Shashi B. Mishra

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EDUCATION

Ph.D., Physics, (*Best Ph.D. thesis in Physics, 2021*) March 2021
Indian Institute of Technology Madras, India
Thesis: Ab initio Modelling and Functionalization of Graphene & TiO_2 Surfaces and Interfaces
Areas of Expertise: Surface Science, Photocatalysis, Magnetism, Heterostructure, Energy storage

M.Sc., Physics June 2013
Utkal University, Odisha, India

B.Sc., Physics June 2011
Fakir Mohan University, Odisha, India

WORK EXPERIENCE

- **April, 2023 - Present** Postdoctoral Researcher, SUNY Binghamton, NY, USA
  Area: Phonon-mediated superconductivity and EPW code development
- **April, 2021 - March, 2023** Postdoctoral Researcher, University of California, Riverside, USA
  Area: First principle study of light-induced magnetic phenomena in metals for magnetic switching devices
- **June, 2020 - March, 2021:** Project Officer at IIT Madras, India
  Area: Development of TiO_2 based materials for gas sensing and solar cell applications

TECHNICAL SKILLS

- Languages: Python, Matlab, Bash Script
- Softwares: Quantum ESPRESSO, VASP, *ab initio* MD, Gaussian, Wannier90, Wannier Berri, EPW.

RESEARCH INTEREST

- First-principles theory for electron-phonon interaction
- Materials for High-T_c superconductivity
- Design of materials for electronic and optoelectronic devices
- Energy storage materials, catalysis, and photocatalysis
- Low-dimensional physics in heterostructures
- Magnetism, Spin Hall effect and magneto-optics

RESEARCH EXPERIENCE

- **Phonon-mediated superconductivity beyond the Migdal approximation:** Revisited the non-adiabatic theory of superconductivity and implemented first-order vertex corrections for electron-phonon interactions in the isotropic approximation within the Eliashberg formalism in the EPW code.
- **Stability-superconductivity map for compressed Na-intercalated graphite** Conducted an *ab initio* study on Na-C binary compounds under moderate pressures, revealing new stable stoichiometries and confirming NaC_4 potential for high-temperature superconductivity with a critical temperature up to 48 K at 10 GPa.
- **Inverse Faraday effect in non-magnetic metals:** Formulated a gauge-invariant theory for IFE for nonmagnetic materials with inversion symmetry.
- **Magnetism through intercalation:** Intrigued formation of a low-dimensional magnetic lattice by intercalating fluorine molecules between graphene layers.
- **Creation of spin-polarized 2D electron gas:** Proposed a heterostructure between Sr_2FeMoO_6 and La_2CoMnO_6 to form spin-polarized 2DEG through quantum confinement and orbital manipulation.
- **Long-range magnetic ordering in double perovskite Ba_2MnTeO_6:** Explained the magnetic exchange interactions in BMTO, where Mn^{2+} with S = 5/2 spins constitute a triangular lattice.

- **Si_2BN for Mg-ion batteries:** Demonstrated low migration energy barrier and good theoretical specific capacity for Mg-ion on Si_2BN, making it a potential candidate for high-performance anode materials for energy storage devices.
- **Semiconductor/2D interface:** Designed a low-stained heterostructure between Graphene and TiO_2(001) surface and the study shows that AB-stacked graphene bilayer opens up a minor bandgap.
- **Atomistic mechanism for surface-adsorbate interactions:** Explained TiO_2-CO_2 interaction using a three-state model and proposed change in exchange-correlation energy as an indicator for adsorption nature.

PUBLICATIONS

1. **S. B. Mishra** Inverse Faraday effect in 3*d*, 4*d*, and 5*d* transition metals *Phys. Rev. B*, **111**, 174413 (2025).
2. Z. Liu*, **S. B. Mishra***, J.-M. Lihm, S. Poncé, and E. R. Margine, Phonon-limited carrier transport in the Weyl semimetal TaAs (Under Review in Phys. Rev. B) (*equal contribution)*arXiv* **2505.16544** (2025).
3. **S. B. Mishra**, H. Mori, and E. R. Margine, First-order vertex corrections to phonon-mediated superconductivity in H_3S and Pb (Submitted).
4. X, Zhang, **S. B. Mishra**, E. R. Margine, and E. Kioupakis, Cubic BeB_2: A metastable *p*-type conductive material from first principles (Submitted).
5. A. Das, Preethi M., **S. B. Mishra**, N. C. Maji, P. Ningthoukhongjame, R. G. Nair, Abhijith T,A. S. Vasenko, Madhumitha R., and , Electrostatic Self-assembly Driven Heterojunction of CeO_2/g-C_3N_4 Nanosheets for Efficient Photocatalytic Hydrogen Evolution and Photoelectrocatalytic Water Splitting: A Hybrid Experimental and Theoretical Study (Under Review in ACS Applied Materials & Interfaces).
6. Y. Rambabu, **S. B. Mishra**, E. Cortes, Defects dynamic in photo-Excited CeO_2 and their influence on CO_2 photoreduction (Revision in Advance Functional Materials).
7. **S. B. Mishra**, E. T. Marcial, S. Debata, A. N. Kolmogorov, and R. Margine, Stability-superconductivity map for compressed Na-intercalated graphite *Phys. Rev. B*, **110**, 174508 (2024).
8. P. Sahoo, **S. B. Mishra**, S. Debata, A. Sharma, B. Sahu, S. Padhan, R. Thangavel, B-K. Lee, Hydrothermally Grown Halogen-Doped ZnO Nanorods for Photoelectrochemical Water Oxidation: Experimental and DFT Insights *J. Phys. Chem. C*, **128**, 18711 (2024).
9. Abhijitha V. G., **S. B. Mishra**, and B. R. K. Nanda, Si_2BN nanosheets as anchoring cathode material for realizing high capacity Al-ion battery *J. Energy Storage*, **77**, 109913 (2024).
10. V. Ortiz, **S. B. Mishra**, L. Voung, S. Coh, and R. B. Wilson, Transient Ellipsometry Measurements of the Specular Inverse Faraday Effect in Transition Metals, *Phys. Rev. Mater*, **7**, 125202 (2023).
11. **S. B. Mishra** and S. Coh, Spin contribution to the inverse Faraday effect of nonmagnetic metals, *Phys. Rev. B*, **107**, 214432 (2023).
12. B. Biswal, **S. B. Mishra**, R. Yadav, S. Poudyal, R. Rajarapu, P. K. Barman, K. R. Pandurang, M. Mandal, R. Singh, B. R. K. Nanda, and A. Misra, Work Function of van der Waals Topological Semimetals: Experiment and Theory, *Appl. Phys. Lett.*, **120**, 093101 (2022).
13. Abhijitha V. G., **S. B. Mishra**, S. Ramaprabhu, and B. R. K. Nanda, Design of Aluminium ion battery with Graphyne host: Lowest volume expansion, High stability, and Low diffusion barriers, *Nanoscale Adv.*, **4**, 3870-3882 (2022).
14. S. Dey, A. Chakravorty, **S. B. Mishra**, N. Khatun, A. Hazra, B. R. K. Nanda, S. Chandran, D. Kabiraj, S. C. Roy, High energy ion induced modification in TiO_2 nanorods: thermal spike driven crystallinity, morphology and electronic structure transformation, *Nanoscale Adv.*, **4**, 241-249 (2022).
15. **S. B. Mishra**, Abhijitha V. G., S. Ramaprabhu, and B. R. K. Nanda, Graphdiyne-A promising Cathode Material for Aluminium dual ion Battery, *ACS Appl. Energy Mater.*, **4**, 7786-7799 (2021).
16. **S. B. Mishra**, S. Marutheeswaran, S. C. Roy, V. Natarajan, P.K. Rai, and B. R. K. Nanda, Adsorption and Degradation Mechanism of 2,4,6-TNT on TiO_2 (110) surface, *Surf. Sci.*, **713**, 171902 (2021).
17. J. Khatua, T. Arh, **S. B. Mishra**, H. Lutekens, A. Zorko, B. Sana, M.S.R. Rao, B. R. K. Nanda, and P. Khuntia, Development of Short and Long-range Magnetic order in the Double Perovskite-based Frustrated Triangular Lattice Antiferromagnet Ba_2MnTeO_6, *Sci. Rep.*, **11**, 6959 (2021).
18. **S. B. Mishra**, S. C. Roy, and B. R. K. Nanda, Electronic Structure of Graphene/TiO_2 Interface: Design and Functional Perspectives, *Appl. Surf. Sci.*, **542**, 148709 (2021).

19. **S. B. Mishra**, S. K. Yadav, D. G. Kanhere and B. R. K. Nanda, Fluorine Intercalated Graphene: Formation of a Two-dimensional Spin Lattice through Pseudoatomization, *Phys. Rev. Mater.*, **4**, 074411 (2020).

20. **S. B. Mishra** and B. R. K. Nanda, Facet Dependent Catalytic Activities of Anatase TiO_2 for CO_2 Adsorption and Conversion, *Appl. Surf. Sci.*, **531**, 147330 (2020).

21. P. Panigrahi*, **S. B. Mishra***, T. Hussain, B. R. K. Nanda and R. Ahuja, Density Functional Theory Studies of Si_2BN Nanosheets as Anode Materials for Magnesium Ion Batteries, *ACS Appl. Nano Mater.*, **3**, 9055 (2020) (*equal contribution).

22. S. Marutheeswaran*, **S. B. Mishra***, S. C. Roy and B. R. K. Nanda, Mechanistic Understanding of NO_2 Dissociation on a Rutile TiO_2(110) Surface: An Electronic Structure Study, *J. Phys. Chem. C*, **124**, 8786 (2020) (*equal contribution).

23. **S. B. Mishra**, A. Choudhary, S. C. Roy, and B. R. K. Nanda, Quantum-Mechanical Process of Carbonate Complex Formation and Large-scale Anisotropy in the Adsorption Energy of CO_2 on Anatase TiO_2(001) Surface, *Phys. Rev. Mater.*, **2**, 115801 (2018).

24. S. Samanta, **S. B. Mishra**, and B. R. K. Nanda, Quantum well Structure of Double Perovskite Superlattice and Formation of Spin-polarized Two-dimensional Electron gas, *Phys. Rev. B*, **98**, 115155 (2018).

25. **S. B. Mishra**, and B. R. K. Nanda, Virtual Synthesis of Crystals using *Ab initio* MD: Case study on $LiFePO_4$, *AIP Conf. Proc.*, **1832**, 090044 (2017).

UNDER PREPARATION

1. **S. B. Mishra**, R. Margine, and R. Akashi, Role of higher-order van Hove singularity effect on self-energy of H_3S.
2. **S. B. Mishra**, Inverse Faraday Effect in Ferromagnets.
3. Z. Liu, **S. B. Mishra**, and E. R. Margine, and R. Akashi, First principle study of transport properties of TaAs-family.
4. S. Tiwari, J. Lafuente-Bartolome, **S. B. Mishra**, M. Zacharias, S. Ponce, E. Kioupakis, E.R. Margine, and F. Giustino, EPWPy: An automated python framework for EPW.
5. Thermoelectric properties of AuX (X=S,Se) monolayers, **S. B. Mishra**, Kulwinder Kaur, and B. R. K. Nanda.
6. Strain Engineering in Monolayer Graphene: A Combined Tight-Binding and DFT Study, **S. B. Mishra**, M. Gupta, and B. R. K. Nanda.
7. Vacancy Induced Magnetic-Exchange Interactions in Graphene, **S. B. Mishra**, M. Harshavardhan, and B. R. K. Nanda.
8. S. Dey, **S. B. Mishra** and Somnath C. Roy, Gas sensing activities of TiO_2 after ion-irradiation.
9. A. B. Swain, **S. B. Mishra** and P. Bohm, Stronger femtosecond excitation and electron-phonon coupling in $BaTiO_3$.
10. **S. B. Mishra** and S. Marutheeswaran, Electronic and Mechanical properties of Heteronanothreads.

CONFERENCES AND WORKSHOPS (8 OUT OF 18)

S. B. Mishra, H. Mori, and R. Margine, First-order vertex corrections to phonon-mediated superconductivity in H_3S and Pb, *APS March 2025*, Anaheim.

S. B. Mishra, E. T. Marcial, S. Debata, A. N. Kolmogorov, and R. Margine, Stability-superconductivity map for compressed Na-intercalated graphite, *APS March 2025*, Anaheim.

S. B. Mishra, H. Mori, and R. Margine, First-principles study of phonon-mediated superconductivity beyond the Migdal approximation, *APS March 2024*, Minnesota.

S. B. Mishra and S. Coh, Inverse Faraday effect for transition metals, *APS March 2023*, Las Vegas.

S. B. Mishra and S. Coh, Theory of inverse Faraday effect for non-magnetic materials, *APS March 2022*, Chicago.

S. B. Mishra, S. C. Roy, and B. R. K. Nanda, Design and Electronic Structure Analysis of Graphene/Anatase TiO_2 (001) Interface, International Center for Theoretical Physics (ICTP), Italy, September 28-30, 2020.

S. B. Mishra, S. K. Yadav and B. R. K. Nanda, ICAMM, Rennes, France, 26 June-6 July, 2019.

TEACHING ASSISTANT (DEPARTMENT OF PHYSICS, IIT MADRAS, CHENNAI, INDIA)

- Designed, prepared, and taught Electronics laboratory exercises to 60 Engineering Physics students
- Prepared and taught Advanced Physics laboratory exercises to 50 Engineering Physics students

AWARDS & RECOGNITION

- **Young Scientist Award 2024** from Odisha Physical Society, Odisha, India
- **Prof. A. L. Lashkar Prize 2021** for **best Ph.D. thesis** in Physics, IIT Madras, India
- **Best Oral Presentation Award** at "**EESTER 2020**", organized by SRMIST, IIT Madras and Uppsala University
- **Young Scientist Scholarship** by DST, India as a Travel grant for attending "**ICAMM 2019**", Rennes, France.
- **Best Poster Award** at "**ICAFM 2017**", Anna University, Chennai, India.
- **First Prize on Evaluation Test** at "I2CAM 2017 School on Clean Energy", JNCASR, Bangalore, India.
- **Institute of Mathematics & Applications Scholarship** by DST, Govt. of Odisha, India (2011-2013).

ACADEMIC ACTIVITIES

- **PI for PHY250052 (2025-2026):** Received ACCESS credit of 150,000 as PI.
- **Session Chair in APS 2024:** Chair a focus session on Electrons, Phonons, Electron-Phonon Scattering, and Phononics in APS March meeting 2024.
- **APS DCOMP Member (2024 - Mar 2025):** Early career representative of APS DCOMP Divison.
- **APS ALM (2025):** Representative of APS DCOMP in Annual Leadership meeting held at Grand Hyatt, DC.
- **Peer Reviewer (2021-2022)**: Reviewer for Chemical Engineering Science, International Journal of Hydrogen Energy, Physics Letters A, Physical Chemistry and Chemical Physics, Solid State Communications, Computer Physics Communications, Scientific Reports, International Journal of Alloys and Compounds, and The Journal of Physics and Chemistry of Solids.
- **Workshop Facilitator (2024)**: TA at the School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows, June 9-16, 2024, University of Texas, Austin, USA.
- TA for hands-on exercises on Quantum ESPRESSO at Evolution of Electronic Structure and Experimental Realization (EESTER) 2018, organized by SRMIST and IIT Madras, India.
- **Developer Team Member**: Contributed to the development of the EPW (Electron-Phonon Physics) and Quantum ESPRESSO software packages.

REFERENCES

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UC Riverside, CA-92507, USA
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