Orbital Selectivity and Magnetic Ordering in Fe intercalated Dirac Semimetal Bi$_2$Se$_3$

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In this paper we investigate the intercalation effects of Iron (Fe) in the van der Waals gap of Bi$_2$Se$_3$ on the magnetic and transport properties using first-principles band structure estimations combined with dynamical mean-field theory. The Dirac cone in the band structure of parent Bismuth Selenide is modified via Fe intercalation at moderate densities. Further inclusion of electronic correlations found to result in the emergence of novel and exotic properties in an intercalated Bi$_2$Se$_3$.

Accompanied by unconventional structural effects, the onset of an orbital selective metal insulator transition in the Fe 3$d$ orbitals brings about a magnetic phase transition in the Fe intercalated Bi$_2$Se$_3$. Additionally we have explored the dependency of the electron-electron correlations on the magnetic ordering and the effects of intercalation in establishing new physical properties.

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I. INTRODUCTION

Topological insulators (TI) denote materials with properties dominated by the bulk insulating states, while their surface electronic structures are found to be metallic in nature. In these TIs, if spin-orbit coupling (SOC) exceeds the band gap and induce a band inversion, a Dirac type band structure emerges, and subsequently, the conducting states appear at the surfaces as demanded by the time-reversal symmetry. In recent times, these topological surface states are engineered in numerous ways to inspect their exotic properties and applicability. Specifically, intercalation and doping by the transition metals (TM) in topological insulators and breaking of the time reversal symmetry are new features that are gathering interest in recent times. In addition, several exciting phenomena such as, the realization of quantum anomalous Hall effect etc. are likely to be possible.

Intercalation by foreign materials into the layered topological insulators changes properties of the parent compounds and possesses versatile applications, such as in superconductors, ambipolar transistors, quantum computers, battery electrodes and solid lubricants. In particular, intercalation by the transition metals are expected to modify the time reversal symmetry induced band inversion and change the linearly dispersing bands by the reformed topological surface states. A well-known three dimensional topological insulator is Bi$_2$Se$_3$ with a 0.3 eV gap in its bulk, alongwith the presence of a Dirac cone in the $K - \Gamma - M$ direction. Ab initio electronic structure calculations and electron scattering experiments have convincingly demonstrated topological properties of Bi$_2$Se$_3$. Further, doped Bi$_2$Se$_3$ is currently being investigated due to the prospects of observing a new phenomenon that occurs when the topological surface states interact with different type of impurities or with other electronic states in the bulk. Intercalating Bismuth Selenide with Cu to get superconductivity below 4K was a potential discovery. Since it is a layered material, there is a van der Waals gap (gap between two consecutive layers of the material and the layers have van der Waals interaction between them) in the crystal structure, making it favourable for intercalation with other materials as well, such as, Fe, Sr, Ag and many others. Intercalation into host materials with these has the prospects of achieving new energy storage materials.

The present paper focuses on the intercalation of topological insulating compound Bi$_2$Se$_3$ with Fe. The percentage of intercalation in these layered materials is determined by the physical size of the inserted material, structural stability and energetically favourable state of the host after insertion. Most of the time, the intercalation is governed by the likelihood of the host to retain its charge neutrality. Intercalation with small alkali metals, such as, Li etc. is relatively easy due to the size, while the ionic nature of the intercalant determines the probability of success of the intercalation in most cases. With all these issues in mind, intercalation with a zerovalent material is of a greater advantage, since it does not change the oxidation state of the host material, which, as a result, allows the insertion of a lot of zerovalent materials (e.g., Au, Ag, Fe, Cu and Ni) in the topological insulators. It does not affect the layered host Bi$_2$Se$_3$, thus enabling an accurate intercalation. Here we used nearly 10 atomic percent of zerovalent Fe into layered Bi$_2$Se$_3$ crystals. Earlier studies have observed that Fe-doped Bi$_2$Se$_3$ is dominated by ferromagnetic interactions. It is relevant to mention here that magnetism can also be achieved by Cr doping, where onset of antiferromagnetic correlations was observed. Further quantum anomalous Hall state was also discovered in vanadium doped topologically insulating films, which makes magnetic topological insulators as candidates for electronic applications. The discovery of the magnetic topological insulators has become interesting with an appearance of integer moments which may be related to half-metallic behaviour.

Parent Bi$_2$Se$_3$, when doped with TM, such as, Cr and Fe, shows an insulating behaviour with reduced band gaps due to the hybridization between the $d$ orbitals of the TM with the Se-$p$ orbitals. Interestingly, in the TI systems, strong spin-orbit coupling results in different
FIG. 1. (Color Online) (a) The crystal structure is shown where the atoms are labelled, (b) Fermi surface and (c) band structure of Fe intercalated Bi$_2$Se$_3$. The Fermi surface reveals impurity d bands crossing the Fermi level. The high intensity region is for electrons, while the low intensity stands for holes. Intercalation results in disappearance of the band inversion at the Γ point and results in increase in the number of conduction electrons.

The spectral function shows partially occupied Se-4p, Bi-6p and Fe-3d bands near the Fermi level for the Fe-intercalated sample. The energy bandgap in parent Bi$_2$Se$_3$ is about 0.3 eV (in good accord with the reported experiments and theory) closes with Fe-intercalation and impurity bands dominate near the Fermi level (see Fig.1c and Fig.2). For performing correlated electronic structure and spectra calculations, a fully charge-self-consistent dynamical mean field theory (DMFT) is employed via the EDMFT package, which implements a combined DFT and DMFT derived from the stationary Luttinger-Ward functional. Here, the exact double-counting of DFT and DMFT and Coulomb interaction are well treated and the Green’s function is determined self-consistently. In strongly correlated systems, DFT+DMFT has been successful in detailing a lot of important results. In the DMFT section, the non-interacting Hamiltonian is added with the Coulomb interaction term, $H_{\text{int}}$, to incorporate the effects of correlated Fe-3d orbitals and also a self energy functional, $\Sigma_{\text{dc}}$ to take care of the double counting. The total Hamiltonian, except the $\Sigma_{\text{dc}}$ term is expressed as,

$$H = \sum_{k,a,\sigma} \epsilon_{k,a} c_{k,a,\sigma}^\dagger c_{k,a,\sigma} + U \sum_{i,a} n_{i\sigma} n_{i\bar{\sigma}} + \text{...}$$
\[ U' \sum_{i,a,b,\sigma,\sigma'} n_{i\alpha\sigma} n_{i\beta\sigma'} - J_H \sum_{i,a,b} S_{i\alpha} S_{i\beta} \]  

where \( \epsilon_{k,a} \) is the band dispersion which includes the effects of SOC, \( \sigma \) stands for up and down spins and \( U \) and \( U' \) are the intra- and inter-orbital Coulomb interaction terms between electrons with opposite spins in the same orbital and between electrons with parallel spins in different orbitals respectively, and \( J_H \) is the Hunds coupling. The inter-orbital term \( (U') \) is reduced by the ferromagnetic coupling due to Hunds first rule that favors the alignment of spins. We also have a relationship between different energy scales, namely, \( U, U' \) and \( J_H \) given by, \( U' = U - 2J_H \). In our work we have considered \( J_H = 1.25 \) eV (reasonable for Fe-3d bands) and varied \( U \) over a realistic range.

Finally the total Hamiltonian is solved using the DMFT method. The correlated five Fe-3d orbitals are treated dynamically within the DMFT based on orbital projection-embedding scheme accomplished via the EDMFT package, while the Bi and Se-p orbitals are treated at the DFT level. The impurity solver used in the DMFT code is the continuous time quantum Monte Carlo (CT-QMC) in the hybridization expansion method. The parameters, namely, the Coulomb interaction \( U \), Hund’s coupling, \( (J_H) \) and the inverse temperature, \( \beta = 1/k_B T \) are varied within an experimentally realizable range to get \( T \) and \( U \) dependence of the intercalated system. The DFT+DMFT calculations are converged up to precision of 0.0001 with respect to the charge density, the chemical potential and the self energy with considering step over \( E \) as \( 10^{-6} \). Finally the maximum entropy method is used for the analytical continuation of the self-energy from the imaginary axis to real frequencies with an auxiliary Green’s function. Then from the real frequency Green’s function, the momentum-resolved spectral functions and the density of states are obtained. To check the stability and accuracy of the result we have used Pade approximation in addition to the maximum entropy method used in the EDMFTF package.

III. RESULTS AND DISCUSSION

We have considered Fe intercalation in between two quintuple layers of Bi₂Se₃, a situation that is energetically more favorable. In each of the quintuple layer, the hexagonal atomic planes are arranged following the sequence of Se1-Bi-Se2-Bi-Se1 along the \( z \)-direction with covalent bonding between the atoms, and the Se1 and Se2 atoms stand for two inequivalent Selenium atoms. So the intercalated Fe atom will be in the environment of a Se1 atom. First we study the change in the band structure of Bi₂Se₃ due to the intercalation by Fe (see Fig.1c).

The validity of the EDMFT package is well established. Moreover our calculated results, such as the momentum resolved spectral function and the magnetic order are consistent with the earlier iron doped Bi₂Se₃ results. We also present DMFT one particle spectrum for Cu intercalated Bi₂Se₃ which shows good agreement with the earlier experiments (zero energy peak in the density of states). Since a Fe-based system consists of unfilled 3d-orbitals and possesses different values of the Coulomb interaction, we varied it within a reasonable range, and determined the final values of \( U \) and \( J_H \) for the system (considering earlier experimental results), which are found as 5.5 eV and 1.25 eV respectively. Large values of \( U \), that is, strong electronic correlations renormalize the spectral function considerably. The total density of states of an intercalated Bi₂Se₃ is presented in Fig.3 for different values of \( U \). In comparison with the DFT DOS, the correlated electronic spectra from the DMFT are very distinct, indicating that this system is a correlated bad metal. It is observed that, the spectral weight at the Fermi level, \( E_F \) reduces with increasing \( U \). The Fe intercalation leads to an abrupt change of the electronic structure and the 3d orbitals of the Fe atom dominate the low-energy properties of the compound (Fig.2). This is in contrast with Fe-doped Bi₂Se₃ which shows an insulating behaviour, and instead here we get bad metal. Further, we obtain the temperature dependence of the DOS, by employing a different value of \( \beta \) in the EDMFTF. This yields that with decreasing temperature, the total spectral weight of the 50K, the \( d_x^2 \) and \( d_{x^2-y^2} \) orbitals undergo an orbital selective metal-insulator transition as shown in Fig.4a. The orbital selectivity is confirmed from the divergence of \( \text{Im} \Sigma(\omega) \) at the Fermi level for the \( d_x^2 \) and \( d_{x^2-y^2} \) orbitals, while the other orbitals provide support for metallic features at low energies. This orbital selectivity at 50K can be related to the onset of a possible magnetic order, as also corroborated by the magnetic susceptibility plot (Fig.4b). The right inset of Fig.4a shows \( \text{Im} \Sigma(\omega) \) at 100 K which reveals non-Fermi liquid features due to high \( T \), while the left inset of Fig.4a depicts the resitiv-
Density data at low temperatures, which shows proportionality to $T$ with a change of slope around 50 K. Change of slope around 50 K in resistivity further confirms an ordering transition to occur. This ordering transition is also coherence restoring transition because resistivity decreases at lower $T$. The transport observation also goes hand in hand with our prediction of a paramagnetic to a ferromagnetic transition, while the paramagnetic order can be considered as fluctuation of magnetic moments at high $T$. The observation of orbital selectivity and related magnetic order in Fe-intercalated systems is not surprising and can be argued to have originated from moderate $U'$ ($U'$ being the inter-orbital Coulomb repulsion) which leads to a selective Mottness in the multi-band situation. Interestingly, stabilization of the magnetic order enhances selective Mott features at low temperatures as a zero energy pole emerges in the $\text{Im} \Sigma(\omega)$ ($d_{z^2}$ and $d_{x^2-y^2}$, along with small mass enhancement in $\text{Re} \Sigma(\omega)$ of three other d-orbitals.

Next we present angle resolved photoemission spectra of Fe intercalated Bi$_2$Se$_3$ in Fig.5a and Fig.5b. In contrast to the conventional DFT band structure results, it shows pronounced renormalized effects in the band structures owing to strong electronic correlations. The characteristic Dirac-like dispersion manifests above the Fermi level at the $\Gamma$ point for both low (50 K) and high (200 K) temperatures. Near the Fermi level (FL), two bands cross the FL along the $K - \Gamma - M$ direction. Further at the lower temperature (that is, 50 K), the lower band sinks below the FL signaling a transition from a hole pocket to an electron pocket in the $\Gamma - K$ and $\Gamma - M$ directions. In comparison with the DFT band structure results, the DMFT momentum resolved spectra indicate a correlation driven Lifshitz transition. It may also be noted that in this study, the intercalation density is 10% (we have examined other (lower) densities, although not presented here), as this scenario seems to be ideal for observing a magnetic phase transition. Our results also indicate emergence of small electron pockets around these two directions (namely, $\Gamma - K$ and $\Gamma - M$), which is further confirmed by the DMFT Fermi surface (FS) results (see
change, that is, from five electron pockets, it becomes
the FS topology shows a sizeable
point and hole pockets around the
Both the results reveal presence of electron pockets
and the DMFT FS (Fig.6) are shown here for compari-
deserves to be investigated. Both the DFT FS (Fig.1b)
correlations is already described above, the DMFT FS
Fermi surface map reveals connection between ordering
Emergence of new pockets in the Brillouin zone edge is evi-
dent, whereas none of the electron pockets around the Γ point
disappear.

Further to address intercalation dependent changes we
calculate the DMFT FS at two different temperatures
(namely, 50 K and 200 K). Combined with intercalation
dependent evolution of the electronic structure, the
Fermi surface map reveals connection between ordering
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tion being considered, the FS topology shows a sizeable
change, that is, from five electron pockets, it becomes
three electron pockets at 50 K and finally a one electron
pocket at 200 K around the Γ point. On the other hand,
the hole pockets around the K and M points also undergo
significant modification. We strongly believe that these
modifications arise due to orbital dependent electronic
structure reconstruction and essentially driving the sys-
tem into a magnetically ordered phase.

To capture the nature of magnetic ordering by elec-
tronic correlations, we have calculated the temperature
variation of the magnetic susceptibility and the moment
from the EDMFT package. In Fig.4b we show the tem-
perature dependence of the magnetic susceptibility, χ
and the inset contains the variation of the magnetic
moment, m with temperature. The parent compound
Bi$_2$Se$_3$ possesses a weak diamagnetic character with al-
most no temperature dependence, while Fe intercalation
makes the compound magnetic. The magnetic nature is
confirmed to be ferromagnetic as χ shows a Curie be-
haviour with χ ∼ (T − Tc)$^{-1}$, with Tc as the Curie tem-
perature. We have observed Tc ∼ 30K. Moreover we
have calculated the spin gap energy (denoted by the en-
ergy difference between the ferromagnetic and the weakly
diamagnetic state), which reveals that the ferromagnetic
state is more energetically stable. In Fe-Bi$_2$Se$_3$ system,
the magnetic moments of Fe is about 3.5µ$_B$ and the other
atoms have smaller magnetic moments (of about 0.001-
0.01µ$_B$) which align antiparallelly with the moments of
the Fe atom. The system turns out to be magnetic with
a value for the magnetic moment as 3.4µ$_B$. The spin
up and spin down states are partially filled with a occu-
pation difference between them resulting in a magnetic
moment which is almost totally contributed by the Fe-3d
orbitals and the relevant electronic correlations.

In conclusion, the electronic correlations along with a
reasonable spin-orbit coupling in Fe intercalated Bi$_2$Se$_3$
have been examined employing the DFT+DMFT method
executed with the CT-QMC impurity solver. A strong
correlation-driven electronic structure modification ac-
companied by a Lifshitz transition is found in the in-
tercalated compound, indicating an ordered phase to set
in at lower temperatures, which is significantly different
than the parent compound. Both the electronic correla-
tions and the spin-orbit coupling play major roles in the
electronic structure and transport properties of interca-
lated compound. These generate tiny electron pockets
around the Γ − K and the Γ − M directions. Our results
are somewhat similar to the Fe-doped (not intercalated)
Bi$_2$Se$_3$ compound, in the sense that it also shows differ-
ent type of magnetic ordering with doping concentration
and temperature. All these results are new in liter-
ature and subject to further experimental study. The
results mainly demonstrate many-body characteristics,
such as many-body self-energy, spectral weight, presence
of quasiparticles near the Fermi level, and a strong renor-
malization of the effective masses. Further explorations
of the low temperature properties and other intercalation
densities need to be undertaken in near future. Moreover
increased Tc due to intercalation can lead to potential ap-
Fig.6) discussed below.

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densities need to be undertaken in near future. Moreover
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Applications in the context of spintronic devices and energy storage materials\textsuperscript{32–35}. Our studies suggest that the Fe-intercalated Bi$_2$Se$_3$ could be an ideal system to identify the role of electronic correlations and spin-orbit coupling in magnetism of iron-based materials.

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