2 S.V. Levchenko, A.M. Rappe, Influence of ferroelectric polarization on the equilibrium stoichiometry of Lithium Niobate (0001) surfaces, Phys. Rev. Lett. 100 (2008) 256101.