Abstract Submitted
for the MAS15 Meeting of
The American Physical Society

Prediction of Weyl semi-metallic phase in inversion-asymmetric BiSb SOBHIT SINGH, IRAIS VALENCIA-JAIME, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505-6315, USA, ANDRES GARCIA-CASTRO, Cinvestav-Unidad Queretaro, Queretaro-76230, Mexico, FRANCISCO MUÑOZ, Departamento de Física, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile, ALDO ROMERO, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505-6315, USA — Recent experimental realization of long sought Weyl fermions in non-magnetic crystals has greatly motivated the condensed matter physicist to search for the materials supporting Weyl fermions [1-3]. Weyl fermions appear to be very promising for the future electronics, often referred as Weyltronics. By means of first-principle calculations, we report a non-magnetic stoichiometric crystal structure of BiSb with broken space-inversion symmetry. This structure is insulating in bulk and has non-trivial band topology. We observe a pressure driven Weyl semi-metallic phase transition in this structure. The obtained Weyl semi-metallic phase exist in the $4.0 - 6.0$ GPa pressure range. We find that 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 yields novel topological transport properties in this system. [1] Science 349, 622 (2015) [2] Nat Phys 11, 748 (2015) [3] Phys. Rev. X 5, 031013 (2015)

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Date submitted: 22 Sep 2015 Electronic form version 1.4