Indian Institute of Science Education and Research Bhopal

Advertisement for the Post of Two Junior Research Fellow (J.R.F.)

Supervisor: Dr. Apurba Nandi, Department of Chemistry

Project: Development of Data-Driven Machine-learned Interatomic Potentials for Quantum Molecular Simulations of Condensed-Phases and Reaction Dynamics

Duration: 1 year, with potential continuation toward PhD subject to performance and Institute criteria

Eligibility:

- Master's degree with ≥60% or 7.0 CPI/CGPA + at least one national-level qualification (UGC-JRF/CSIR-JRF/NET-LS/JEST/valid GATE score etc.)
- Or completed BS-MS form National level institutes such as IIT/IISER/IISc with ≥ 8 CPI.

Disciplines: Chemistry | Chemical Engineering | Physics | Data Science | Computer Science | Related fields

Fellowship: Rs. 37000/- +HRA (20 %)

No. of positions: 2 JRF position

Last date of application: 4th November, 2026

Preferable Skills: Candidates with experience in computer programming (Python, C++, Fortran, etc.), data analysis, molecular dynamics (MD) simulations, and algorithm development will be preferred.

Applications are invited for a **Junior Research Fellow (JRF)** position in an interdisciplinary research project focused on developing **data-driven interatomic potentials for molecular simulations of condensed-phase systems and chemical reaction dynamics**.

The project lies at the exciting intersection of **Artificial Intelligence/Machine Learning, Quantum Molecular Simulations, Computational Chemistry, and Molecular Dynamics Simulations.** The selected candidate will have the opportunity to develop and apply modern **AI/ML-based approaches** to learn molecular interactions from quantum-mechanical data and use them for large-scale simulations of chemically complex systems.

This is an excellent opportunity for candidates interested in working at the interface of Artificial Intelligence and Quantum Molecular Simulations. The project will provide hands-on exposure to both AI/ML-based data-driven approaches and quantum-mechanical molecular simulations, offering an opportunity to develop skills at the rapidly growing intersection of computational science and AI-driven molecular research.

How to Apply: Candidates with an interest in combining AI/ML with quantum molecular simulations are particularly encouraged to apply. Interested candidates should submit a cover letter, detailed CV, valid NET/GATE/JEST qualifying certificate with rank, names and contact details of one or two referees, and a brief description of prior research experience. Applications should be submitted by email only to **Dr. Apurba Nandi** at apurba@iiserb.ac.in on or before 4th November 2026. Incomplete applications will not be considered and no correspondence will be entertained in this regard. Only shortlisted candidates will be notified with the date of the interview. The interview will be via online platform.

Contact address of the PI:

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