

Abstract Submitted  
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**Band gap engineering of BaZrS<sub>3</sub> by Ti doping**<sup>1</sup> XIUCHENG WEI, SAMANTHE PERERA, CHUAN ZHAO, HAO ZENG, University at Buffalo-SUNY, YI-YANG SUN, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, HAOLEI HUI, Xi'an Jiaotong University — Although first synthesized some 5 decades ago, the chalcogenide perovskites are scarcely investigated compared to their oxide counterparts. The recent advances in organic-inorganic halide-perovskites as solar absorbers demonstrating power conversion efficiencies in the 20% range has led to revived interests in these materials, in an effort to address the instability and toxicity issues that plague halide perovskites. BaZrS<sub>3</sub> is a prototypical chalcogenide perovskite. It is shown to be a direct band gap semiconductor with a band gap of 1.7-1.8 eV, slightly higher than the optimum value for a single junction solar cell of 1.3-1.5 eV. In this work, we report band gap engineering of BaZrS<sub>3</sub> by cation alloying with Ti. Since the Ti 3d states have energy lower than 4d states of Zr, substitutional Ti doping can lower the band gap by pushing down the conduction band minimum. A series of BaZr<sub>1-x</sub>Ti<sub>x</sub>S<sub>3</sub> powder samples (with X smaller than 0.2) were synthesized. XRD results showed a systematic shift of the diffraction peaks to higher angles with increasing x, suggesting a decrease in lattice spacing. UV-Vis absorption was also measured to determine the bandgaps. The band gap was found to be reduced to 1.5 eV with moderate Ti doping; while at higher doping concentration, secondary phases were detected. Our work demonstrates that cation alloying is a viable approach for band gap engineering of chalcogenide perovskite for PV applications.

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