

Supplemental Material for “Microscopic origin of magnetic anisotropy in the d^0 ferromagnetic multiferroic monolayer TiCdO_4 ”

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1. DFT + U calculations for MAE.

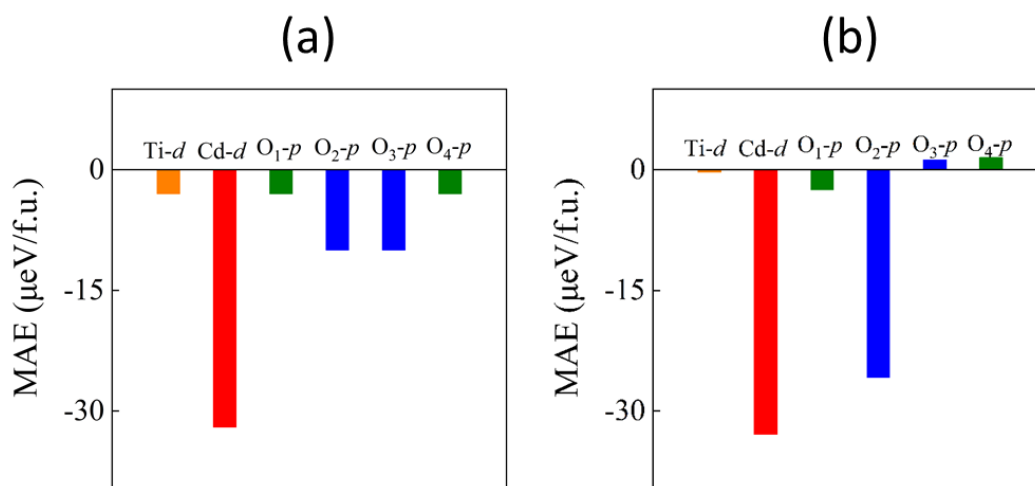


Fig. S1. Atomic- and orbital-resolved MAE contributions in the (a) $P2/m$ and (b) $P1$ phases, obtained using DFT + U calculations.

2. PDOS of O p orbitals in the $P2/m$ and $P1$ phases.

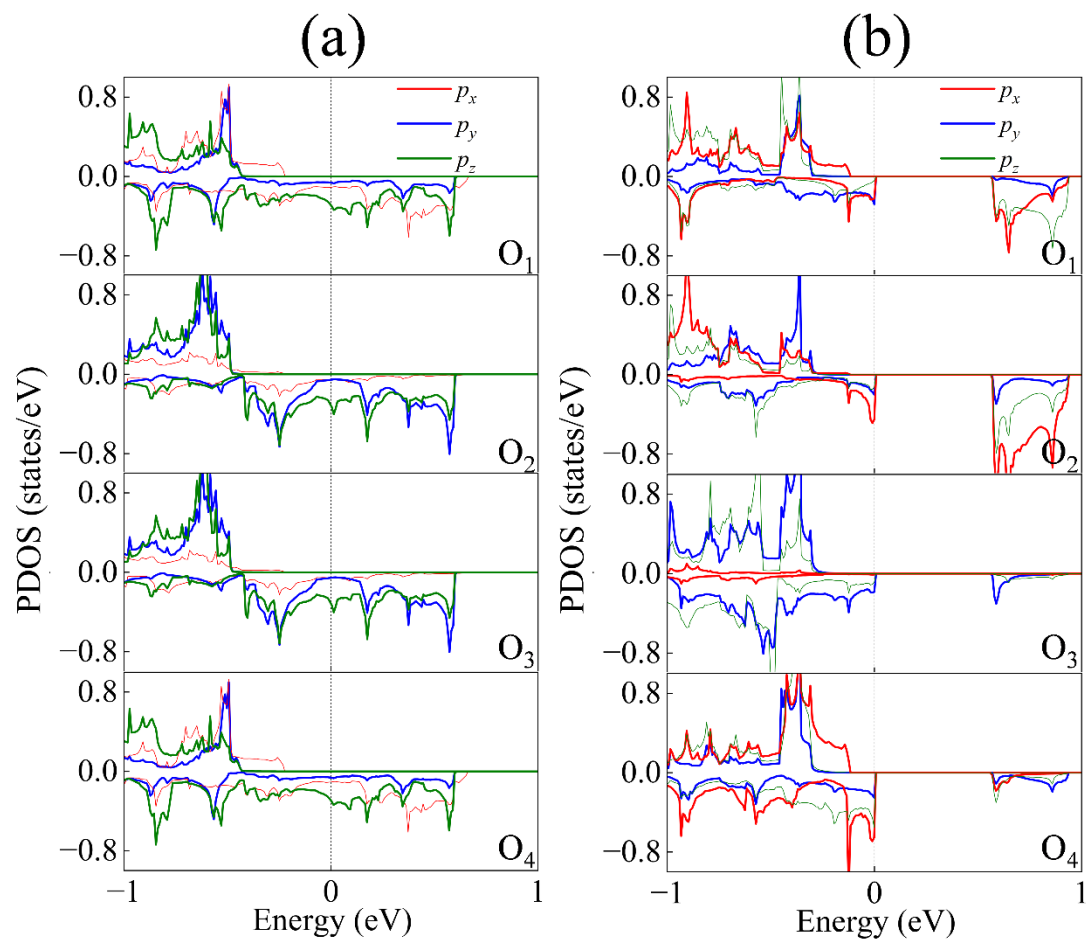


Fig. S2. Calculated PDOS of $O_1, O_2, O_3,$ and O_4 p orbitals in the (a) $P2/m$ and (b) $P1$ phases.