Abstract Submitted
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First principles investigation of ternary Na-V-VI2 chalcogenides and their semi-classic transport coefficients[1] ISHAN KHARE, Ottawa HIlls High School, Ottawa Hills, OH; The University of Toledo, Toledo, OH, NATHAN SZYMANSKI, RICHARD IRVING, The University of Toledo, Toledo, OH — Ternary chalcogenides have been of recent investigation for applications such as solar cells and thermoelectrics. We study the structural, energetic, electronic, optical, and thermoelectric properties of nine ternary Na-V-VI2 chalcogenides, NaAB2, where A represents pnictogens As, Sb, Bi and where B represents chalcogens S, Se, Te, using first principles methods based on density functional theory and beyond. Optimized lattice parameters have been computed using the generalized gradient approximation (GGA). Phonon density of states computed at zero-temperature shows that only four compounds, NaAsS2, NaAsTe2, NaSbS2, and NaSbSe2, of the nine compounds, are dynamically stable. These layered crystal structures result in computations that show highly anisotropic electronic and optical properties. Thermoelectric properties and semi-classic transport coefficients such as Seebeck coefficient and power factor are also studied by applying Boltzmann statistics. The compounds are predicted to have promising thermoelectric properties at 300 K, which indicates that these materials can be used for thermoelectric devices. Experimental verification is suggested.

[1]University of Toledos Research in Science and Engineering Program; Ohio Supercomputer Center, http://osc.edu/ark:/19495/f5s1ph73

Ishan Khare
Ottawa HIlls High School, Ottawa Hills, OH; The University of Toledo

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