Tanusri Saha Dasgupta

Senior Professor & Director (Additional Charge)
CMPMS
tanusri@bose.res.in

Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Shreya Das; Correlated Electrons; Under progress; Tanusri Saha-Dasgupta
2. Edwine Tandong; Soft Matter; Under progress; Tanusri Saha-Dasgupta and Jaydeb Chakrabarti
3. Shiladitya Karmakar; Application Materials; Under progress; Tanusri Saha-Dasgupta
4. Samir Rom; Electronic Structure of Complex Materials; Under progress; Tanusri Saha-Dasgupta
5. Aishwaryo Ghosh; Application of Machine Learing to Materials Science; Under progress; Tanusri Saha-Dasgupta
6. Koushik Pradhan; Spin-orbit materials; Under progress; Tanusri Saha-Dasgupta
7. Manoj Gupta; Toplogical compounds; Under progress; Tanusri Saha-Dasgupta
8. Rajdeep Biswas; 2D Materials; Under progress; Tanusri Saha-Dasgupta

b) Post-Docs

1. Tanmoy Pal; Battery Materials
2. Dipayan Sen; Hybrid perovskites
3. Soumendu Datta; Alloy nanoclusters

c) External Project Students / Summer Training

1. Arnab Paul; Magnetism in Hubbard Model
2. Soham Mukherjee; 2D magnetism

Teaching

1. Autumn semester; Advanced Condensed Matter Physics; PhD; 5 students; Yes with Manoranjan Kumar (co-teachers)
2. Spring semester; Advanced Condensed Matter Physics; Integrated PhD; 12 students; Yes with Thirupathaiah Setti (co-teachers)

Publications

a) In journals

1. Rafikul Ali Saha, Anita Halder, **Tanusri Saha-Dasgupta**, Desheng Fu, Mitsuru Itoh, and Sugata Ray, *Covalency driven modulation of paramagnetism and development of lone pair ferroelectricity in multiferroic* $Pb_3TeMn_3P_2O_{14}$, Physical Review B, 101, 180406(R), 2020
2. Shreya Das, Anita Halder, Atasi Chakraborty, Indra Dasgupta, and **Tanusri Saha-Dasgupta**, *Understanding the curious magnetic state of* Sr_3OsO_6, Physical Review B, 101, 184422, 2020
3. Santu Baidya, Aabhaas Vineet Mallik, Subhro Bhattacharjee, and **Tanusri Saha-Dasgupta**, *Interplay of Magnetism and Topological Superconductivity in Bilayer Kagome Metals*, Physical Review Letters, 125, 026401, 2020
4. Dipayan Sen, Gour Jana, Nitin Kaushal, Anamitra Mukherjee, and **Tanusri Saha-Dasgupta**, *Intrinsic ferromagnetism in atomically thin two-*

dimensional organic-inorganic van der Waals crystals, Physical Review B, 102, 054411, 2020

5. Priyo Adhikary, Subhadeep Bandyopadhyay, Tanmoy Das, Indra Dasgupta, and **Tanusri Saha-Dasgupta**, *Orbital-selective superconductivity in a two-band model of infinite-layer nickelates*, Physical Review B, 102, 100501(R), 2020
6. Anita Halder, Samir Rom, Aishwaryo Ghosh and **Tanusri Saha-Dasgupta**, *Prediction of the Properties of the Rare-Earth Magnets* $Ce_2Fe_{17-x}Co_xCN$*: A Combined Machine-Learning and Ab Initio Study*, Physical Review Applied, 14, 034024, 2020
7. Essam M. Hussein, Nizar El Guesmi, Ziad Moussa, Uttam Pal, Samir K. Pal, **Tanusri Saha Dasgupta**, and Saleh A. Ahmed, *Unprecedented Regio- and Stereoselective Synthesis of Pyrene-Grafted Dispiro[indoline-3,2 -pyrrolidine-3 ,3 -indolines]: Expedient Experimental and Theoretical Insights into Polar [3 + 2] Cycloaddition*, ACS Omega, 5, 24081-24094, 2020
8. N. Roy, A. Chakrabarty, B.Koley, **T.Saha-Dasgupta** and Partha P.Jana, *Site preference and atomic ordering in the structure of* In_3Pd_5*: A theoretical study*, Journal of Solid State Chemistry, 290, 121567, 2020
9. Swati Rani, Damayanti Bagchi, Uttam Pal, Mamta Kumari, Manisha Sharma, Arpan Bera, Javaid Shabir, Samir Kumar Pal, **Tanusri Saha-Dasgupta**, and Subho Mozumdar, *The Role of Imidazolium-Based Surface-Active Ionic Liquid to Restrain the Excited-State Intramolecular H-Atom Transfer Dynamics of Medicinal Pigment Curcumin: A Theoretical and Experimental Approach*, ACS Omega, 5, 25582 – 25592, 2020
10. A. Koshelev, L. Shvanskaya, O. Volkova, K. Zakharov, F. Theuss, C. Koo, R. Klingeler, S. Kamusella, H.-H. Klauss, S. Kundu, S. Bachhar, A. V. Mahajan, P. Khuntia, D. Khanam, B. Rahaman, **T. Saha-Dasgupta** and A. Vasiliev, *Thermodynamic and resonant properties of mixed spin compounds* $ACuFe_2(VO_4)_3$ *(A = Li, Na)*, Journal of Alloys and Compounds, 842, 155763, 2020
11. Debankur Das, Jürgen Horbach, Peter Sollich, **Tanusri Saha-Dasgupta**, and Surajit Sengupta, *Wrinkles, folds, and ripplocations: Unusual deformation structures of confined elastic sheets at nonzero temperatures*, Physical Review Research, 2, 043284, 2020
12. E. S. Kozlyakova, K. N. Denisova, A. A. Eliseev, A. V. Moskin, A. Y. Akhrorov, P. S. Berdonosov, V. A. Dolgikh, B. Rahaman, S. Das, **T. Saha-Dasgupta**, P. Lemmens, A. N. Vasiliev, and O. S. Volkova, *Short-range and long-range magnetic order in Fe* $(Te_{1.5}Se_{0.5})O_5Cl$, Physical Review B, 102, 214405, 2020
13. Subhadeep Bandyopadhyay, Priyo Adhikary, Tanmoy Das, Indra Dasgupta, and **Tanusri Saha-Dasgupta**, *Superconductivity in infinite-layer nickelates: Role of f orbitals*, Physical Review B 102, 220502(R), 2020
14. Basant Roondhe, Vaishali Sharm, Hardik L. Kagdada, Dheeraj K. Singh, **Tanusri Saha Dasgupta** and Rajeev Ahuja, *Enhancing the electronic and phonon transport properties of two-dimensional hexagonal boron nitride through oxygenation: A first principles study*, Applied Surface Science, 533, 147513, 2020
15. Shiladitya Karmakar and **Tanusri Saha-Dasgupta**, *First-principles prediction of enhanced thermoelectric properties of double transition metal MXenes:* $Ti_{3-x}Mo_xC_2T_2$*;* $(x = 0.5, 1, 1.5, 2, 2.5, T = -OH/-O/-F)$, Physical Review Materials, 4, 124007, 2020
16. **Tanusri Saha-Dasgupta**, *The Fascinating World of Low-Dimensional Quantum Spin Systems: Ab Initio Modeling*, Molecules, 26(6), 1522, 2021
17. Swastika Chatterjee, Sujoy Ghosh and **Tanusri Saha-Dasgupta**, *Ni Doping: A Viable Route to Make Body-Centered-Cubic Fe Stable at Earth's Inner Core*, Minerals, 11, 258, 2021
18. Rafikul Ali Saha, Anita Halder, Desheng Fu, Mitsuru Itoh, **Tanusri Saha-Dasgupta** and Sugata Ray, *The Critical Role of Stereochemically Active Lone Pair in Introducing High Temperature Ferroelectricity*, Inorganic Chemistry, 60, 4068 – 4075, 2021

19. Aniruddha Adhikari, Susmita Mondal, Monojit Das, Pritam Biswas, Uttam Pal, Soumendra Darbar, Siddhartha Sankar Bhattacharya, Debasish Pal, **Tanusri Saha Dasgupta**, Anjan Kumar Das, Asim Kumar Mallick and **Samir Kumar Pal**, *Incorporation of a Biocompatible Nanozyme in Cellular Antioxidant Enzyme Cascade Reverses Huntington's Like Disorder in Preclinical Model*, Advanced Healthcare Materials, 10, 2001736, 2021

Talks / Seminars Delivered in reputed conference / institutions

1. ICTS web seminar; Jun 2, 2020; ICTS Bangalore; 1 hour
2. Physics Symposium (Online); Dec 3, 2020; IIT Delhi; 1 hour
3. PRL colloquium; Mar 17, 2021; PRL Ahmedabad; 1 hour
4. Third International Conference on Current Trends in Materials Science and Engineering 2021(CTMSE 2021); Mar 13, 2021; Institute of Engineering & Management, Kolkata; 1 hour
5. National Level Lecture Workshop in Frontiers in Science and Engineering by Women in Science; Feb 9, 2021; Deen Dayal Upadhyaya College; 1 hour
6. Nakshatra Talks: 'Women in Science - Breaking the Glass Ceiling'; Mar 7, 2021; Bennett University; 1 hour

Administrative duties

1. Dean (Academic), Director (Additional charge)

Patents Taken and Process Developed with Details

1. Patent Appl.No.202031038150 dated 04.09.2020 on "Development of Tribo-electroceutical Fabric for Potential Application in Self Sanitizing Personal Protective Equipment (PPE)"; Applied
2. Patent Appl.No.202031038152 dated 04.09.2020 on "A Nanoceutical Fabric for source control to prevent COVID-19 spread including through expelled respiratory droplets"; Applied

Awards, Recognitions

1. J. C. Bose National Professor; Adjunct Professor of IISER Kolkata, Vice president of Indian Physics Association

Membership of Learned Societies

1. American Physical Society, Indian Physics Association

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

1. J.C.Bose Fellowship; SERB; 5 years; PI
2. TRC; DST; 5 years; PI

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

1. Subhro Bhattacharjee, ICTS, Bangalore, Joint publication, Serial 3; National
2. Indra Dasgupta, IACS, Joint publication, Serial 5, 13; National
3. Tanmoy Das, IISc, Joint publication, Serial 5, 13; National
4. A. Vasiliev, Moscow State University, Joint publication, Serial 10, 12; International
5. S. K. Pal, SNBNCBS, Joint publication, Serial 7, 9, 19; National
6. Surajit Sengupta, TIFR Hyderabad, Joint publication, Serial 11; National
7. R. Ahuja, Uppsala University, Joint publication, Serial 14; International
8. Swastika Chatterjee, IISER Kolkata, Joint publicatiom, Serial 17; National
9. Sujoy Ghosh, IIT KGP, Joint publication, Serial 17; National

Outreach program organized / participated

1. Participated in outreach program on popularization of Science in Bennett University and Pabna University, Bangladesh

Areas of Research

Computational Condensed Matter and Materials Physics

Interplay of Magnetism and Topological Superconductivity in Bilayer Kagome Metals

The binary intermetallic materials, M_3Sn_2 (M = 3d transition metal) present a new class of strongly correlated systems that naturally allows for the interplay of magnetism and metallicity. Using first principles calculations we confirm that bulk Fe_3Sn_2 is a ferromagnetic metal, and show that M = Ni and Cu are paramagnetic metals with nontrivial band structures. Focusing on Fe_3Sn_2 to understand the effect of enhanced correlations in an experimentally relevant atomistically thin single kagome bilayer, our *ab initio* results show that dimensional confinement naturally exposes the flatness of band structure associated with the bilayer kagome geometry in a resultant ferromagnetic Chern metal. We use a multistage minimal modeling of the magnetic bands progressively closer to the Fermi energy. This effectively captures the physics of the Chern metal with a nonzero anomalous Hall response over a material relevant parameter regime along with a possible superconducting instability of the spin-polarized band resulting in a topological superconductor. (Phys. Rev. Lett. **125**, 026401)

Orbital-Selective Superconductivity in infinite-layer Nickelates: Role of nonzero *f*-ness

We propose a first-principles derived low-energy model Hamiltonian in infinite-layer nickelate compounds, consisting of two orbitals: Ni x2-y2, and an axial orbital. The axial orbital is constructed out of A-site d, Ni 3z2-r2, and Ni-s characters. Calculation of the superconducting pairing symmetry and pairing eigenvalue of the spin-fluctuation mediated pairing interaction underlines the crucial role of the interorbital Hubbard interaction in

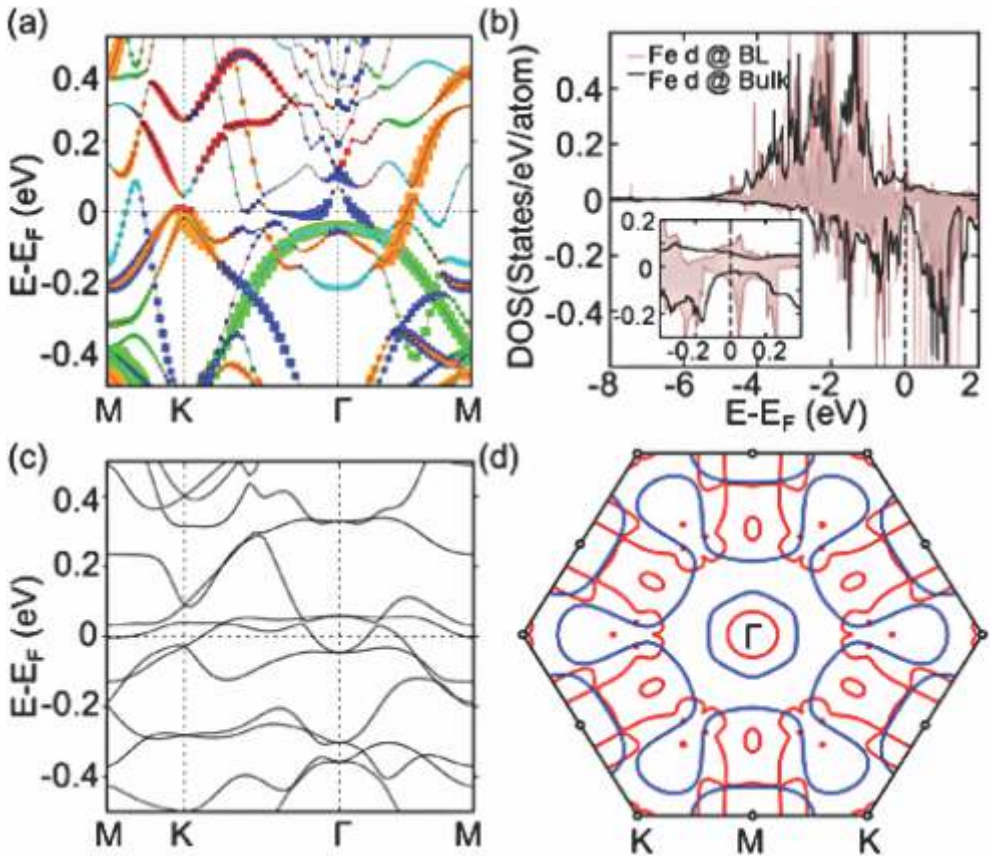

Figure 1: Calculated Band structure (a), Density of states (b) + (c), and Fermi surface of bilayer of Fe_3Sn_2 (see Phys. Rev. Lett. 125, 026401 for details)

superconductivity, which turns out to be orbital selective.The axial orbital brings in material dependence to the problem, making $LaNiO_2$ different from $NdNiO_2$ or $PrNiO_2$, thereby controlling the interorbital Hubbard interaction-assisted superconductivity (Phys. Rev. B **102**, 100501(R); Phys. Rev. B **102**, 220502(R))

Plan of Future Work Including Project

1. i) Application of machine learning for battery materials ii) Segregation trend in alloyed nanoclusters iii) Construction of force field for 2D materials iv) 2D magnets v) Oxide heterostructures vi) Spin liquids

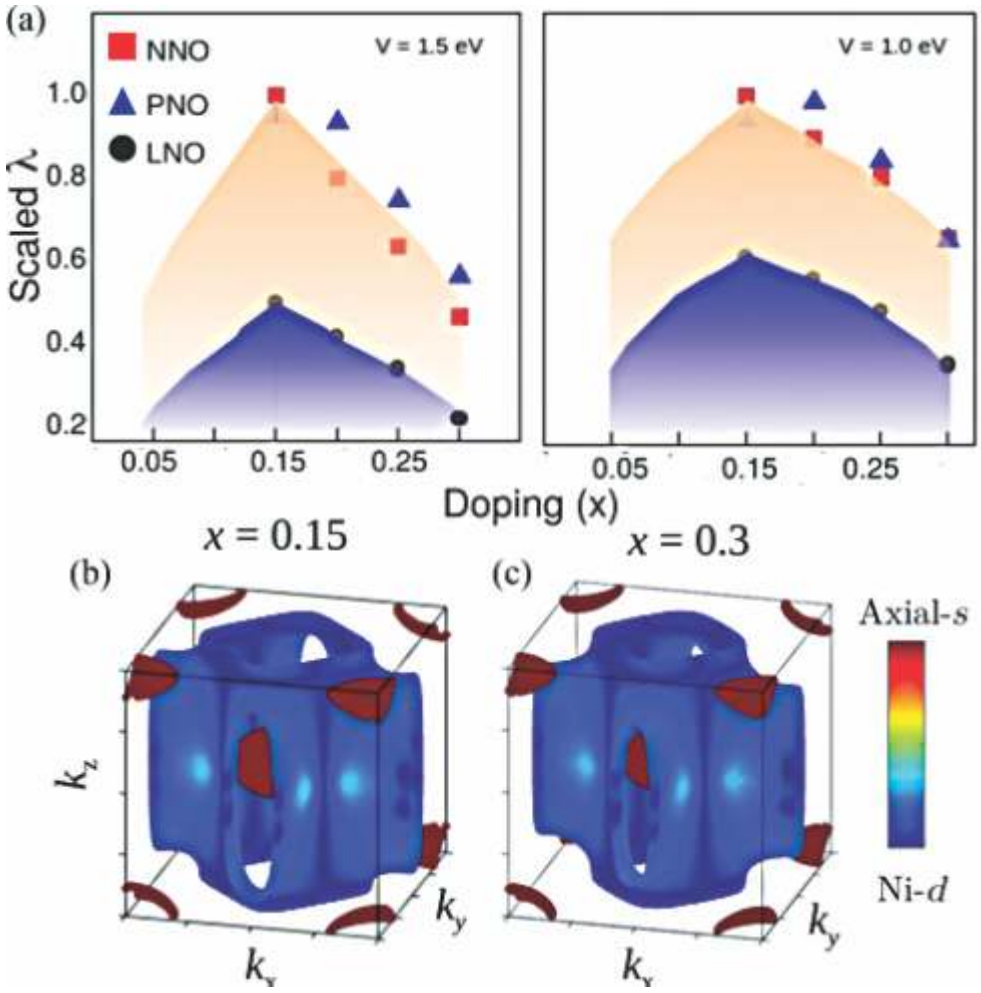

Figure 2: Calculated superconducting phase diagram (a) and Fermi surfaces for nickelate compounds.