

CAREER OBJECTIVE

Dedicated Physics researcher and educator with a Ph.D. in Computational Material Science, specializing in DFT simulations and nanomaterial-based toxic gas sensing. Committed to fostering a dynamic and intellectually stimulating learning environment through innovative teaching methodologies, interdisciplinary research collaborations, and mentorship. Currently serving as an Assistant Professor, with a focus on effective undergraduate teaching, laboratory instruction, student mentoring, and research in computational materials science.

EXPERTISE

Computational Material Science | Density Functional Theory (DFT) | Nanomaterial-Based Toxic Gas Sensing | Solid-State Physics | Electronic Structure Calculations | Research Mentorship & Student Guidance | Curriculum Development | Interdisciplinary Research Collaboration | Scientific Writing & Publications | Advanced Physics Laboratory Instruction

EDUCATION QUALIFICATIONS

Doctor of Philosophy (PhD) in Physics

Sep 2021 – Mar 2025

The Maharaja Sayajirao University of Baroda

- **Thesis Title:** Development of Toxic Gas Sensors using 2D Materials: A First Principles Study
- **Supervisor:** Dr. Keyur N. Vyas

Master of Science in Physics

Jun 2016 – Jun 2018

The Maharaja Sayajirao University of Baroda

- **Specialization:** Spectroscopy
- **CGPA:** 6.52

Bachelor of Science in Physics

Jun 2013 – Jun 2016

The Maharaja Sayajirao University of Baroda

- **CGPA:** 6.76

ACHIVEMENT AND ACADEMIC EXCHANGE

- **Invited Research Visit:** May 2023
 - Received a formal invitation from the Faculty of Mechanical Engineering, Bialystok University of Technology, Poland, under the **NAWA-PROM academic exchange program** by the Government of Poland.

TEACHING EXPERIENCE

Assistant Professor

Sep 2026 – Present

Usha Mittal Institute of Technology, SNDT Women's University, Mumbai, Maharashtra

- Conducting lectures and laboratory sessions and supporting students in developing strong conceptual and analytical skills.
- Teaching Physics to undergraduate engineering students.
- Contributing to academic activities, student mentoring, and curriculum-related initiatives.

Temporary Assistant Professor

Aug 2021 – Jun 2023, Jun 2024 – Jun 2025

Department of Physics, The Maharaja Sayajirao University, Vadodara.

- Delivered engaging lectures on Thermodynamics, Classical Mechanics to undergraduate and postgraduate students.
- Supervised student research projects and dissertations, fostering scientific curiosity and analytical skills.
- Developed innovative laboratory experiments integrating real-world applications of physics concepts.
- Actively participated in curriculum development, ensuring alignment with industry and research advancements.
- Organized seminars, guest lectures, and student workshops on advanced topics in physics.

Ad-hoc Lecturer

Jun 2019 – Jan 2021

V.S. Patel College of Arts & Science, Veer Narmad South Gujarat University, Bilimora.

- Taught Classical Mechanics ensuring a strong conceptual foundation for students.
- Designed and conducted laboratory sessions, incorporating experimental techniques and error analysis methods.
- Provided academic mentorship, assisting students in project work and career guidance.
- Developed innovative laboratory experiments integrating real-world applications of physics concepts.

TECHNICAL SKILLS

- **Computational Tools:**
 - Density Functional Theory (DFT) Codes: **Quantum Espresso**
 - Electronic Transport Simulation: **BoltzTrap**
 - Material Visualization Software: **Xcrysden, VESTA**
 - Data Analysis & Office Automation: **OriginLab**, MS Office
- **Soft Skills:**
 - Research writing & Scientific communication
 - Mentorship & Student Engagement
 - Curriculum Design & Academic Leadership

RESEARCH INTERESTS

- Computational modelling of hazardous gas adsorption on 0D and 2D nanomaterials.
- Hydrogen evolution and storage studies for energy applications.
- Application of DFT-based simulations in material property analysis.
- Development of new sensing materials for industrial and environmental applications.

CONFERENCE AND PRESENTATIONS

- **International Union of Materials Research Society – International Conference in Asia (IUMRS-ICA 2024)**
 - **Poster Presentation**, Devi Ahilya Vishwavidyalaya, Indore, India.
- **Advances in Materials Science: Challenges and Opportunities (AMSCO-2023)**
 - **Poster Presentation**, Maharaja Krishnakumarsinhji Bhavnagar University.
- **Solid State Physics Symposium (DAE-SSPS 2022)**
 - **Poster Presentation**, BIT-Mesra, Ranchi.

PUBLICATIONS

1. Heli Mistry, Darshil Chodvadiya, Shardul Vadalkar, Keyur N. Vyas, and Prafulla K. Jha.
“Interaction study of CO and NO pollutant gases with pristine, defected, and doped α -CX (X= N, P) monolayers using density functional theory” - Surfaces and Interfaces 46 (2024): 103958
DOI: [10.1016/j.surfin.2024.103958](https://doi.org/10.1016/j.surfin.2024.103958)
2. Heli Mistry, Bhautik R. Dhori, Maitry Joshi, Keyur N. Vyas, and Prafulla K. Jha.
“Hazardous CO, NO, NH₃ Gases over Boron and Beryllium Doped α -CN Monolayers: A First Principles Study for Sensing and Removal Applications.” - Materials Chemistry and Physics 327 (2024): 129875
DOI: [10.1016/j.matchemphys.2024.129875](https://doi.org/10.1016/j.matchemphys.2024.129875)
3. Shardul Vadalkar, Darshil Chodvadiya, Heli Mistry, Narayan N. Som, Keyur N. Vyas, and Prafulla K. Jha.
“Toxic gas removal using transition metal-decorated Cyclo [18] carbon: A first principles prevision.” Computational and Theoretical Chemistry 1238 (2024): 114724
DOI: [10.1016/j.comptc.2024.114724](https://doi.org/10.1016/j.comptc.2024.114724)
4. Heli Mistry, Shardul Vadalkar, Keyur N. Vyas, and Prafulla K. Jha.
“Adsorption Mechanism of Ni Decorated α -CN Monolayer towards CO, NO, and NH₃ Gases: Insights from DFT and Semi-classical Studies” - Materials Science in Semiconductor Processing 186 (2025): 109106
DOI: [10.1016/j.mssp.2024.109106](https://doi.org/10.1016/j.mssp.2024.109106)

EXTRA CURRICULAR ACTIVITIES

- BA (Visharad) in Hindustani Classical Vocal
- Intermediate-level proficiency in Harmonium and Sitar
- Performed in cultural events and academic gatherings, integrating music with science education

REFERENCES

1. **Prof. Prafulla K. Jha**
HOD, Department of Physics
The Maharaja Sayajirao University of Baroda
Email: prafullaj@yahoo.com
2. **Mr. Sanjeev R. Kane**
Scientific Officer -H
Raja Ramanna Centre for Advanced Technology (RRCAT), Indore
Email: kanesanjeev@gmail.com