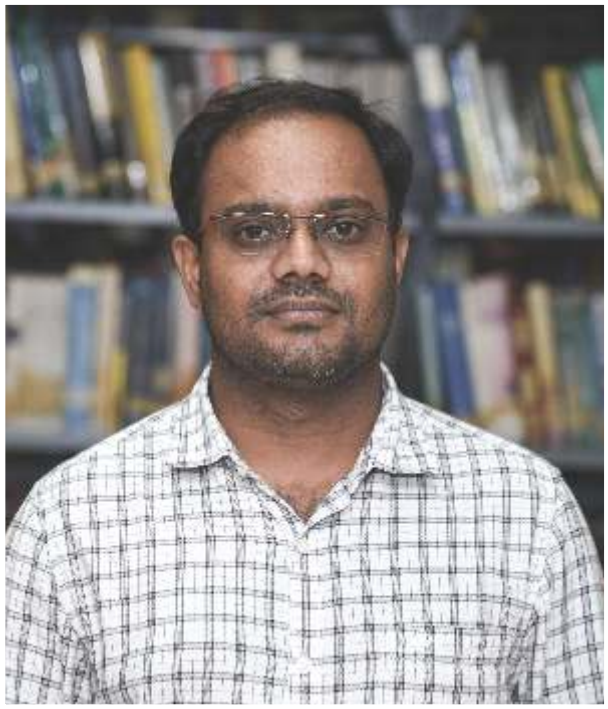


Thirupathaiah Setti

Assistant Professor
CMPMS
setti@bose.res.in

Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Indrani Kar; Transition metal dichalcogenides; Under progress
2. Susmita Changdar; Topological semimetals; Under progress
3. Achintya Low; Quantum Spin Liquids; Under progress
4. Sayan Routh; Topological Superconductors; Under progress; Prof. Prasenjit Singha Deo (Supervisor)
5. Shubham Purwar; 2D Magnetism; Under progress
6. Susanta Ghosh; Topological Quantum Materials; Under progress

b) Post-Docs

1. Ayana Mukhopadhyay; Synthesis and characterisation of 2D magnetic single crystals
2. Reena Goyal; Synthesis and characterisation of single crystals of the high Tc superconductors

Teaching

1. Autumn semester; Condensed Matter Physics-PHY302; Integrated PhD; 16 students; with 1 (Prof. Tanusri Saha-Dasgupta,) co-teacher
2. Spring semester; Lab Course: PHY391; Integrated PhD; 12 students; with 4 (Prof. Kalyan Mandal, Prof. Rajib K Mitra, Dr. Manik Pradhan and Dr. Ramkrishna Das) co-teachers

Publications

a) In journals

1. Indrani Kar, Joydeep Chatterjee, Luminita Harnagea, Y. Kushnirenko, A. V. Fedorov, Deepika Shrivastava, B. Büchner, **P. Mahadevan** and **S. Thirupathaiah**, *Metal-chalcogen bond-length induced electronic phase transition from semiconductor to topological semimetal in ZrX_2 (X = Se and Te)*, Physical review B, 101, 165122, 2020
2. Susmita Changdar, S. Aswartham, Anumita Bose, Y. Kushnirenko, G. Shipunov, N. C. Plumb, M. Shi, Awadhesh Narayan, B. Büchner, and **S. Thirupathaiah**, *Electronic structure studies of FeSi: A chiral topological system*, Physical Review B, 101, 235105, 2020
3. **S. Thirupathaiah**, Y. S. Kushnirenk, K. Koepernik, B. R. Piening, B. Buechner, S. Aswartham, J. van den Brink, S. V. Borisenko, I. C. Fulga, *Sixfold fermion near the Fermi level in cubic $PtBi_2$*, SciPost Physics, 10, 004, 2021
4. Indrani Kar, Kapildeb Dolui, Luminita Harnagea, Yevhen Kushnirenko, Grigory Shipunov, Nicholas C. Plumb, Ming Shi, Bernd Büchner, and **Setti Thirupathaiah**, *Experimental Evidence of a Stable 2H Phase on the Surface of Layered 1T -$TaTe_2$*, The Journal of Physical Chemistry C, 125, 1150-1156, 2021

b) Conference proceedings / Reports / Monographs / Books

1. Observation of surface Dirac state in transition metal dichalcogenide NiTe2 using ARPES, Indrani Kar, Luminita Harnagea, Soma Banik, Surjeet Singh, and Setti Thirupathaiah, AIP Conference Proceedings 2265, 030361 (2020).
2. Angle Resolved Photoemission Spectroscopy Study on Electronic Band Structure of Topological Insulator Bi2Se3 in the Presence of Magnetic Impurities, Susmita Changdar, Rabia Sultana, Soma Banik, V. P. S. Awana, and Setti Thirupathaiah, AIP Conference Proceedings 2265, 030355 (2020).

Talks / Seminars Delivered in reputed conference / institutions

1. Annual Conference on Quantum Condensed Matter (QMAT 2020); Sep 10, 2020; SNBNCBS; 7th to 11th Sept. 2020
2. C. K. Majumdar Memorial Workshop 2020; Dec 31, 2020; SNBNCBS; 28th Dec. 2020 to 4th Jan. 2021

Extramural Projects (DST, CSIR, DAE, UNDP, etc.)

1. Startup Research Grants; DST-SERB; 12/2020 to 12/2022; PI

Conference / Symposia / Schools organized

1. Annual Conference on Quantum Condensed Matter (QMAT 2020); Dec 28, 2020; SNBNCBS; 28th Dec. 2020 to 4th Jan. 2021

Scientific collaborations with other national / international institutions (based on joint publications)

1. SNBNCBS; Lab Course: PHY391; National
2. IISER Pune; Sl. No. 1, 4, and Conf. Paper 1; National
3. SSCU, IISc.; Synthesis and characterisation of 2D magnetic single crystals; National
4. NPL, Delhi; Conf. Paper 2; National
5. RRCAT, Indore; Conf. Paper 1 and 2; National
6. IFW Dresden, Germany; Sl. No. 1-4; International
7. University of Delaware, New York; 28th Dec. 2020 to 4th Jan. 2021; International
8. SLS, PSI, Switzerland; Sl. No. 1, 2 and 4; International

Areas of Research

Synthesis, Structural, Physical Properties, and Electronic Structure Studies of Quantum Materials

1. Electronic Structure Studies of FeSi: A Chiral Topological System [Susmita Changdar *et al.*, PRB 101, 235105 (2020)]

Most recent observation of topological Fermi arcs on the surface of manyfold degenerate B20 systems, CoSi and RhSi, have attracted enormous research interests. Although another isostructural system, FeSi, has been predicted to show bulk chiral fermions, it is yet to be clear theoretically and as well experimentally that whether FeSi possesses the topological surface Fermi arcs associated with the exotic chiral fermions in vicinity of the Fermi level. In this contribution, using angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT), we present the low-energy electronic structure of FeSi. We further report the surface state calculations to provide insights into the surface band structure of FeSi near the Fermi level. Unlike in CoSi or RhSi, FeSi has no topological Fermi arcs near the Fermi level as confirmed both from ARPES and surface state calculations. Further, the ARPES data show spin-orbit coupling (SOC) band splitting of 40 meV, which is in good agreement with bulk band structure calculations. We noticed an anomalous temperature dependent resistivity in FeSi which can be understood through the electron-phonon interactions as we find a Debye energy of 80 meV from the ARPES data.

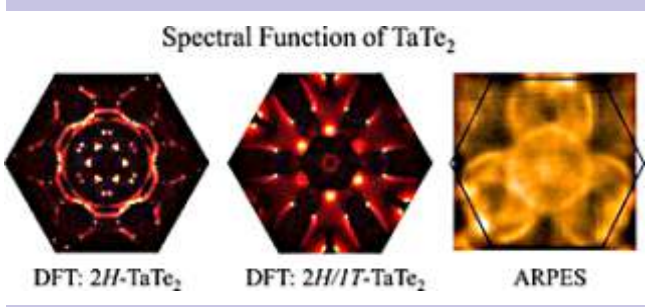
2. Metal-chalcogen bond-length induced electronic phase transition from semiconductor to topological semimetal in ZrX_2 (X = Se and Te) [Indrani Kar *et al.*, Phys. Rev. B 101, 165122 (2020)]

Using angle resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations

we studied the low-energy electronic structure of bulk $ZrTe_2$. ARPES studies on $ZrTe_2$ demonstrate free charge carriers at the Fermi level, which is further confirmed by the DFT calculations. An equal number of hole and electron carrier density estimated from the ARPES data, points $ZrTe_2$ to a semimetal. The DFT calculations further suggest a band inversion between Te *p* and Zr *d* states at the point, hinting at the non-trivial band topology in $ZrTe_2$. Thus, our studies for the first time unambiguously demonstrate that $ZrTe_2$ is a topological semimetal. Also, a comparative band structure study is done on $ZrSe_2$ which shows a semiconducting nature of the electronic structure with an indirect band gap of 0.9 eV between (*A*) and *M*(*L*) high symmetry points. In the below we show that the metal-chalcogen bond-length plays a critical role in the electronic phase transition from semiconductor to a topological semimetal ingoing from $ZrSe_2$ to $ZrTe_2$.

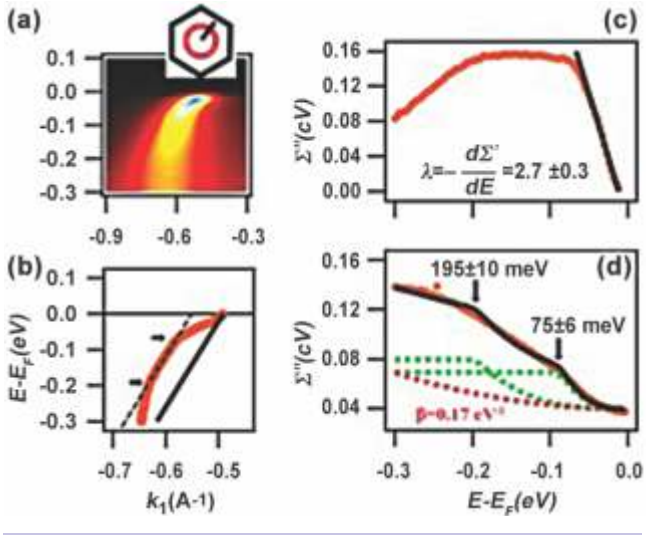
3. Experimental Evidence of a Stable 2H Phase on the Surface of Layered 1T′-$TaTe_2$ [Indrani Kar *et al.*, J. Phys. Chem. C 125, 1, 1150 (2021)]

The low-energy electronic structure of 1*T* -$TaTe_2$ is studied using high-resolution angle-resolved photoemission spectroscopy (ARPES) and density functional theory calculations. We observe that the Fermi surface of 1*T* -$TaTe_2$ is in the hexagonal symmetry, which is in contradiction to its monoclinic crystal structure. We observe a totally different electronic structure of $TaTe_2$ when compared with the isostructural compound $NbTe_2$. Further, despite being in the hexagonal symmetry, the Fermi surface topology of $TaTe_2$ is quite different when compared to the isovalent compounds $TaSe_2$ and TaS_2. To fully understand the experimentally obtained electronic band structure of $TaTe_2$, we disentangled the surface states from the bulk with the help of slab calculations. Thus, we realize that the surface states resemble the 2*H* phase electronic structure, while the bulk states replicate the 1*T* phase electronic structure of $TaTe_2$. This is an interesting discovery as $TaTe_2$ does exist neither in the 1*T* phase nor in the 2*H* phase as per the observation of the crystal structure. We further notice that the 1*T* phase electronic structure shows substantial band dispersion in the k_z direction. We realize that the band structure of $TaTe_2$ is temperature independent above and below the CDW transition temperature.



4. Anomalous band renormalization due to high energy kink in the colossal thermoelectric material $K_{0.65}RhO_2$ [Susmita Changdar et al., arXiv:2007.02016v1 (2020)]

We report on low-energy electronic structure and electronic correlations of $K_{0.65}RhO_2$, studied using high-resolution angle-resolved photoemission spectroscopy (ARPES) technique and density functional theory (DFT) calculations. We observe a highly correlated hole pocket on the Fermi surface. We further notice that the correlations are momentum dependent. Most importantly, two kinks at binding energies of 75 meV and 195 meV have been observed from the band dispersion in the vicinity of the Fermi level. While the low energy kink at 75 meV can be understood as a result of the electron-phonon interaction, the presence of high energy kink at 195 meV is totally a new discovery of this system leading to an anomalous band renormalization. Based on systematic analysis of our experimental data, we propose high frequency bosonic excitations as a plausible origin of the high energy anomaly. Further, we notice that the high energy anomaly has important implications in obtaining the colossal thermoelectric power of $K_{0.65}RhO_2$.



Plan of Future Work Including Project

1. Since the discovery of chiral magnetic and topological properties in Mn3X systems, several research groups have been trying to understand the electronic, physical and structural properties of these systems for their technological applications in topological spintronics and quantum computations. However, to date, very few studies are available on these systems. Especially, the so-far existing studies are limited to the structural and electronic properties of the pristine Mn3Sn, Mn3Ge, Mn3Pt and Mn3Ir systems. Some of these studies suggest interesting magnetic properties of Mn3Sn systems that a magnetic phase change as a function of temperature. That means, at around 275 K a magnetic transition from non-collinear antiferromagnetic phase to a spiral magnetic structure and below 50 K the system becomes to be a spin glass. Such magnetic transitions are expected to reflect in the electronic band structure and physical properties as well. It is further anticipated that the magnetic reorientation generates a gap at the band crossing Weyl point below the transition temperature due to the time-reversal symmetry. Experimental studies in this direction are not done so far. Thus, we recently had grown the single crystals of (Mn1-xFex)3Sn (x = 0, 0.03, 0.05, and 0.1) systems and will be performing thorough physical and electronic properties studies of these systems for the next one year.