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Electronic properties of TlFe2Se2 using density functional theory

Doping and anion height are found to drastically affect the electronic structures of superconductors [1-2]. In this study, we investigated the composition-dependence of the electronic properties of the newly discovered intercalated $TlFe_2Se_2$ superconductor using density functional theory. We calculated the electronic structures of $Tl_xFe_2Se_2$ with various Tl concentrations (x = 1.00, 0.75 and 0.50) using a 2 x 2 x 1 supercell. Fractional coordinate z_{Se} of Se which essentially controls the anion height are taken from "relaxed"nonmagnetic and magnetic configurations of $TlFe_2Se_2$ which have values of z_{Se} = 0.341 Å and 0.348 Å, respectively. We also used the experimental value of z_{Se} = 0.357 Å taken from [3], which is higher than the simulated ones. We also added a hypothetical value of z_{Se} = 0.364 Å which is the highest among the fractional coordinate values used. All calculations of the electronic structures are done using QUANTUM ESPRESSO [4]. Generalized gradient approximation of Perdew-Burke-Ernzerhof [5] is used for exchange-correlation potentials.

The density of states (DOS) for various Tl content has shown metallic properties where states near the Fermi energy (E_F) are mostly from Fe-d states. This is consistent with the typical features of iron-based superconductors. For various fractional coordinates, z_{Se}, the DOS have also shown similar characteristics. Band structure calculations on the other hand revealed different results. For x = 1.00, no pocket is found around the zone center (Γ point) of the First Brillouin zone. For x = 0.75 and 0.50 on the other hand, hole-like pockets are being observed around the Γ point which is typical of Fe-based superconductors. The appearance of the hole-like pockets might be due to the shifting of the E_F towards lower energy when Tl content is reduced. This indicates a possible doping effect in this material (i.e. hole doping).

Furthermore, we also studied the possible three dimensionality of $Tl_xFe_2Se_2$ with various Tl content by observing the Z point of the first Brillouin zone. As Tl content is reduced, a shift of bands is observed towards higher energies which resulted to an appearance of a shallow electron-like pocket around the Z point when x = 0.75. The electron-like pocket is mainly of Fe-d_{xz}+d_{yz} character. This is not consistent though with the experiments where the observed electron-like pocket has Fe-d_{xy}+Se-p_z character [6]. Looking at the band structure calculations for various z_{Se}, the electron-like band found around the Z-point above E_F for z_{Se} = 0.341 Å seems to shift towards lower energies as the z_{Se} increases, which eventually crossed the E_F for z_{Se} = 0.357 Å. This electron-like pocket is now consistent with the experimental results where the orbital character is found to be of Fe-d_{xy}+Se-p_z. Increasing further the z_{Se} to 0.364 Å, the bands split and a hole-like band is formed below E_F.

In conclusion, these results suggest that the Tl content plays a significant role in tuning the electronic properties of $Tl_xFe_2Se_2$ where doping effect might occur with the appropriate value of Tl concentration. In addition, the anion height shows strong control of the band topology of this material.

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Primary authors: Ms TAGDULANG, Nikki D. (Department of Physics, Mindanao State University - Iligan

Institute of Technology); Ms JACOSALEM, Naomi Jane P. (Department of Physics, Mindanao State University - Iligan Institute of Technology); Dr AMBOLODE II, Leo Cristobal C. (Department of Physics, Mindanao State University - Iligan Institute of Technology, Premier Research Institute of Science and Mathematics (PRISM), Mindanao State University - Iligan Institute of Technology)

Presenter: Dr AMBOLODE II, Leo Cristobal C. (Department of Physics, Mindanao State University - Iligan Institute of Technology, Premier Research Institute of Science and Mathematics (PRISM), Mindanao State University - Iligan Institute of Technology)

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