



# SANTU BAIDYA

## CONTACT

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## CORE COMPETENCIES

- Studying quantum materials using first principles simulation
- Using tight-binding and k.p model to understand microscopic physics of materials
- Carrying out high-throughput calculation using DFT method



## PROFILE SUMMARY

Motivated and passionate to working in the field of applied material science for the research and development and taking real-life challenges in the field of science. Having long years of experience in material science with excellent track record of research success with multiple published articles. Seeking an opportunity to leverage skills and use expertise to solve practical scientific challenging problems



## EDUCATION

**Ph.D. in Physics (Computational Material Science) 2009-2014**  
University of Calcutta, 68.00%

Research carried out at *S. N. Bose National Centre For Basic Sciences*, Kolkata, West Bengal, India

**Supervisor:** Prof. Tanusri Saha-Dasgupta

**Title:** Interplay of Charge, Orbital and Spin in Correlated Transition Metal Oxides

**Description:** The thesis explores the idea, using density functional theory (DFT), that the interplay between the three degrees of freedom charge, spin, and orbital associated with the electrons along with strong correlation between electrons in materials produces many complex phenomena like magnetic phase transitions, spintronics, metal-insulator transition, large magnetoresistance, multiferroicity etc. which brings interest both from academic and application point of view.

**Master of Science in Physics 2007-2009**  
University of Calcutta, 65.10%, First Class

**Bachelor of Science in Physics honours 2004-2007**  
University of Calcutta, 60.13%, First Class



## WORK EXPERIENCE

**Postdoctoral Research Associate 03/2021 - Present**  
Material Research Centre, Indian Institute of Science, Bangalore, India  
**Supervisor:** Prof. Abhishek K. Singh

- Using Wannier function to study physical and chemical properties
- Developing codes for studying various bulk properties of materials
- Using machine learning for studying large number of materials

## TECHNICAL SKILLS

- Parallel computation, Linux, MS Windows, MS Powerpoint, MS Word, LaTeX, Machine Learning
- Programming Languages: Fortran, Python, Scripting
- Computational Packages: VASP, Quantum Espresso, Wien2k, Abinit, OpenMx, TB-LMTO-ASA, NMTO, Wannier90, Python-TB
- Visualizing Softwares: Xcrysden, VESTA, Blender, MATLAB, GNUPLOT, Photoshop

## EXECUTIVE SKILLS

- Ability to independently solving problems
- Ability to do team work on any project
- Leading any project
- Quick learner
- Guiding students in projects

- Defect transition levels studied using DFT for power electronic devices with DRDO
- Topological properties studied for transition metal superlattices using DFT
- DFT study electronic and magnetic properties of 2D materials, bulk materials and superlattices

### **Postdoctoral Research Associate** 04/2019 – 02/2021

Department of Physics and Astronomy, Rutgers University  
New Jersey, USA

**Supervisor:** Prof. David Vanderbilt

- Collaborated with experimental group of John Hopkins University to study topological materials
- Independently solved problem of Weyl semimetal phase of a Dirac semimetal under magnetic field using DFT
- Studied phonon spectra in bulk materials collaborating with experimentalists
- Experience in Wannier90 based tight-binding to study topological properties

### **Postdoctoral Fellow** 05/2016 – 01/2019

IBS-CCES, Department of Physics and Astronomy, Seoul National University, Seoul, South Korea

**Supervisor:** Dr. Choong Hyun Kim and Prof. Jaejun Yu

- Worked in 2D materials for studying electronic and magnetic properties
- Studied 2D materials using DFT to propose new QAHI
- Experience in working with metal-organic-framework based materials

### **Postdoctoral Fellow** 04/2015 – 03/2016

Faculty For Physics, University of Duisburg-Essen, Duisburg, Germany

**Supervisor:** Prof. Rossitza Pentcheva

- Worked in transition metal based heterostructures using DFT
- DFT used to propose new QAHI in magnetic heterostructures
- Experience in studying excited state spectra of bulk and heterostructures using DFT

### **Visiting Scientist** 10/2014 – 01/2015

Theoretical Sciences Unit, JNCASR, Bangalore, Karnataka, India

**Supervisor:** Umesh V. Waghmare

- DFT study of polar transition metal based heterostructure
- Experience in tight-binding to study band structures

## RESEARCH INTEREST

- Magnetic materials
- Two dimensional materials
- Spintronics
- Ferroelectric materials
- Topological phases
- Surface science
- Magnetoelectric effect
- Lattice dynamics
- Metal-organic framework,
- Machine-learning
- Excited state properties

## REVIEWED JOURNALS

- Physical Review B
- Physical Review Letter
- Physical Review materials
- Physica B
- ACS Applied Materials and Interface

## LANGUAGES KNOWN

English, Hindi, Bengali

## D.O.B. AND NATIONALITY

02.01.1987 and Indian



## RESEARCH EXPERIENCE

- Studied materials with correlated electrons for microscopic understanding of electronic and magnetic properties.
- Studied excited state properties like XAS, XMCD and EELS for materials using DFT method to support experimental observation.
- Used maximally localized Wannier function (MLWF) based tight-binding and k.p model to understand bulk properties of materials related to electronic bands.
- Studied topological properties of two dimensional as well as bulk materials.
- Experienced with using Machine learning to propose new materials with ferromagnetic insulating properties.
- Experience in writing code to analyze electronic properties using both Fortran and python.



## AWARDS AND ACHIEVEMENTS

- National Level examinations: CSIR-UGC NET (2009), GATE (2009), JEST (2009)
- Best oral presentation award at Bose Fest conference in 2013 and 2014 organized in S. N. Bose National Centre For Basic Sciences, Kolkata



## PUBLICATIONS

“Phonon spectrum of and as evidence of coupling of the lattice with electronic and magnetic degrees of freedom”, Physical Review B volume=105, page=075137 (2022), Yuanyuan Xu, Huiyuan Man, Nan Tang, Takumi Ohtsuki, **Santu Baidya**, Satoru Nakatsuji, David Vanderbilt, Natalia Drichko

“Weyl-mediated helical magnetism in NdAlSi”, Nature Materials volume=20, page=1650 (2021), Impact factor=43.8, Jonathan Gaudet, Hung-Yu Yang, **Santu Baidya**, Baozhu Lu, Guangyong Xu, Yang Zhao, Jose A. Rodriguez-Rivera, Christina M. Hoffmann, David E. Graf, Darius H. Torchinsky, Predrag Nikolić, David Vanderbilt, Fazel Tafti & Collin L. Broholm.

“Importance of dynamic lattice effects for crystal field excitations in the quantum spin ice candidate  $\text{Pr}_2\text{Zr}_2\text{O}_7$ ”, Phys. Rev. B volume=104, page=075125 (2021), Yuanyuan Xu, Huiyuan Man, Nan Tang, **Santu Baidya**, Hongbing Zhang, Satoru Nakatsuji, David Vanderbilt, and Natalia Drichko.

“First principles theory of Dirac semimetal  $\text{Cd}_3\text{As}_2$  under Zeeman magnetic field”. Phys. Rev. B volume=102.

- "Interplay of Magnetism and Topological Superconductivity in Bilayer Kagome Metals", Phys. Rev. Lett. volume=125, page=026401 (2020), Impact factor=9.227, **Santu Baidya**, Aabhaas Vineet Mallik, Subhro Bhattacharjee, and Tanusri Saha-Dasgupta.
- "Theoretical evidence of spin-orbital-entangled  $J_{\text{eff}} = 1/2$  state in the 3d transition metal oxide  $\text{CuAl}_2\text{O}_4$ ", Phys. Rev. B (Rapid Communication) volume=100, page=161104 (2019), Impact factor=3.736, Choong H. Kim, **Santu Baidya**, Hwanbeom Cho, Vladimir V. Gapontsev, Sergey V. Streltsov, Daniel I. Khomskii, Je-Geun Park, Ara Go, and Hosub Jin.
- "Chern insulator with a nearly flat band in the metal-organic-framework-based Kagome lattice", Scientific Reports volume=9, page=13807 (2019), Impact factor=4.525, **Santu Baidya**, Seungjin Kang, Choong H. Kim and Jaejun Yu.
- "Tunable Magnetic Topological Insulating Phases in Monolayer  $\text{CrI}_3$ ", Phys. Rev. B volume=98, page=155148 (2018), Impact factor=3.736, **Santu Baidya**, Jaejun Yu and Choong H. Kim.
- "Confinement-driven electronic and topological phases in corundum-derived 3d oxide honeycomb lattices", Phys. Rev. B volume=97, page=035126 (2018), Impact factor=3.736, Okan Köksal, **Santu Baidya** and Rossitza Pentcheva.
- "High-temperature large-gap quantum anomalous Hall insulating state in ultrathin double perovskite films", Phys. Rev. B volume=94, page=155405 (2016), Impact factor=3.736, **Santu Baidya**, Umesh V. Waghmare, Arun Paramekanti and Tanusri Saha-Dasgupta.
- "Design of Mott and topological phases on buckled 3d-oxide honeycomb lattices", Phys. Rev. B volume=93, page=165145 (2016), Impact factor=3.736, D. Doennig, **Santu Baidya**, W. E. Pickett and R. Pentcheva.
- "Controlled confinement of half-metallic two-dimensional electron gas in  $\text{BaTiO}_3/\text{Ba}_2\text{FeReO}_6/\text{BaTiO}_3$  heterostructures: A first-principles study", Phys. Rev. B (Rapid Communication) volume=92, page=161106 (2015), Impact factor=3.736, **Santu Baidya**, Umesh V. Waghmare, Arun Paramekanti, Tanusri Saha-Dasgupta.
- "Breakdown of  $J=0$  nonmagnetic state in d4 iridate double perovskites: A first-principles study", Phys. Rev. B (Rapid Communication) volume=92, page=121113 (2015), Impact factor=3.736, Sayantika Bhowal, **Santu Baidya**, Indra Dasgupta, Tanusri Saha-Dasgupta.

- "Covalency driven low-temperature structural distortion and its effect on electronic structure of  $\text{Hg}_2\text{Ru}_2\text{O}_7$ ", Phys. Rev. B volume=91, page=075123 (2015), Impact factor=3.736, **Santu Baidya**, Tanusri Saha-Dasgupta.
- "Covalency-driven structural instability and spin-phonon coupling in barium cobalt oxychloride", Phys. Rev. B volume=90, page=235147 (2014), Impact factor=3.736, Tanushree Chakraborty, **Santu Baidya**, Carlo Meneghini, Tanusri Saha-Dasgupta, Giulia Veronesi, Marco Merlini, Hiroko Yokota, Mitsuru Itoh, S. Majumdar, and Sugata Ray.
- "A real-space study of random extended defects in solids: Application to disordered Stone-Wales defects in graphene", Physica E (Low-dimensional systems and nanostructures) volume=61, page=191-197 (2014), Impact factor=3.176, Suman Chowdhury, **Santu Baidya**, Dhani Nafday, Soumyajyoti Halder, Mukul Kabir, Biplab Sanyal, Tanusri Saha-Dasgupta, Debnarayan Jana, Abhijit Mookerjee.
- "Copper rubidium diphosphate,  $\text{Rb}_2\text{Cu}_3(\text{P}_2\text{O}_7)_2$ : synthesis, crystal structure, thermodynamic and resonant properties", New. J. Chem., volume=37, page=2743-2750 (2013), Impact factor=3.069, Larisa Shvanskaya, Olga Yakubovich, Anna Ivanova, **Santu Baidya**, Tanusri Saha-Dasgupta, Elena Zvereva, Alexey Golovanov, Olga Volkova and Alexander Vasiliev.
- "Crystal structure and magnetic properties of new layered sodium nickel hydroxide phosphate,  $\text{Na}_2\text{Ni}_3(\text{OH})_2(\text{PO}_4)_2$ ", Dalton Trans., volume=42, page=14718-14725 (2013), Impact factor=4.052, Olga Yakubovich, Galina Kiriukhina, Olga Dimitrova, Anatoli Volkov, Alexey Golovanov, Olga Volkova, Elena Zvereva, **Santu Baidya**, T. Saha-Dasgupta and Alexander Vasiliev.
- "Interplay of localized and itinerant character of Ru ions:  $\text{Tl}_2\text{Ru}_2\text{O}_7$  vs.  $\text{Hg}_2\text{Ru}_2\text{O}_7$ ", Phys. Rev. B volume=86, page=125117 (2012), Impact factor=3.736, **Santu Baidya**, Soumyajit Sarkar, T. Saha-Dasgupta and D. D. Sarma.
- "Effect of A cation on magnetic properties of double perovskite compounds: From ferromagnetic  $\text{Ca}_2\text{CrSbO}_6$  to antiferromagnetic  $\text{Sr}_2\text{CrSbO}_6$ ", Phys. Rev. B volume=86, page=024440 (2012), Impact factor=3.736, **Santu Baidya**, and T. Saha-Dasgupta.
- "Electronic Structure and phonons in  $\text{La}_2\text{CoMnO}_6$ : A ferromagnetic insulator driven by Coulomb-assisted spin-orbit coupling", Phys. Rev. B volume=84, page=035131 (2011), Impact factor=3.736, **Santu Baidya**, and T. Saha-Dasgupta.

"Understanding neutron scattering data in  $\text{YMn}_2\text{O}_5$ : An effective spin Hamiltonian", Phys. Rev. B volume=84, page=054444 (2011), Impact factor=3.736, **Santu Baidya**, Prabuddha Sanyal, Hena Das, Bertrand Roessli, Tapan Chatterji, and T. Saha-Dasgupta.

"Configuration and self-averaging in disordered systems", Indian Journal of Physics volume=90, page=649 (2016), Impact factor=1.407, S Chowdhury, D Jana, B Sadhukhan, D Nafday, **S Baidya**, T Saha-Dasgupta and A Mookerjee.



## SCHOOLS / CONFERENCES ATTENDED

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"Autumn school on Correlated electrons: From Models to Materials" - in Forschungszentrum Julich, Germany, 2012. Presented a poster.

"International Conference on Functional Oxides and New Carbon Materials" - organized by S N Bose National Centre for Basic Sciences, Kolkata, 2012.

"Summer school on Functionality of Correlated Materials" - in Frauenwoerth im Chiemsee, Germany, 2015. Presented a poster.

"8-th IACS-APCTP-KIAS Joint Conference On Emergent Phenomena in Novel Oxide Materials And Low Dimensional Systems" – organized by IACS, APCTP and KIAS, Pohang, 2016, presented a poster.

"9-th IACS-APCTP Joint Activity on Novel Quantum Phases in Oxide Materials and Low Dimensional Systems" – organized by Indian Association for the Cultivation of Science (IACS), Kolkata, and Asia-Pacific Center for Theoretical Physics (APCTP), 2017, invited oral presentation.

## HOBBIES

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