

Computational Materials Discovery group at IIT Gandhinagar has an immediate opening for a postdoctoral position. The appointment is on a one-year basis, with a maximum term of three years, subject to satisfactory research performance and continued availability of funding.

Project: Optimizing Ligand-Perovskite Nanocrystal Interfaces for Enhanced CO₂ Photoreduction: A Computational Framework.

Job title: Post-Doctoral Researcher.

Employment period: 12 months.

Fellowship: INR 72,000/- to 84,000/- per month (Consolidated).

Essential qualification: Ph.D. in Chemistry, Physics, Materials Science, Chemical Engineering, or related discipline. The percentage/grade points with respect to the academic qualifications will be a minimum of 60% or equivalent grade from Graduation onward and 55% or equivalent grade in class 10th and 12th.

Preferred skills: Prior experience in two or more of the following areas: Density Functional Theory, *Ab initio* Molecular Dynamics, Classical Molecular Dynamics, and Kinetic Monte Carlo. Excellent programming abilities (preferably in Python, Fortran, or C++), analytical skills, and knowledge of high-performance computing are also required. Expertise in high-throughput computing, machine-learning methods, and optimization methods will be an added advantage.

Documents required:

1. A detailed CV indicating academic track records, fellowships, awards, publications, contributed/invited talks and poster presentations, and computational expertise.
2. One cover letter explaining why the candidate is suitable for the advertised position.
3. A short research statement (not more than 1 page).
4. Two letters of recommendations, should be sent directly to the email id: amondal@iitgn.ac.in.
5. A scanned copy of a Ph.D. certificate (a formal confirmation of a Ph.D. degree or thesis expected to be submitted). The selected candidate must provide originals of all degree certificates for verification. Failure to do that will cancel the position.

Application procedure: Candidates must send their applications along with the required documents as a single pdf file to the email id: amondal@iitgn.ac.in.

Last date of application: February 6, 2026.

In case of any queries, please contact:

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