Supplementary Information

Prediction of two-dimensional narrow-gap Janus TiOXY (X, Y=Cl, Br, I; X≠Y) monolayers for electronic and optoelectronic applications

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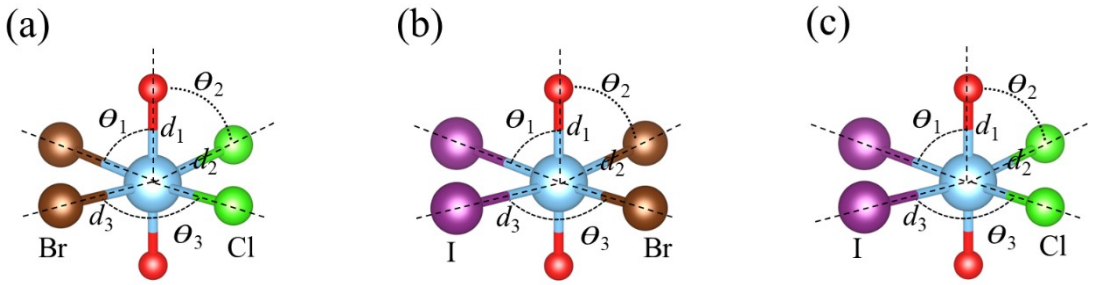

Fig. S1 The labeled bond lengths d_1, d_2, and d_3 (in units of Å) and bond angles θ_1, θ_2, and θ_3 (in units of degree) of the Janus TiOClBr (a), TiOBrI (b), and TiOClI (c) monolayers.

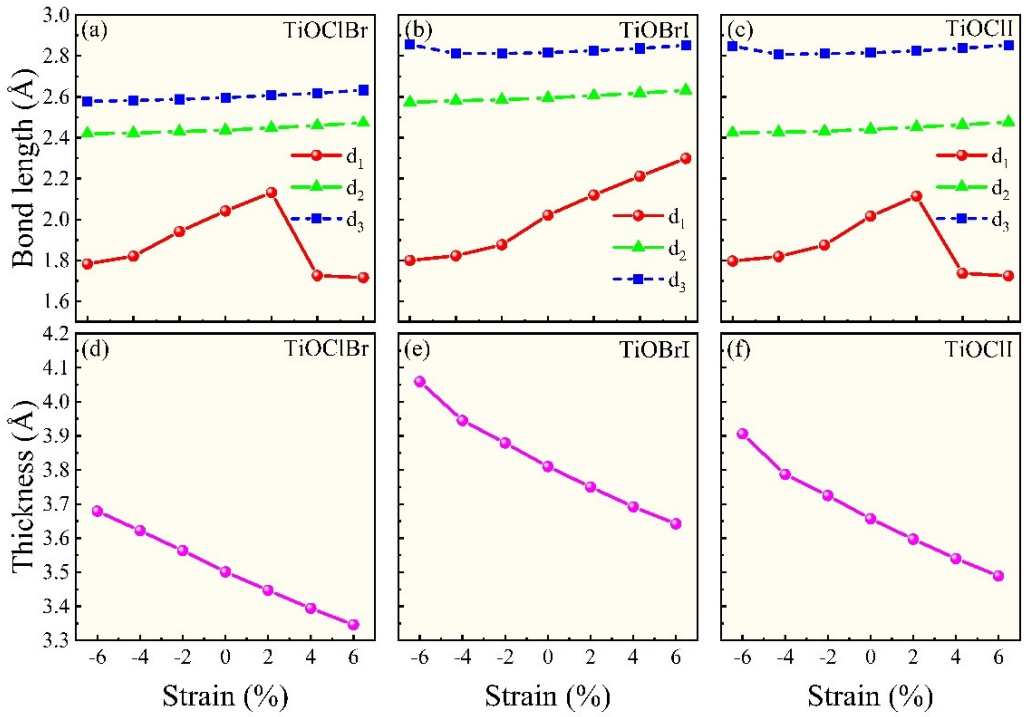

Fig. S2 The variation of (a)-(c) bond lengths d_1, d_2, and d_3 (as denoted by the red-sphere marked solid, green-triangle marked dashed, and blue-sphere marked dashed-dot lines) and (d)-(f) thickness h (as shown by magenta-sphere marked solid lines) under the in-plane biaxial strain in range from -6% to 6% of the Janus TiOClBr, TiOBrI, and TiOClI monolayers, respectively.

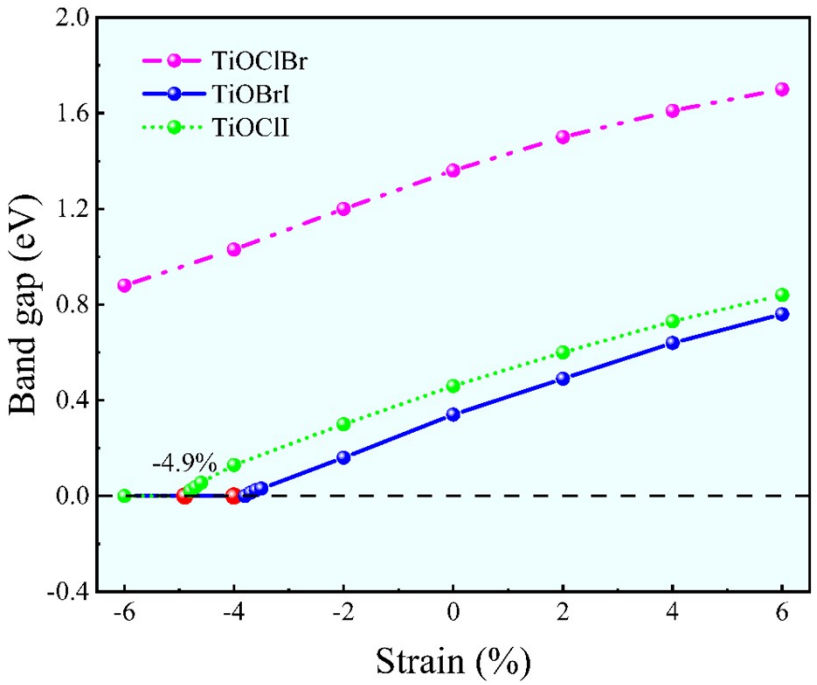

Fig. S3 The variation of band gaps under the in-plane biaxial strain in range from -6% to 6% of the Janus TiOClBr, TiOBrI, and TiOClI monolayers, as denoted by the magenta-sphere marked double-dashed, blue-sphere marked solid and green-sphere marked dot lines, respectively. Where the red-sphere indicates the critical point of strain.

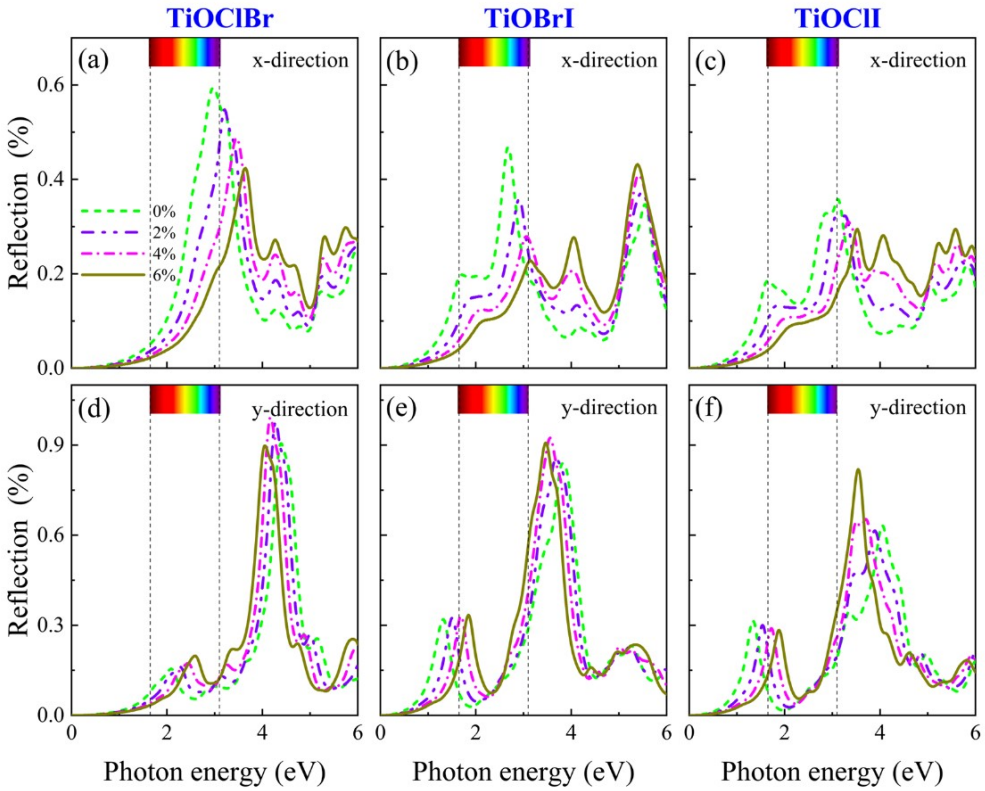

Fig. S4 The photon energy dependent optical reflection coefficients along x directions (a)-(c) and y directions (d)-(f) of the Janus TiOClBr, TiOBrI, and TiOClI monolayers under different in-plane biaxial strains, respectively. The optical reflection coefficients under the biaxial tensile strains of 0%, 2%, 4%, and 6%, are indicated by the green dashed, purple double-dotted dashed, magenta dashed-dot, and brown solid curves, respectively.

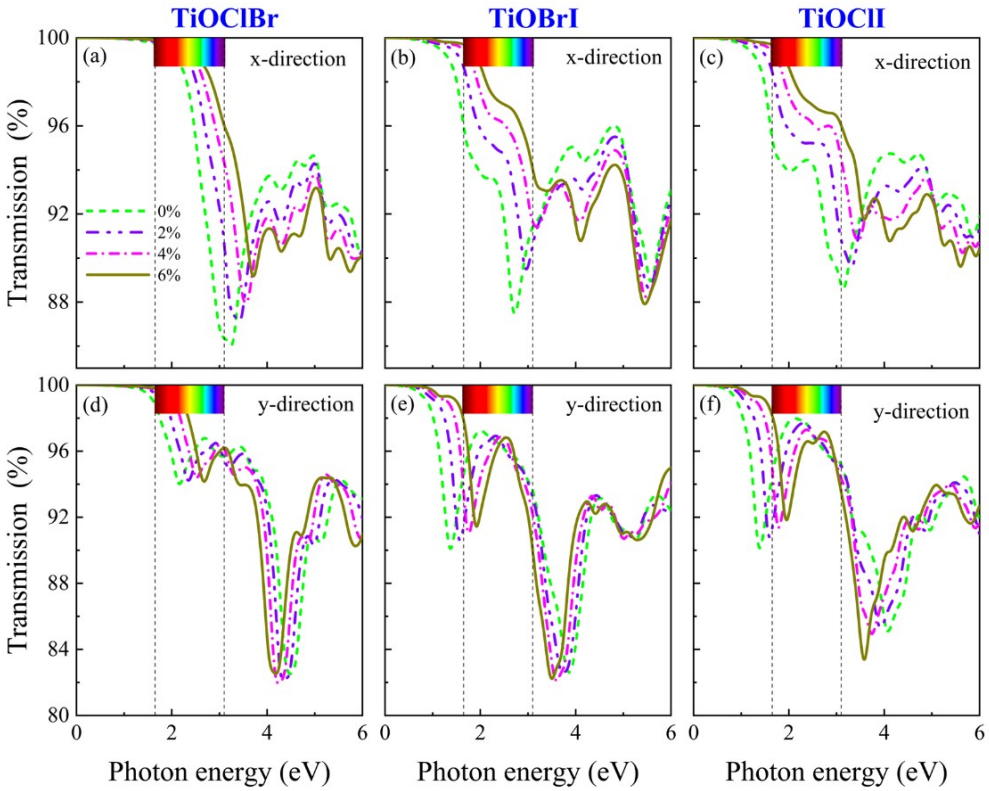

Fig. S5 The photon energy dependent optical transmission coefficients along x directions (a)-(c) and y directions (d)-(f) of the Janus TiOClBr, TiOBrI, and TiOClI monolayers under different in-plane biaxial strains, respectively. The optical transmission coefficients under the biaxial tensile strains of 0%, 2%, 4%, and 6%, are indicated by the green dashed, purple double-dotted dashed, magenta dashed-dot, and brown solid curves, respectively.