

# Single-Crystal Structures, Optical Absorptions, and Electronic Distributions of Thorium Oxychalcogenides ThOQ (Q = S, Se, Te)

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## Supplementary Material

Table S1

Experimental Optical Bandgap Results for ThOQ (Q = S, Se, Te). All values in eV.

| Measurement type | ThOS | ThOSe | ThOTe |
|------------------|------|-------|-------|
| Direct           | 2.27 | 1.91  | 1.46  |
|                  | 2.24 | 1.86  | 1.46  |
|                  | 2.24 |       |       |
| Average          | 2.25 | 1.89  | 1.46  |
| Indirect         | 2.25 | 1.70  | 1.46  |
|                  | 2.21 | 1.60  | 1.46  |
|                  | 2.20 |       |       |
| Average          | 2.22 | 1.65  | 1.46  |

Figure S1. Absorbance vs. energy (eV) spectrum for ThOTe obtained with the visible detection scheme. The bandgap, 1.46 eV, is beyond the 3.2 – 1.5 eV range.

Figure S2. Absorption coefficients of ThOS and ThOTe obtained with the IR detection scheme. As expected from its 2.22 eV bandgap, the ThOS crystal has a flat and low absorption coefficient over the range 1.8 – 1.08 eV.