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Pressure-induced Lifshitz and Weyl Semi-metallic Phase Transitions in BiSb SOBHIT SINGH, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505, IRAIS VALENCIA-JAIME, ANDRES GARCIA-CASTRO, Cinvestav-Unidad Querétaro,Querétaro-76230, México, FRANCISCO MUÑOZ, Departamento de Física, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago 7800024, Chile, ALDO ROMERO, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505 — By means of first-principle calculations, we report a non-magnetic stoichiometric crystal structure of BiSb with broken space-inversion symmetry. This structure belongs to the $R3m$ space group and it was obtained after a systematic study of the low-energy phases of $Bi_{1-x}Sb_x$ $(0 < x < 1)$ compounds found by using minima hopping structure search method [1]. This structure is insulating in bulk and has non-trivial band topology. We observe pressure-induced Lifshitz and Weyl semi-metallic phases as electronic phase transitions in this system. The obtained Weyl semi-metallic phase exist in the $4.0 - 6.0$ GPa pressure range. We find that a total 12 pairs of Weyl points, 12 monopoles and 12 antimonopoles, exist in the bulk Brillouin zone. The Weyl points with opposite chirality are located at different energy values yielding separate electron and hole Fermi-surfaces, which drives novel topological transport properties in this system. The surface state calculations reveal reminiscence of the Fermi-arcs at (001) surface of the BiSb slab, which further confirm the existence of Weyl semi-metallic phase in BiSb [2-4]. [1] J. Chem. Phys. 120, 9911 (2004) [2] Science 349, 622 (2015) [3] Nat Phys 11, 748 (2015) [4] Phys. Rev. X 5, 031013 (2015)

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