



INDIAN INSTITUTE OF TECHNOLOGY GANDHINAGAR

Research & Development Office

ADVERTISEMENT NO. OTH/13515/Advt0307 DATED 31.08.2026

Applications are invited for a temporary position of **Post-Doctoral Fellow** at IIT Gandhinagar.

The details are as below:

Name of PI	Prof. Anirban Mondal	Department	Chemistry
Project title	Data-Driven Inverse Design of Multifunctional TADF Materials for Optoelectronics, Photocatalysis, and Solar Thermal Storage		
Designation	Post-Doctoral Fellow		
Number of positions	1		
Application Link	http://recruitment.iitgn.ac.in/projectstaff/		
Last date of application submission	20-09-2026		
Consolidated Monthly Remuneration	Rs. 1,00,000/- per month		
Duration of appointment	01 year, extendable subject to performance and fund availability.		
Eligibility Norms	☒ Institute norms ☐ Funding Agency norms		
Essential Qualification/Experience as per the norms	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 10 th and 12 th .		
Desirable Qualification/Experience	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.		
Job Description	The selected candidate will work on the computational and data-driven design of multifunctional TADF (organic/inorganic) materials for optoelectronics, photocatalysis, and solar thermal storage. The work will involve quantum-chemical calculations, molecular simulations, high-throughput screening, machine learning, and optimization to establish structure–property relationships and identify promising materials, along with development of computational workflows using Python/Fortran/C++ on high-performance computing platforms.		

For Query, Please Contact
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“Merely meeting the minimum eligibility criteria will not guarantee the shortlisting and/or appointment. A higher cutoff level may be used. The Institute reserves all rights, not to call an applicant for a selection test or not to fill up a position through this round of selection process without assigning any reason.”