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Electronic properties of giant ferroelectric Rashba semiconductor BiSb: A first-principle study of bulk and monolayer SOBHIT SINGH, A. C. GARCIA-CASTRO, I. VALENCIA JAIME, W. IBARRA-HERNANDEZ, A. H. ROMERO, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505, USA, F. MUNOZ, Departamento de Fisica, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile — We investigate the electronic properties of layered BiSb compound in bulk and two-dimensions. Our first-principle calculations reveal that BiSb is a ferroelectric Rashba semiconductor that inherits large Rashba effect due to the presence of strong spin-orbit interactions and broken inversion-symmetry of the crystal. The theoretical maximum value of the Rashba energy (E_R) and Rashba constant (α_R) in bulk BiSb is 147.3 meV and 10.43 eVÅ, respectively [1]. We notice that the strength of the Rashba spin-splitting can be effectively tuned by applying an external stress or bi-axial strain. Interestingly, a novel Weyl semimetallic phase emerges in the bulk BiSb when the external applied pressure is in the 4.0-6.0 GPa range [2]. This Weyl semimetallic phase can be efficiently harnessed by gaining control over the ferroelectric polarization of the bulk BiSb [2]. We further study the electronic and vibrational properties of the BiSb monolayer and BiSb/BN heterostructure. Our calculations suggest that BiSb monolayer and BiSb/BN heterostructure systems are thermodynamically stable and exhibit intriguing electronic properties. [1] Sobhit Singh et al., *Phys. Chem. Chem. Phys.* 18, 29771-29785 (2016) [2] Sobhit Singh et al., *Phys. Rev. B* 94, 161116(R) (2016)

Sobhit Singh
West Virginia University

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