Electron transport and optical properties of high spin-orbit materials

George J. de Coster [1,2]

[1] *DEVCOM Army Research Laboratory, Adelphi, Maryland 20783, USA*
[2] *Institute of Physics, Faculty of Electrical Engineering and Information Technology, University of the Bundeswehr Munich, 85577 Neubiberg, Germany*

High spin orbit materials have long been studied for their spintronic applications, and ability to affect adjacent magnetic materials for relatively low energy costs. In the last two decades the field of topological materials has paved the way for many new 'topologically non-trivial' materials where strong spin-orbit coupling gives rise to special surface (or edge) states that carry Dirac like spin-orbit coupled conduction states. In this talk we focus on two such materials, Bi_2Se_3 [1] and $PtSe_2$ [2]. We will show how non-linear optical responses such as the circular photogalvanic effect make these materials unbiased photodetectors when illuminated by circularly polarized light, which has opened a whole new space of applications for strong spin-orbit coupling. In the case of Bi_2Se_3 the polarization sensitive photoresponse can be understood in Fig. 1 where the strong spin splitting of the surface states (red and blue) result in selection rules that require the spin flip of an electron when excited from the valence to the conduction band. For a particular handedness of circularly polarized light, only one side of the Dirac cone permits excitations.

We will present a combination of theoretical and experimental studies on Bi_2Se_3 and $PtSe_2$ that explore the ways in which disorder, strain, and external fields impact the quality of the polarization sensitive photoresponse. We will show how both the symmetries of the crystal structure and the details of its band structure impact the non-linear optical response and show that depending on the underlying material properties disorder can be advantageous or disadvantageous depending on the application of interest.

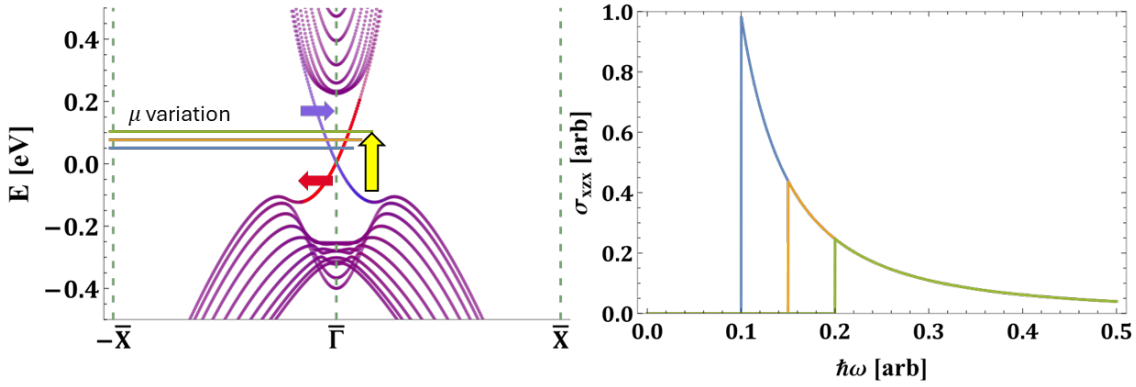

Figure 1: Schematic Bi_2Se_3 band structure (left) and corresponding analytical non-linear optical resonse tensor element (right) responsible for the circular photogalvanic response. The topological surface states are colored red and blue corresponding to their spin polarization, while bulk bands are colored purple. The chemical potential, μ, is varied across the indicated colored lines, and the corresponding non-linear optical tensor element calculation shows that due to Pauli blocking the minimum energy threshold for the optical excitation is 2μ.

[1] B.C.Connelly, P.J. Taylor, G.J. de Coster, PNAS 121 (5) e2307425121 (2024)
[2] C. Yim et al. npj 2D Materials and Applications **2**, 5 (2018)