Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Material: Oxygen functionalized InSe and TlTe two-dimensional materials: Transition from tunable bandgap semiconductors to quantum spin Hall insulators

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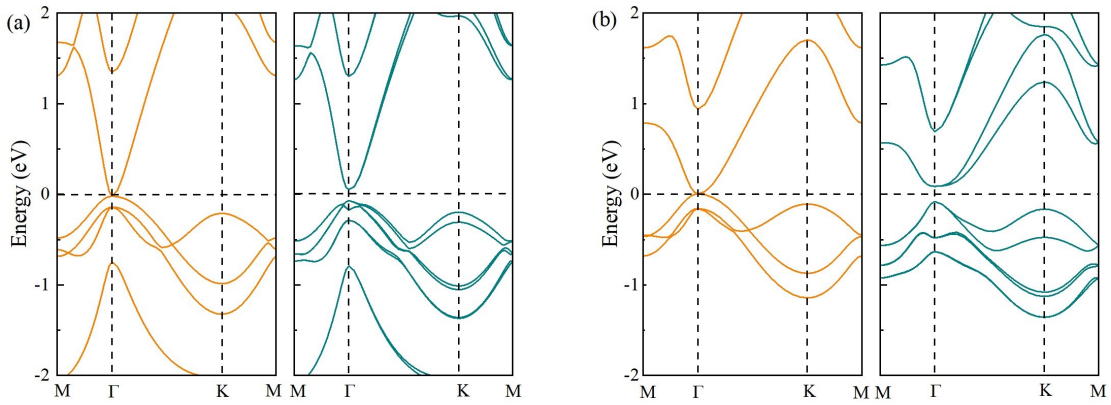

Fig. S1. Band structure of (a) InSeO and (b) TlTeO by HSE06. Orange and dark gray curves represent the band structures without and with SOC, respectively.

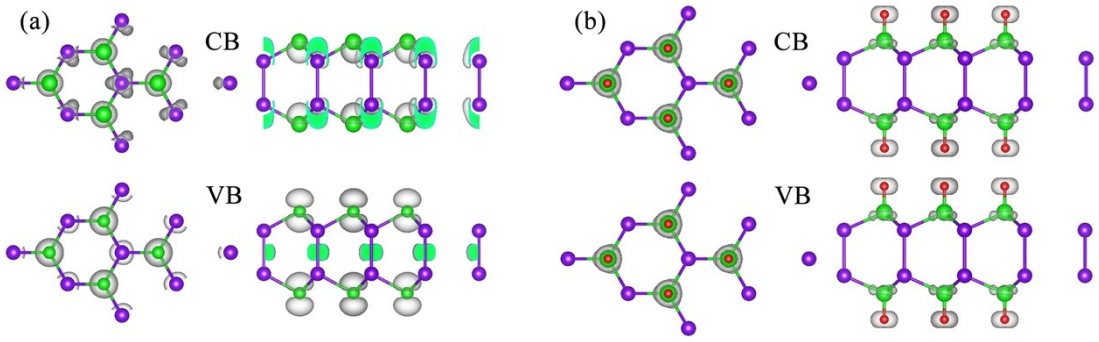

Fig. S2. The partial charge densities of the conduction band bottom (CB) and valence band top (VB) of InSe and InSeO, respectively (top and side views). The blue, green and red balls represent In, Se and O atoms respectively.

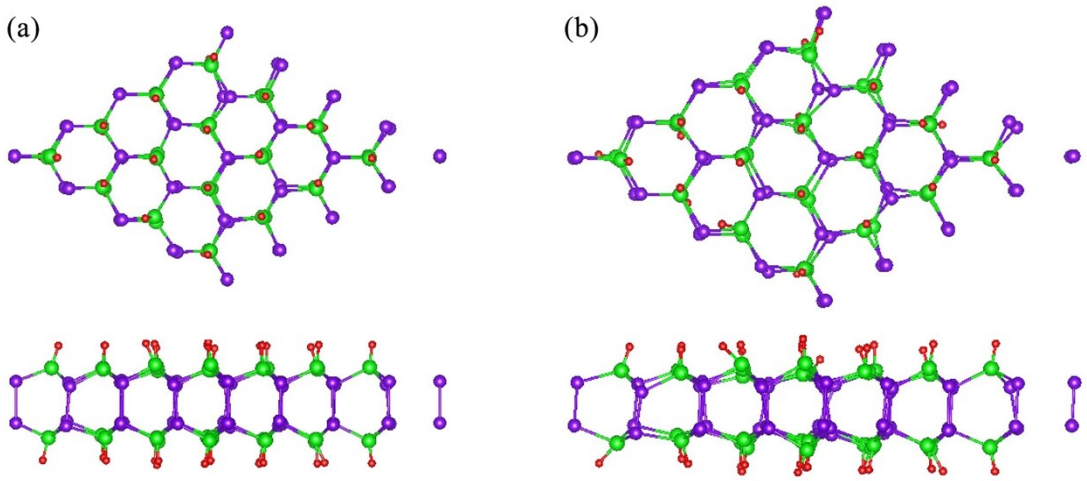

Fig. S3. The snapshot of atomic configuration of (a) InSeO and (b) TlTeO at 300 K. Neither structure reconstruction nor structure disruption appeared in InSeO and TlTeO.