Tanusri Saha-Dasgupta

Senior Professor
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Professor Tanusri Saha-Dasgupta is a Computational Condensed Matter Physicist interested in novel materials properties both in bulk and in nanoscale.

Supervision of Research / Students

Ph.D. Students

1. Kartik Samanta; First principle study on Transition Metal compound using Density Functional Theory (DFT); Completed, to be submitted in July 2017.
2. Hrishit Banerjee; Electronic Structure Study of Organic and Inorganic complexes; Ongoing.
3. Dhani Nafday; Electronic Structure of graphene and related materials; Ongoing.
4. Ransell D'souza; First-principles Study of 2D materials; Ongoing.
5. Paulomi Chakraborty; Mechanical and Electronic Properties of Technological Important Materials; Ongoing.
6. Anita Haldar; Study and prediction in Double Perovskite Compounds; Ongoing.
7. Shreya Das; Computational Study of Oxohalides; Ongoing.

Projects of M.Sc./ M.Tech./ B.Tech./ Post B.Sc. students

1. Mitrajyoti Ghosh; St. Stephen's College, Delhi, Summer Student sponsored by Indian Academy of Sciences.

Post Doctoral Research Scientists

1. Tilak Das
2. Shamik Chakrabarti

Teaching activities at the Centre

1. Post-BSc; PHY302 course; 7 students; co-teacher: Dr. Shreemoyee Ganguly.

Publications in journals

1. R D'Souza, S Mukherjee, **T Saha-Dasgupta;** *Influence of interface geometry on phase stability and bandgap engineering in boron nitride substituted graphene: A combined first-principles and Monte Carlo study;* Journal of Alloys and Compounds; 2017; **708**; 437.
2. K Samanta, **T Saha-Dasgupta;** *Rocksalt versus layered ordering in double perovskites: A case study with La_2CuSnO_6 and La_2CuIrO_6;* Physical Review B; 2017; **95;** 235102.
3. P Chakraborty, T Das, D Nafday, L Boeri, **T Saha-Dasgupta;** *Manipulating the mechanical properties of Ti_2C MXene: Effect of substitutional doping;* Physical Review B; 2017; **95;** 184106.
4. S Ganguly, M Kabir, **T Saha-Dasgupta;** *Magnetic and electronic crossovers in graphene nanoflakes;* Physical Review B; 2017; **95;** 174419.
5. S Datta, AK Raychaudhuri, **T Saha-Dasgupta;** *First principles study of bimetallic $Ni_{13-n}Ag_n$ nano-clusters (n= 0–13): Structural, mixing, electronic, and magnetic properties;* The Journal of Chemical Physics; 2017; **146;** 164301.
6. Hajime Hojo, Ryo Kawabe, Keisuke Shimizu, Hajime Yamamoto, Ko Mibu, Kartik Samanta, **Tanusri Saha-Dasgupta,** Masaki Azuma; *Ferromagnetism at Room Temperature Induced by Spin Structure Change in $BiFe_{1-x}Co_xO_3$ Thin Films;* Advanced Materials; 2017; **29;** 1603131.
7. A Valli, A Amaricci, A Toschi, **T Saha-Dasgupta,** K Held, M Capone; *Effective magnetic correlations in hole-doped graphene nanoflakes;* Physical Review B; 2016; **94;** 245146.
8. H Banerjee, S Chakraborty, **T Saha-Dasgupta;** *Cationic Effect on Pressure Driven Spin-State Transition and Cooperativity in Hybrid Perovskites;* Chemistry of Materials; 2016; **28;** 8379.
9. Santu Baidya, Umesh V. Waghmare, Arun Paramekanti, and **Tanusri Saha-Dasgupta;** *High-temperature large-gap quantum anomalous Hall insulating state in ultrathin double perovskite films;* Physical Review B; 2016; **94;** 155405.

10. Olga S Volkova, Larisa V Shvanskaya, Evgeny A Ovchenkov, Elena A Zvereva, Anatoly S Volkov, Dmitriy A Chareev, Kaimujjaman Molla, Badiur Rahaman, **Tanusri Saha-Dasgupta,** Alexander N Vasiliev; *Structure–Property Relationships in* α-, β'–, *and* γ-*Modifications of* $Mn_3(PO_4)_2$; Inorganic Chemistry; 2016; **55;** 10692.
11. Nagamalleswararao Dasari, SRKC Sharma Yamijala, Manish Jain, **T Saha Dasgupta,** Juana Moreno, Mark Jarrell, NS Vidhyadhiraja; *First-principles investigation of cubic* $BaRuO_3$*: A Hund's metal;* Physical Review B; 2016; **94;** 085143.
12. KV Zakharov, EA Zvereva, MM Markina, MI Stratan, ES Kuznetsova, SF Dunaev, PS Berdonosov, VA Dolgikh, AV Olenev, SA Klimin, LS Mazaev, MA Kashchenko, Md A Ahmed, A Banerjee, S Bandyopadhyay, A Iqbal, B Rahaman, **T Saha-Dasgupta,** AN Vasiliev; *Magnetic, resonance, and optical properties of* $Cu_3Sm(SeO_3)_2O_2Cl$*: A rare-earth francisite compound;* Physical Review B; 2016; **94;** 054401.

Other Publications

1. P Das, **T Saha-Dasgupta,** S Puri; Kinetics of Order-Disorder Transitions in Binary Mixtures: A Monte Carlo Study; Journal of Physics: Conference series; 2016; 759; 012010.

Lectures Delivered

1. Oxide Heterostructures; Max-Planck-Partnergroup workshop, IOP; Bhubaneswar; March; 2017.
2. Heterostructures based on double perovskites; Indo-US conference; Kolkata; January; 2017.
3. A site cations in oxides; Solid State Chemistry Symposium, JNCASR; December; 2016.
4. Modeling of strongly correlated electron materials; Indian Academy of Sciences meeting, special session on Walter Kohn; December; 2016.
5. Designing Anomalous Quantum Hall Effect; APCTP; Pohang, South Korea; December; 2016.
6. Materials modeling through first-principles; IISER; Pune; October; 2016.
7. First-principles way of understanding Physical and Chemical processes; RSC-CRSI joint symposium; Edinburg; May; 2016.

Membership of Committees

External Committee

Member, PAC under Physical Sciences; Member, Sectional Committee (Physics), Indian Academy of Sciences, Bangalore; Member, Sectional Committee (Physics), National Academy of Sciences India, Allahabad; Member, International Advisory Committee, CIMTEC conference, Italy.

Internal Committee

Associate Dean (Faculty); Convener, Advanced Post Doctoral Manpower Program; Convener, Faculty search committee; Chairperson, Computer Services Cell Advisory Committee & Working Group Committee.

Awards / Recognitions

1. "Outstanding Referees" recognition of American Physical Society (2017).

Sponsored Projects

1. Thematic Unit on Computational Materials Science; DST-Nanomission; 2012-2017 (PI).
2. Indo-Austrian; DST bilateral program; 2015-2017 (PI).
3. Indo-Russian; DST bilaterial program; 2014-2016 (PI).
4. Technical Research Centre; DST; 2016-- (Co-PI).

Conference / Symposia / Workshops / Seminars etc. organized

1. Indo-US conference on Physics and Chemistry of Oxide Materials; January 2017.

Collaborations including publications (Sl. No. of the paper listed in 'Publications in journals' jointly published with collaborators)

National

1. M. Kabir (IISER, Pune) (Sl No. 4)
2. U. Waghmare (JNCASR, Bangalore) (Sl No. 8)

International

1. L. Boeri, Technical Uni , Graz, Indo-Austrian project (Sl No 3)
2. M. Azuma, Tokyo Tec, Collaboration sponsored by Visiting Professorship at Tokyo Inst of Technology (Sl no 6)
3. A. Vasiliev, Moscow State Univ, Indo-Russian (Sl no. 10, 12)
4. K Held, Techinal Univ Vienna, Indo-EU project (Sl no. 7)

Member of Editorial Board

1. Pramana

Significant research output / development during last one year

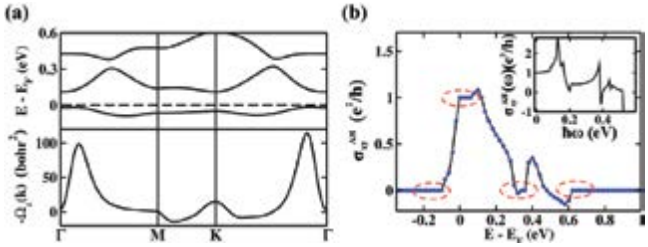
General research areas and problems worked on

Oxide heterostructures; 2D materials; Double perovskites; Organic-inorganic hybrid materials; Quantum Spin Systems

Interesting results obtained

Prediction of High-temperature large-gap quantum anomalous Hall insulating state in ultrathin double perovskite films (Santu Baidya, Umesh V. Waghmare, Arun Paramekanti, and Tanusri Saha-Dasgupta, Phys. Rev. B 94, 155405 , 2016)

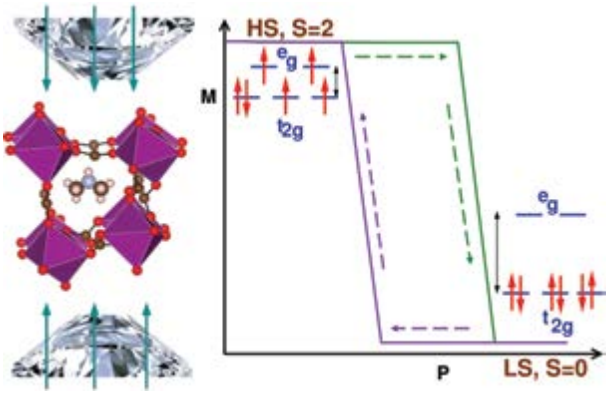
Towards the goal of realizing topological phases in thin films of correlated oxide and heterostructures, we propose here a quantum anomalous Hall insulator (QAHI) in ultrathin films of double perovskites based on mixed 3d–5d or 3d–4d transition-metal ions, grown along the [111] direction. Our finding of the QAHI state in ultrathin Ba_2FeReO_6 is expected to stimulate experimental verification along with possible practical applications of its dissipationless edge currents.



(a): The band structure in minority spin channel (top panel) and calculated Berry curvature (bottom panel) plotted along the high symmetry directions in the BZ. (b): Anomalous Hall conductivity of the band structure in (a), in units of e^2/h. Quantized plateaus are highlighted. Inset: Frequency dependence of the real part of the antisymmetric optical conductivity.

Cationic Effect on Pressure driven Spin-State Transition and cooperativity in Hybrid Perovskites (H Banerjee, S Chakraborty, T Saha-Dasgupta, Chemistry of Materials 28, 8379, 2017)

Hybrid or metal organic framework (MOF) perovskites of general composition, ABX_3, are known to show interesting properties which can lead to a variety of technological applications. Our first principles study shows they are also potential candidates for exhibiting cooperative spin-state transitions upon application of external stimuli.



Hybrid perovskites and cooperativity, manifested as hysteresis in spin-state transition under pressure.

Proposed research activities for the coming year

1. High-throughput Computational Materials Design
2. Problems of geological interest
3. Light induced Spin-Cross Transition in Metalorganic Complexes