SHASHI B. MISHRA

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RESEARCH SUMMARY

I am a theoretical condensed matter physicist working at the intersection of quantum many-body theory, computational materials science, and machine learning. Currently, I focus on pushing the boundaries of electron-phonon physics by developing methodologies that go beyond the Migdal approximation. These efforts enable more accurate predictions of superconducting properties in systems such as high-Tc hydrides where conventional adiabatic theories break down. I am also interested in integrating machine learning with first-principles calculations to accelerate the discovery of materials with tunable quantum properties, especially for transport and superconductivity applications. My research emphasizes bridging fundamental physics with real-world applications that include design of quantum materials for next-generation computing, light-induced magnetism for ultrafast devices, and materials for sustainable energy storage.

EDUCATION

Ph.D. in Physics March 2021
Indian Institute of Technology Madras, India
Dissertation: Ab initio Modelling and Functionalization of Graphene & TiO_2 Surfaces and Interfaces
Advisor: Prof. B. R. K. Nanda
Award: **Prof. A. L. Lashkar Prize for Best Ph.D. Thesis in Physics (2021)**

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

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

PROFESSIONAL APPOINTMENTS

Postdoctoral Researcher April 2023 - Present
Department of Physics, SUNY Binghamton, NY, USA
Advisor: Prof. Roxana Margine
- Developing first-order vertex corrections for electron-phonon interactions beyond Migdal approximation
- Implementing machine learning approaches to accelerate superconductor discovery
- Contributing to EPW (Electron-Phonon Wannier) code development
- Investigating transport properties of Weyl Semimetals

Postdoctoral Researcher April 2021 - March 2023
Department of Mechanical Engineering, University of California, Riverside, USA
Advisor: Prof. Sinisa Coh
- Formulated gauge-invariant theory for inverse Faraday effect in nonmagnetic metals
- Investigated light-induced magnetic phenomena for ultrafast magnetic switching applications

Project Officer June 2020 - March 2021
Indian Institute of Technology Madras, India
- Developed TiO_2-based materials for gas sensing and solar cell applications

RESEARCH INTERESTS

- **Quantum Many-Body Theory:** Phonon-mediated superconductivity, electron-phonon interactions, vertex corrections, strongly correlated systems
- **Superconductivity:** High-T_c cuprates, iron-based superconductors, nickelates, superconducting mechanisms beyond BCS theory
- **Topological Quantum Matter:** Topological superconductivity, Weyl and Dirac semimetals, topological phase transitions, quantum anomalous Hall effect
- **Transport Properties:** Electron-phonon limited transport, Berry phase effects on conductivity, anomalous transport in topological materials, ultrafast carrier dynamics

- **Machine Learning for Materials Physics:** ML-accelerated discovery of phonon-mediated superconductors, neural network potentials for electron-phonon coupling, data-driven approaches for predicting critical temperatures
- **Magnetism and Spintronics:** Altermagnets, frustrated magnetism, 2D magnetic materials, spin-orbit coupling effects, magnetic exchange interactions
- **Computational Materials Design:** High-T_c superconductors, 2D materials, heterostructures
- **Light-Matter Interactions:** Inverse Faraday effect, magneto-optics, ultrafast phenomena
- **Energy Materials:** Battery materials, photocatalysis, surface chemistry
- **Code Development:** Contributing to EPW and Quantum ESPRESSO packages

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. Y. Rambabu, **S. B. Mishra**, O. Henrotte, and E. Cortes, "Defects Dynamic in Photo-Excited CeO_2 and their Influence on CO_2 Photoreduction", *Adv. Funct. Mater.*, e13933 (2025).
3. **S. B. Mishra**, H. Mori, and E. R. Margine, "Electron-phonon vertex correction effect in superconducting H_3S" *arXiv:2507.01897* (2025), Under Review in *npj. Comp. Mat.*
4. Z. Liu*, **S. B. Mishra***, J.-M. Lihm, S. Poncé, and E. R. Margine, "Phonon-limited carrier transport in the Weyl semimetal TaAs," (*equal contribution) *arXiv:2505.16544* (2025), Revision in *Phys. Rev. B.*
5. X. Zhang, **S. B. Mishra**, E. R. Margine, and E. Kioupakis, "Cubic BeB_2: A metastable *p*-type conductive material from first principles", *arXiv:2506.00769* (2025), Revision in *Phys. Rev. B.*
6. A. Das, Preethi M., **S. B. Mishra**, N. C. Maji, P. Ningthoukhongjame, R. G. Nair, Abhijith T, A. S. Vasenko, Madhumitha R., "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" (Revision in *ACS Applied Materials & Interfaces*).
7. **S. B. Mishra**, E. T. Marcial, S. Debata, A. N. Kolmogorov, and E. 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. Vuong, 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. Luetkens, 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).

Manuscripts in 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**, and R. Margine, "Vertex correction, anharmonicity and isotope effect on superconductivity of H_3S"
3. **S. B. Mishra**, "Inverse Faraday Effect in Ferromagnets"
4. Z. Liu, **S. B. Mishra**, and E. R. Margine, "First principle study of transport properties of TaAs-family"
5. S. Tiwari, J. Lafuente-Bartolome, **S. B. Mishra**, M. Zacharias, S. Poncé, E. Kioupakis, E.R. Margine, and F. Giustino, "Automation and Abstraction for Many-Body Physics: Bridging complexity using EPWpy"
6. **S. B. Mishra**, K. Kaur, and B. R. K. Nanda, "Thermoelectric properties of AuX (X=S,Se) monolayers"
7. **S. B. Mishra**, M. Gupta, and B. R. K. Nanda, "Strain Engineering in Monolayer Graphene"
8. S. Dey, **S. B. Mishra**, and S. 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"

RESEARCH FUNDING

- **Principal Investigator**, PHY250052 (2025-2026): ACCESS computational resources, 150,000 credit hours
- **DST Young Scientist Travel Grant** (2019): International Conference ICAMM, Rennes, France

TEACHING EXPERIENCE

Teaching Assistant, Department of Physics, IIT Madras 2015-2018

- Designed and taught Electronics Laboratory (60 students)
- Taught Advanced Physics Laboratory (50 students)
- Developed course materials for Mathematical Physics

Workshop Instructor

- School on Electron-Phonon Physics, University of Texas, Austin (2024)

- EESTER Workshop on Quantum ESPRESSO, SRMIST/IIT Madras (2018)

AWARDS AND HONORS

- **Young Scientist Award 2024**, Odisha Physical Society
- **Prof. A. L. Lashkar Prize 2021** for Best Ph.D. Thesis in Physics, IIT Madras
- **Best Oral Presentation Award**, EESTER 2020 International Conference
- **DST Young Scientist Scholarship**, International Travel Grant (2019)
- **Best Poster Award**, ICAFM 2017, Anna University
- **First Prize**, I2CAM School on Clean Energy, JNCASR (2017)
- **Institute of Mathematics & Applications Scholarship**, DST India (2011-2013)

PROFESSIONAL SERVICE

Leadership Positions

- **Early Career Representative**, APS Division of Computational Physics (DCOMP) (2024-2025)
- **Session Chair**, APS March Meeting 2024: "Electrons, Phonons, and Electron-Phonon Scattering"
- **APS Annual Leadership Meeting**: Representative at Washington DC, DCOMP Division (2025)

Editorial Service

- Peer Reviewer: *Physical Chemistry Chemical Physics*, *Scientific Reports*, *International Journal of Hydrogen Energy*, *Computer Physics Communications*, *Chemical Engineering Science*, *Physics Letters A*, *Solid State Communications*, *International Journal of Alloys and Compounds*, and *The Journal of Physics and Chemistry of Solids*.

Software Development

- Developer Team Member: EPW (Electron-Phonon Wannier) code
- Contributor: Quantum ESPRESSO package

SELECTED PRESENTATIONS (8 OF 18 TOTAL)

- "Stability-superconductivity map for compressed Na-intercalated graphite," *APS March Meeting*, Anaheim (2025)
- "Phonon-mediated superconductivity beyond the Migdal approximation," *APS March Meeting*, Minnesota (2024)
- "Inverse Faraday effect for transition metals," *APS March Meeting*, Las Vegas (2023)
- "Theory of inverse Faraday effect for non-magnetic materials," *APS March Meeting*, Chicago (2022)
- "Formation of 2D spin lattice in fluorinated graphene," *EESTER International Conference* (2020)
- "Design and Electronic Structure Analysis of Graphene/Anatase TiO_2 Interface," *ICTP*, Italy (2020)
- "Induced Magnetism in Graphene Bilayer," *ICAMM*, Rennes, France (2019)

TECHNICAL SKILLS

Computational Methods: DFT, electron-phonon interactions, Wannier functions, molecular dynamics, machine learning
Software: Quantum ESPRESSO, VASP, EPW, Wannier90, WannierBerri, Gaussian
Programming: Python, MATLAB, Bash, Fortran
HPC: Experience with parallel computing, job scheduling (SLURM), optimization

REFERENCES

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