Bhakti Mangesh Kshirsagar

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Professional Summary

I am a final-stage PhD candidate in Computational Materials Science and recently submitted my thesis. I have good experience in Density Functional Theory (DFT). Skilled in calculating and analyzing structural, electronic, optical, polarization, thermodynamic, and mechanical properties of materials. Experienced in scripting using Fortran and Python for scientific computing and automating workflows with Bash on HPC clusters. Demonstrated ability to publish research in peer-reviewed journals and present findings at national and international conferences.

Education

- Ph.D. (Physics) thesis-submitted : *Savitribai Phule Pune University, India*,
  Thesis: Ab-initio DFT-based Investigations on Some Perovskites
- M.Phil. (Physics), 2017 : A Grade, *Savitribai Phule Pune University*
- M.Sc. (Physics), 2010 : B^+ Grade, *University of Pune*
- B.Sc. (Physics), 2008 : 87.16%, *University of Pune*

Awards

- Qualified State Eligibility Test (SET) for Assistant Professorship (2016)
- Department of Science and Technology Women Scientist - A Research Fellowship (DST-WOS-A) (2020-2023)

Research Work Experience

Ph.D. Research — Computational Materials Science

- Conducted DFT-based investigations on materials for optoelectronics, piezoelectrics, spintronics, photocatalysis, and hydrogen fuel cell applications.

M.Phil. Research — Nuclear Battery Development

- Developed a nuclear battery using radioactive sources.
- Investigated radiation effects on MOSFETs as dosimeters.

Teaching Experience

- Lecturer at H.V. Desai College, Pune (PG level).
- Lecturer at New Arts, Commerce, and Science College, Ahmednagar.

- Visiting Lecturer at Bakulabai Tambat Nursing College, Pune.

Publications

1. J. Phys. Chem. C (2021): DFT study on $CsSnX_3$ quantum dots for photovoltaics.
2. Mater. Chem. Phys. (2023): $BaSnTiO_3$ as a lead-free analogue to $PbTiO_3$.
3. Comput. Condens. Matter (2024) : Dopant effects in $GaNbO_4$ for photocatalysis.
4. AIP Conf. Proc. (2024) : Pressure-dependent properties of $BaSnTiO_3$.

Certifications and Training

- Basic Linux Workshop (SPPU, 2015)

Selected Conferences and Workshops

- AAPALI PSI-K, International Conference on Density Functional Theory and Applications (2025)
- Asia-Pacific Condensed Matter Physics Conference (2021)
- Webinar Series on Simulation Methods (2020-2021)