Rajender Prasad Tiwari, Ph.D.

Assistant Professor
Department of Electronics
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Education

- Ph.D. (Nanoscience, 2021), Jawaharlal Nehru University, New Delhi, India
  Thesis title: "Ferroelectric oxides and van der Waals materials for photovoltaic applications: experiment and theory".
- Master of Science (Electronic Science) 2012, Jamia Millia Islamia, New Delhi, India.
- Bachelor of Science (Electronics Hons.) 2009, Hansraj College, University of Delhi, India.
- UGC NET-JRF (Electronic Science) 2015.
- UGC NET-JRF (Electronic Science) 2014.

Positions Held

- Assistant Professor (Permanent, since 10/2022), Department of Electronics, Hansraj College, DU.
- Young Scientist, Post Doctoral Fellow (04/2021 – 10/2022), Asia Pacific Center for Theoretical Physics, South Korea.
- System Engineer (10/2012 – 08/2015), Tata Consultancy Services, India.

Teaching Experience

Since 10/2022 – Present

Subjects:

- Digital Electronics and HDL.
- Analog Electronics.
- Programming Fundamentals using Python.
- Printed Circuit Board Designing.

Grants and Awards

- Young Scientist Training Program, South Korea. Funded 80M KRW.
- Junior Research Fellowship and Teaching Assistantship award from the Government of India, 2015-2020.
- Graduate Aptitude Test in Engineering (GATE)-2015.
- Best poster presentation award on the title "Origin of ferroelectricity in $KNbO_3$: A DFT study" on national science day, February 2019, Jawaharlal Nehru University, India.

Contribution To Committees/ Administrative work in College

- HRC Journal of Contemporary Science, Managing Editor.
- HRC Research Cell, Department representative.
- Hostal Admissions, Department representative.
- NAAC criteria 5.2, Student Progression.

Recent Training/Workshop/Webinar

- One-month faculty induction program/orientation course.
- Webinar: Transistor Discovery and Microelectronics Evolution.
- Webinar: Horizons of High-Energy Physics

Mentorship and Supervision

- Mentoring graduate students via the HRC Mentorship program.
- Mentored and supervised the M.Tech. and M.Sc. students in their six months major, and three months minor projects.

Research Specialization

Materials modeling and simulation using density functional theory, molecular dynamics, and many-body perturbation theory of 3D bulk and two-dimensional materials for bulk photovoltaic applications. Synthesis and characterization of perovskite materials using various techniques. Photovoltaic device fabrication using RF-DC magnetron-sputtering system, pulsed laser deposition system, and spin coating.

Research Interests

Condensed Matter Physics: Theoretical exploration of various material systems for novel applications and implement the theoretical results in experiments to fabricate highly efficient devices.

Electronic Devices: Simulation and modeling of electronic devices, with a particular focus on understanding the fundamental physics underlying their behavior.

Research Milestones

Asia Pacific Center for Theoretical Physics, South Korea, 04/2021-10/2022
(Young scientist postdoctoral researcher)

- Worked independently on a project titled "Theoretical development of a pathway for achieving enhanced photoconversion efficiency via bulk photovoltaic effect for next-generation solar cells".
- Using first-principles calculations, it is discovered that lead-free oxychalcogenide perovskites are a promising alternative to the toxic lead-halide hybrid and bulky complex oxide perovskites for the bulk photovoltaic effect (BPVE) application. The bulk photovoltaic properties of this novel class of materials are

convincingly demonstrated by calculating the shift current in the $KNbO_{3-x}Q_x$ (x=0, 1, 2; Q=S, Se) oxychalcogenides. Furthermore, to provide a more realistic view of these materials for optoelectronic applications, the state-of-art many-body perturbation theory (MBPT) is used to investigate their excited state properties.

- In a significant breakthrough in addressing the major challenges of organometal perovskites in large-scale application of perovskite-based solar cells, a novel Rashba ferroelectric semiconductor 'α-GeTe' is proposed which is endowed with ferroelectricity and the spin degree of freedom that can be exploited to improve the bulk photovoltaic efficiency. Further, it is discovered that, in contrast to the conventional perovskite ferroelectrics, the characteristic features of the 3D-bulk α-GeTe are retained up to its 2D-nanostructure limit and an enhanced photoconversion is possible via BPVE at this nanoscale limit.

Jawaharlal Nehru University, India, 08/2015-04/2021
(Graduate researcher)

- Investigated and engineered, both experimentally and theoretically, the BPVE properties of ABO_3 ferroelectric perovskites such as $KNbO_3$ and its derivatives, and 2D van der Waals materials (α-In_2Se_3, h-NbP) for the fabrication of highly efficient solar cells.
- Using DFT calculations I established for the first time that the electronic and optical properties of $KNbO_3$ can be tuned suitable for the BPVE applications by applying the triaxial tensile strain which can be achieved experimentally by doping $KNbO_3$ by a bigger-sized dopant than Nb^{5+} at B-site. The $KNbO_3$-based ferroelectric and multiferroic complex compounds are realized by doping, investigating their optical and electronic properties, and fabricating thin-film solar cell devices based on these materials.
- Elucidated for the first time that, of the co-existing in-plane and out-of-plane polarization in α–In_2Se_3, the shift current BPVE response of this 2D material is influenced *only* by the former component of the polarization. Also, the tuning of shift current in the visible light is possible by doping *only* at the tetrahedral site.
- Successfully demonstrated using DFT study that the monolayered buckled-honeycomb and puckered-tetragonal 2D lattice forms of NbP are naturally derivable from the (110) and (001) orientations, respectively, of its bulk Weyl semimetallic form. The physical properties of these monolayers are spectacularly different as the tetragonal lattice is metallic, and the honeycomb lattice is a semiconductor, exhibits intrinsic ferroelectricity originating from a rare sd^2-sp^2 hybridization, and yields a large shift current response at the atomistic thickness of 1.21 Å.

Research Skills

A. Software Skills

Analytical and computational tools	Quantum Espresso, QuantumWise, VASP, FULLPROF, EAGLE, XILINX, Z-View, VESTA, Origin, Image-J.

Programming Languages	Assembly language 8085/86 Microprocessor, C#, C++, Python, HTML, UNIX, PL-SQL, FORTRAN, and MATLAB.
Operating Systems	Ubuntu, Windows.

B. Technical Skills

Operation and Maintenance of-

- Dell Servers for computational works
- RF-DC sputtering system
- Rigaku X-ray diffractometer
- UV-Vis-NIR spectrometer.
- WITec Raman spectroscopy
- Radiant and aixACCT ferroelectric test systems
- Wayne-Kerr Impedance Analyzer
- High and low-temperature furnaces

C. Experimental Skills

- Characterization of samples using X-ray Diffraction (XRD), Raman spectroscopy, Dielectric measurement, P-E hysteresis of bulk and thin films, Ellipsometry, Impedance spectroscopy, UV-Visible-NIR spectroscopy.
- Rietveld Refinement of XRD data.
- Characterization using Secondary Electron Microscopy (SEM), Energy Dispersive X-Ray (EDX), Atomic Force Microscopy (AFM), M-H hysteresis, and solar cell simulator.
- Cross-sectional Transmission Electron Microscopes (TEM) sample preparation.
- Thin-film deposition (metals, oxides, and magnetic materials) using RF-DC sputtering system, pulsed laser deposition (PLD), and spin coating.

Recent Publications

[1] **R. P. Tiwari** "Visible-Light-Activated Enhanced Shift Current Bulk Photovoltaic Effect in Lead-Free Oxychalcogenide Perovskites: Emergence of Fully Inorganic Photovoltaic Materials" *J. Phys. Chem. C*, vol. 126, no. 25, pp. 10258–10265, 2022.

[2] **R. P. Tiwari**, "Enhanced Shift Current Bulk Photovoltaic Effect in Ferroelectric Rashba Semiconductor α-GeTe: Ab Initio Study from Three- to Two-dimensional van der Waals Layered Structures" *J. Phys.: Condens. Matter*, vol 34, no. 43, pp. 435404, 2022.

[3] **R. P. Tiwari**, B. Birajdar, and R. K. Ghosh, "First-principles calculation of shift current bulk photovoltaic

effect in two-dimensional α–In_2Se_3," *Phys. Rev. B*, vol. 101, no. 23, pp. 235448–235456, 2020.

[4] **R. P. Tiwari**, S. Z. H. Hashmi, R. Sharma, S. A. Khan, and B. Birajdar, "Synthesis of highly pure and dense 0.9($KNbO_3$)—0.1($BaNi_{1/2}Nb_{1/2}O_{3-\delta}$) ceramic with superior magnetic properties," *J. Am. Ceram. Soc.*, vol. 102, pp. 4659–4669, 2019.

[5] **R. P. Tiwari**, B. Birajdar, and R. K. Ghosh, "Strain engineering of ferroelectric $KNbO_3$ for bulk photovoltaic applications: an insight from density functional theory calculations," *J. Phys. Condens. Matter*, vol. 31, pp. 505502–505512, 2019.

[6] **R. P. Tiwari**, J. Shah, R. K. Kotnala, and B. Birajdar, "Electrical microstructure properties of 0.9$KNbO_3$—0.1($BaNi_{1/2}Nb_{1/2}O_{3-\delta}$) electroceramic," *J. Alloys Compd.*, vol. 753, pp. 642–645, 2018.

[7] **R. P. Tiwari**, V. Kumar, S. Singh, J. Shah, R. K. Kotnala, and B. Birajdar, "Structural phase transition, impedance spectroscopy and narrow optical band Gap in (1-x)$KNbO_3$—x $Ba(Sc_{1/2}Nb_{1/2})O_3$," *J. Eur. Ceram. Soc.*, vol. 38, pp. 1427–1433, 2018.

[8] **R. P. Tiwari** and B. Birajdar, "Ferroelectric, magnetic and optical properties of Ba and Sc co-doped $KNbO_3$," in *AIP Conference Proceedings*, 2018, p. 030014.

[9] **R. P. Tiwari**, B. Birajdar, and R. K. Ghosh, "Intrinsic ferroelectricity and large bulk photovoltaic effect in novel two-dimensional buckled honeycomb-like lattice of NbP: first-principles study" *J. Phys. Condens. Matter*, vol. 33, pp. 385302-9, 2021.

[10] **R. P. Tiwari**, B. Birajdar, and M. Saini, "Effect of $Ba(M_{0.5}Nb_{0.5})O_{3-\delta}$ (M=Ni^{2+}, Sc^{3+}) doping in $KNbO_3$: a Comparative Study of 10KBNNO and 10KBSNO", *HRC-JCS*, 2023.

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