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Computational investigation of structural, magnetic, elastic, and electronic properties of Half-Heusler ScVX (X = Si, Ge, Sn, and Pb) compounds

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Abstract

In this paper, we report some physical properties of Half-Heusler ScVX (X = Si, Ge, Sn, and Pb) compounds using the first-principle investigations employing density functional theory (DFT) within the WIEN2k. Simulations are carried out using the generalized gradient approximation with the addition of the Hubbard U-term (GGA + U), which takes into consideration the effect of on-site Coulombic interactions. All the compounds are found