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Synthesis, Characterization and Chemical Stability of Silicon Dichalcogenides, $\text{Si}(\text{Se}_x\text{S}_{1-x})_2$

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ABSTRACT

Silicon dichalcogenides have an intriguing crystal structure consisting of long tetrahedral chains held together by van der Waals forces but the electronic and optical properties have been less explored. In the present work, bulk SiSe_2 , SiS_2 , and $\text{Si}(\text{Se}_x\text{S}_{1-x})_2$ were synthesized by the congruent melt growth method and characterized by Raman spectroscopy, X-ray Diffraction and UV/visible/IR transmission measurements supported by first-principles calculations. First-principles calculations reveal a nearly linear decrease of band gap energy in $\text{Si}(\text{Se}_x\text{S}_{1-x})_2$ with increasing Se content, i.e., from SiS_2 to SiSe_2 which corresponds with a blue-shift in the transmission spectra from bulk SiSe_2 to $\text{Si}(\text{Se}_{0.6}\text{S}_{0.4})_2$, and to SiS_2 . Air stability tests demonstrate the formation of toxic $\text{H}_2\text{Se}/\text{H}_2\text{S}$ gas from sample oxidation at room temperature upon exposure to ambient air, and great care should be paid when handling these materials.

KEYWORDS

A1. Characterization, A1, Computer simulation, A2. Growth from melt, B1. Sulfides, B3. Solar cells,

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