Abstract Submitted
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p-type transparent conducting chalcogenides[1] HONGLIANG SHI, BAYRAMMURAD SAPAROV, DAVID SINGH, ATHENA SEFAT, MAO-HUA DU, Oak Ridge National Lab, MATERIALS SCIENCE & TECHNOLOGY DIVISION COLLABORATION — Transparent conducting materials are an important component in many optoelectronic devices ranging from solar cells to transparent electronics. A good transparent conducting material must allow high optical transmittance across a wide optical spectrum, requiring a large optical band gap (>3.0 eV), and have high conductivity. However, in materials high conductivity and large band gaps usually do not coexist. At present, only a few materials are known to be reasonably good n-type transparent conducting oxides (TCOs). The p-type TCOs are still plagued by their poor hole conductivity, usually two orders of magnitudes lower than the highest electron conductivity in the n-TCOs. Chalcogenides usually have better hole conductivity, but their band gaps are usually too small. In this study, first-principles calculations are used to design new chalcogenides with large band gaps. New ternary chalcogenides, i.e.,$Cs_2Zn_3Se_4$ and $Cs_2Zn_3Te_4$, are found by calculations to be chemically stable and have both large band gaps (>3.0 eV) and small effective masses. These new ternary chalcogenidesare are synthesized and found to be air stable.

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