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Prediction of New Crystal Structures of Bi-Sb Compounds using Minima Hopping Structural Search Method SOBHIT SINGH, IRAIS VALENCIA-JAIME, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26506, USA, ANDRES GARCIA-CASTRO, Cinvestav-Unidad Queretaro, Queretaro-76230, Mexico, ALDO ROMERO, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26506, USA
— In the last few years, semi-conducting alloy $Bi_{1-x}Sb_x$ has emerged as a potential candidate for topological insulators [1]. In this work, we present systematic study of the low-enthalpy phases of $Bi_{1-x}Sb_x$ alloys at zero pressure by using the ab-initio minima hopping structural prediction method [2]. Even though, Bi and Sb crystallize in the same 166 space group, our calculations indicate that the $Bi_{1-x}Sb_x$ alloys can have several other thermodynamically stable crystal structures. Additionally to the configurations on the convex hull, we also find a large number of metastable structures which are dynamically and elastically stable. Band structure calculations of the stable phases reveal the presence of strong spin-orbit interaction leading to the Rashba spin splitting of the bands which is of great interest for spintronics applications.

[1] J. C. Y. Teo, L. Fu and C. L. Kane; Phys. Rev. B 78, 045426 (2008)
[2] S. Goedecker; J. Chem. Phys. 133, 224104 (2004)

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