

# Nirmal Ganguli

Associate Professor

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## Career

- 2023–now **Associate Professor**, *Department of Physics, Indian Institute of Science Education and Research Bhopal*, Bhopal Bypass Road, Bhauri, Bhopal 462066, MP, India.
- 2016–'23 **Assistant Professor**, *Department of Physics, Indian Institute of Science Education and Research Bhopal*, Bhopal Bypass Road, Bhauri, Bhopal 462066, MP, India.
- 2015–'16 **Scientist**, *Department of Electronic Structure Theory, Max Planck Institute for Solid State Research*, Heisenbergstraße 1, 70569 Stuttgart, Germany.
- 2011–'14 **Postdoctoral Researcher**, *Faculty of Science and Technology and MESA<sup>+</sup> Institute for Nanotechnology, University of Twente*, P.O. Box 217, 7500 AE Enschede, The Netherlands.

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## Education

- Doctor of Philosophy* **Indian Institute of Technology Bombay, Mumbai, India**, 2012 (within the framework of M.Sc. and Ph.D. dual degree program, Department of Physics, IIT Bombay).  
Area of research work: Theoretical and computational condensed matter physics
- Master of Science* **Indian Institute of Technology Bombay, Mumbai, India**, 2007 (within the framework of M.Sc. and Ph.D. dual degree program, Department of Physics, IIT Bombay).  
Subject of study: Physics
- Bachelor of Science* **Ramakrishna Mission Vidyamandira (University of Calcutta), Kolkata, India**, 2005.  
Subjects of study: Physics (Honors), Chemistry, Mathematics
- Higher Secondary* **West Bengal Council of Higher Secondary Education, India**, 2002.  
Subjects of study: Physics, Chemistry, Mathematics, Biology, Bengali, English
- Secondary* **West Bengal Board of Secondary Education, India**, 2000.  
Subjects of study: Physical Science, Life Science, Mathematics, Geography, History, Bengali, English, Physics (additional)

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## Research

### Research interests

- Spin-Orbit coupling* Spin-orbit coupling and its influence on materials properties like magnetism and transport properties are also our area of interest, where the Rashba-like effect at the heterostructure interface is at the focus. Topologically protected properties of materials also interest us.
- Magnetism* Our interest is to understand the magnetic properties in various materials and find out the mechanism leading to the magnetic ground state.
- Nano-materials* Nanocrystals of semiconducting materials exhibit a host of interesting properties mainly because of two reasons: (a) the band gap is widened due to quantum confinement, (b) the lattice periodicity no longer exists. The focus of our research is the magnetic and optical properties in nanoscale semiconducting materials that are potentially useful for technological applications.

*Hetero-junctions* Heterostructures of oxide materials with another oxide material are very interesting for a number of counter-intuitive properties like high mobility electron gas, magnetism, superconductivity, etc. Heterostructures of oxide and 2-dimensional transition metal dichalcogenides are interesting for the electron-phonon interaction at the interface. Heterostructures of nanoscale semiconductor materials offer the possibility of tuning their optical properties for technological applications.

*Strong correlation* We are interested in investigating physical properties arising from strong electron-electron correlation, primarily in transition metal compounds. The magnetic and transport properties of materials with strong electron-electron correlation are of particular interest.

### **Research group**

*Leader* Dr. Nirmal Ganguli

*PhD* Mr. Avishek Singh (submitted PhD thesis for evaluation on 9 April 2023), Ms. Sugandha Saxena, Mr. Ramsamoj Kewat, Mr. Vivek Kumar, Mr. Suman Rooj, Ms. Purba Dutta, Mr. Shayan Garai

*MS* Mr. Suhas Bhat, Mr. Abhijeet Kumar, Mr. Kunal

*Former members* Mr. Jayant Singh Bhati (MS, project JRF), Mr. Praphull Kabtyal (MS), Ms. Silpa S (MS), Mr. Kartveer Singh (MS) Dr. Jayita Chakraborty (Postdoc), Dr. Preeti Khare (Postdoc)

### **Methods and codes**

*DFT* Plane wave PAW based: VASP, PWscf (Quantum espresso), Wannier90  
All electron based: TB-LMTO-ASA, Wien2k

*QMC* *n*-electron configuration interaction (neci) solver that implements full configuration interaction quantum Monte Carlo (FCIQMC) method

### **Research grants**

2022–'25 SERB Core Research Grant for project titled “**Designing oxide heterostructures for quantum technology through first-principles calculations**”; **Total Budget: ₹ 31 02 264**

2017–'20 SERB Early Career Research Award for project titled “**Magnetism and spin-orbit interaction at complex oxide interfaces for technology: An ab initio investigation**”; **Total Budget: ₹ 47 25 600**

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## **Teaching experience**

### **IISER Bhopal**

*PHY 102* Electromagnetism (2016 - T, 191 students; 2017 - 196 students)

*PHY 401* Electrodynamics and Special Theory of Relativity (2016 - 40 students; 2017 - 69 students)

*PHY 312* Numerical Methods and Programming (2018 - 30 students, 2023 - 63 students)

*PHY 203* Electrodynamics (2018 - T, 161 students)

*PHY 603* Advanced Quantum Mechanics (2018 - 20 students, 2021 - 12 students)

*PHY 626* Electronic Structure of Materials (2019 - 13 students, 2020 - 9 students, 2021 - 15 students, 2022 - 13 students)

*PHY 106* Quantum Mechanics (2019 - T, 322 students)

*PHY 403* Condensed Matter Physics (2019 - 49 students, 2020 - 95 students)

*PHY 601* Advanced Mathematical Methods for Physics (2022 - 8 students; 2023 - 30 students)

## NPTEL

- 12 weeks Electromagnetism (January 2020 - 4025 students; January 2021 - 4005 students)  
8 weeks Solid State Physics (July 2021 - 3638 students)

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## Awards and Achievements

- 2015 • Awarded Max Planck Society's fellowship for foreign scientists, Germany. *Duration: 1 year.*
- 2011 • Awarded postdoctoral research position by Stichting voor Fundamenteel Onderzoek der Meterie (FOM), The Netherlands. *Duration: 3 years.*
- 2009 • Qualified Graduate Aptitude Test in Engineering (GATE) jointly conducted by IITs and IISc with percentile 96.83.
- 2008 • Qualified National Eligibility Test (NET) jointly conducted by Council of Scientific and Industrial Research (CSIR) and University Grants Commission (UGC).
- 2005 • Qualified Joint Admission Test for M.Sc. (JAM) conducted by IITs (All India Rank 68 in Physics and 24 in Geophysics).
- Qualified Joint Entrance Screening Test (JEST) conducted by few premier Indian research institutions (after B.Sc. (candidates after M.Sc. and B.Sc. compete together), All India Rank 189).
- Among the top 1% candidates in terms of performance in the National Graduate Physics Examination (NGPE) conducted by Indian Association of Physics Teachers (IAPT) and attended a workshop at Scottish Church College, Kolkata on experimental physics (invited).
- 2002 • Recipient of Indubhushan Pal Chowdhury scholarship as the topper of Higher Secondary Examination in Kaliyaganj Parbati Sundari High School (as well as Kaliyaganj block).
- 1998 • Recipient of National Scholarship for Talented Students from Rural Areas.

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## Invited presentations

- 2023 • **Asymmetry-Driven Spin-Splitting for Spintronics and Topological Quantum Technology**, Namma  $\Psi_k$  workshop 2023, IISc Bangalore, India
- **Designing oxide heterostructures for antiferromagnetic spin-orbitronics**, Quantum Matter Heterostructures (QMH 2023) conference, IIT Hyderabad, India
- **Analyzing materials properties and designing functional materials from computer simulations**, In-House Symposium on Progress in Metallurgy and Materials (ISPMM 2023), IIT Indore, India
- **Antiferromagnetism and spin-orbit interaction driven spin splitting in centrosymmetric hexagonal MnTe**, Evolution of Electronic Structure Theory and Experimental Realization (EESTER 2023), Chennai, India
- 2022 • **Antiferromagnetic materials and heterostructures for spintronic technology**, Second Asian Conference on Molecular Magnetism (ACMM-II 2022), Bhopal, India
- **Rashba spin-orbit interaction at  $\text{KTaO}_3$  surface for oxide spintronics**, Young Investigator Meet on Quantum Condensed Matter Theory (YIMQCMT 2022), Bhubaneswar, India
- **Antiferromagnetic Spintronics: The future of electronics**, Shodh Shikhar conference, Bhopal, India
- 2021 • **Magnetic quantum materials and heterostructures with Rashba-like spin-orbit interaction for technology**, Young Investigator Meet on Quantum Condensed Matter Theory (YIMQCMT 2021), Bhubaneswar, India (Online)

- **Quantum mechanics and relativity all set to revolutionize electronic devices**, Invited seminar at Jagadis Bose National Science Talent Search, Kolkata, India (Online)
- **Antiferromagnetic Spintronics: The future of electronics**, Invited colloquium at Department of Physics, IIT (ISM) Dhanbad, India (Online)
- 2020
  - **Perovskite oxide heterojunction for Rashba-Dresselhaus assisted antiferromagnetic spintronics**, Young Investigator Meet on Quantum Condensed Matter Theory (YIMQCMT 2020), Bhubaneswar, India (Online)
  - **Rashba effect and proximity-driven spintronics in 2-dimension**, National Conference on Quantum Matter Heterostructures (QMH 2020), Puri, India
- 2019
  - **A design for 2-dimensional antiferromagnetic spintronics via the coexistence of Rashba effect and noncollinear antiferromagnetism**, Young Investigator Meet On Quantum Condensed Matter Theory (YIMQCMT 2019), Kolkata, India
  - **Antiferromagnetic spintronics at perovskite oxide interface**, Workshop and Symposium on Advanced Simulation Methods: DFT, MD and Beyond (ASM 2019), New Delhi, India
- 2018
  - **Two-dimensional antiferromagnetic spintronics at perovskite oxide heterostructure**, Workshop on Evolution of Electronic Structure Theory & Experimental Realization (EESTER-2018), Chennai, India
- 2016
  - **Role of dielectric perovskite oxides in interface electronics**, 19<sup>th</sup> National Seminar on Ferroelectrics and Dielectrics (XIX NSFD-2016), Bhopal, India

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## Community services

- Reviewed articles for the following journals: Advanced Materials Letters, Applied Physics Letters, Journal of Applied Physics, Scientific Reports (Nature Publishing Group), Crystal Growth & Design (ACS)
- Reviewed poster and oral presentation abstracts for DAE Solid State Physics Symposium, India
- Reviewed thesis abstracts for the best thesis award at DAE Solid State Physics Symposium, India
- Reviewed Extra Mural Research and Early Career Research proposals for SERB, India

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## Publications and patent

### *Important journal publications*<sup>†</sup>

- 2023
  - **Hexagonal MnTe with Antiferromagnetic Spin Splitting and Hidden Rashba - Dresselhaus Interaction for Antiferromagnetic Spintronics**; Suman Rooj, Jayita Chakraborty, and Nirmal Ganguli\*; [Advanced Physics Research 2, 2300050](#).
- 2022
  - **Rashba-like spin-orbit interaction and spin texture at the KTaO<sub>3</sub>(001) surface from DFT calculations**; Vivek Kumar and Nirmal Ganguli\*; [Physical Review B 106, 125127](#).
  - **Implications of electron and hole doping on the magnetic properties of spin-orbit entangled Ca<sub>4</sub>IrO<sub>6</sub> from DFT calculations**; Avishek Singh, Jayita Chakraborty, and Nirmal Ganguli\*; [Journal of Magnetism and Magnetic Materials 563, 169861](#).
- 2020
  - **Perovskite oxide heterojunction for Rashba-Dresselhaus assisted antiferromagnetic spintronics**; Jayita Chakraborty and Nirmal Ganguli\*; [Physical Review B 102, 214425](#).
- 2019
  - **DFT study of itinerant ferromagnetism in p-doped monolayers of MoS<sub>2</sub>**; Yuqiang Gao, Nirmal Ganguli\*, Paul J. Kelly; [Physical Review B 100, 235440](#).

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<sup>†</sup>Link to the complete list of publications: <https://orcid.org/0000-0002-9718-8016>

\*Corresponding author

- **Defect Engineered MoS<sub>2</sub> Nanostructures for ROS Generation in Dark: Anti-pollutant and Anti-fungal Performances;** Parbati Basu, Jayita Chakraborty, Nirmal Ganguli, Khushi Mukherjee, Krishnendu Acharya, Biswarup Satpati, Sudipta Khamrui, Suman Mandal, Debmalya Banerjee, Dipak Goswami, Padinharu Madathil Gopalakrishnan Nambissan, Kuntal Chatterjee; [ACS Applied Materials & Interfaces 11, 48179](#).
- **Itinerant ferromagnetism in *p*-doped monolayers of MoS<sub>2</sub>;** Yuqiang Gao, Nirmal Ganguli\*, Paul J. Kelly; [Physical Review B 99, 220406\(R\)](#).
- **Neutron diffraction and short range ordering study in multiferroic Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub>;** A. K. Singh, S. R. Mohapatra, Preeti Khare, Nirmal Ganguli, A. Wildes, V. Siruguri, and S. D. Kaushik; [Materials Research Express 6, 066107](#).
- 2018 • **Enhancement of the superconducting transition temperature by Re doping in Weyl semimetal MoTe<sub>2</sub>;** Manasi Mandal, Sourav Marik, K. P. Sajilesh, Arushi, Deepak Singh, Jayita Chakraborty, Nirmal Ganguli, and R. P. Singh; [Physical Review Materials 2, 094201](#). **Editors' Suggestion**
- 2017 • **Channel-Assisted Proton Conduction Behavior in Hydroxyl-Rich Lanthanide-Based Magnetic Metal-Organic Frameworks;** Soumava Biswas, Jayita Chakraborty, Vijay Singh Parmar, Siba Prasad Bera, Nirmal Ganguli, and Sanjit Konar; [Inorganic Chemistry 56, 4956](#).
- **A comparative study of magnetic and optical properties of Mn-, Gd-, and Nd-doped ZnO nanowires;** Arup Chakraborty, Chol-Sam Jong, Nirmal Ganguli, and I. Dasgupta; [International Journal of Modern Physics B 30, 1650241](#).
- 2014 • **Tuning Ferromagnetism at Interfaces Between Insulating Perovskite Oxides;** Nirmal Ganguli\* and Paul J. Kelly; [Physical Review Letters 113, 127201](#).
- **First-principles study of the electronic structure of CdS/ZnSe coupled quantum dots;** Nirmal Ganguli\*, S. Acharya, and I. Dasgupta; [Physical Review B 89, 245423](#).
- 2013 • **Role of Te in the low-dimensional multiferroic material FeTe<sub>2</sub>O<sub>5</sub>Br;** Jayita Chakraborty, Nirmal Ganguli, Tanusri Saha-Dasgupta, and Indra Dasgupta; [Physical Review B 88, 094409](#).
- 2012 • **How Crucial are Finite-Temperature and Solvent Effects on Structure and Absorption Spectra of Si<sub>10</sub>?;** N. Arul Murugan, Indra Dasgupta, Arup Chakraborty, Nirmal Ganguli, Jacob Kongsted, and Hans Ågren; [Journal of Physical Chemistry C 116, 26618](#).
- **Magnetic properties of Mn-doped Ge<sub>46</sub> and Ba<sub>8</sub>Ge<sub>46</sub> clathrates;** Nirmal Ganguli, K. V. Shanavas, and Indra Dasgupta; [Journal of Physics: Condensed Matter 24, 505501](#). **Journal Cover**
- 2011 • **Long-range visible fluorescence tunability using component-modulated coupled quantum dots;** Sucheta Sengupta, Nirmal Ganguli, I. Dasgupta, D. D. Sarma, and Somabrata Acharya; [Advanced Materials 23, 1998](#). **Highlighted in Nature India**
- 2010 • **Electronic structure and magnetism of transition metal doped Zn<sub>12</sub>O<sub>12</sub> clusters: Role of defects;** Nirmal Ganguli, Indra Dasgupta, and Biplab Sanyal; [Journal of Applied Physics 108, 123911](#).
- **Electronic structure and magnetic properties of (Fe,Co)-codoped ZnO: Theory and experiment;** Debjani Karmakar, T. V. Chandrasekhar Rao, J. V. Yakhmi, A. Yaresko, V. N. Antonov, R. M. Kadam, S. K. Mandal, R. Adhikari, A. K. Das, T. K. Nath, Nirmal Ganguli, I. Dasgupta, and G. P. Das; [Physical Review B 81, 184421](#).
- 2009 • **The making of ferromagnetic Fe doped ZnO nanoclusters;** Nirmal Ganguli, Indra Dasgupta, and Biplab Sanyal; [Applied Physics Letters 94, 192503](#).

### **Patent**

- 2010
- **Asymmetric Heterostructure for Synergistic Tunability of Visible Emissions;** D. D. Sarma, I. Dasgupta, S. Acharya, Sucheta Sengupta, and **Nirmal Ganguli;** Filed on September 21, 2010 at Indian Patent Office; application number 1050/KOL/2010.