Electronic Supplementary Material (ESI) for Dalton Transactions.

The non-centrosymmetric layered compounds $IrTe_2I$ and $RhTe_2I$

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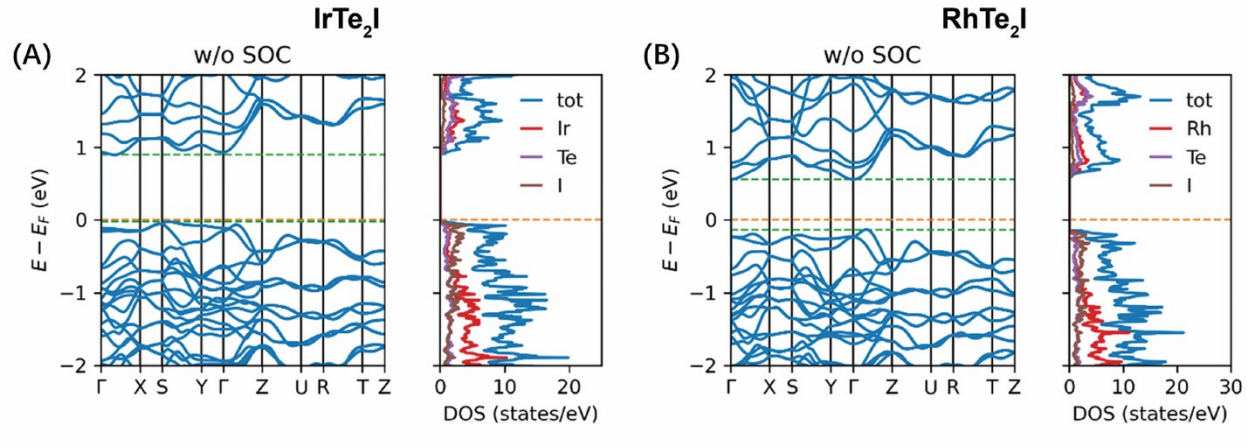

Figure S1. Electronic band structure and DOS for (A) $IrTe_2I$ and (B) $RhTe_2I$ without SOC included. Fermi level (E_F), conduction band minimum (CBM), and valence band maximum (VBM) were highlighted by orange dash lines and green dash lines.

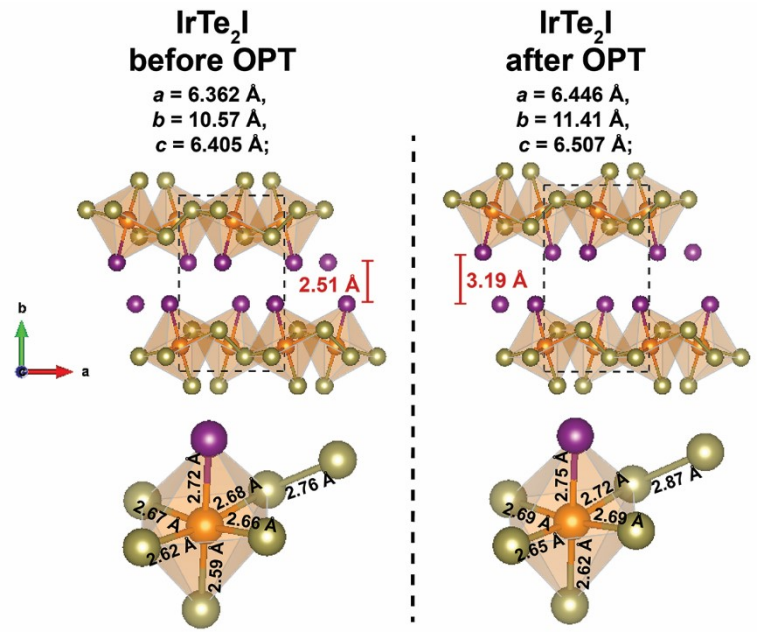

Figure S2. Comparison between experimental structure and the optimized structure ($IrTe_2I$ using as the representative). The latter is used for calculations of band structures and densities of states. The orange colored sphere represents Ir, the purple represents I, and the olive is Te.