Indian Institute of Technology Delhi

School of Interdisciplinary Research (SIRe)

Project Proposal for Ph.D.

SIRe Project Number

2025-01-12

(will be assigned by SIRe)

Project Details	
Project Title	Graph based Generative Models for Materials Discovery
Project Summary (Minimum 500 and maximum 2000 characters)	This research project explores the application of graph-based generative models to accelerate the discovery and design of novel materials with targeted properties. By representing materials as graphs—where atoms are nodes and chemical bonds are edges—these models can capture complex structural relationships and property correlations that traditional computational methods may overlook. The approach leverages recent advances in graph neural networks and deep generative frameworks to learn the underlying distribution of existing materials, enabling both the prediction of properties for candidate materials and the inverse design of new structures with desired characteristics. This computational framework aims to navigate the vast chemical space more efficiently than conventional high-throughput screening methods, potentially reducing the time and resources required for materials development in applications spanning energy storage, catalysis, and electronic devices.

Ph.D. Supervisors

Role	Name of Faculty	Academic Unit in IITD/Institute/University	Email ID (Official)
Supervisor 1	N. M. Anoop Krishnan	Department of Civil Engineering, Yardi School of Artificial Intelligence	krishnan@iitd.ac.in
Supervisor 2	Sayan Ranu	Department of Computer Science and Engineering, Yardi School of Artificial Intelligence	sayanranu@iitd.ac.in

Project requirements (Student qualifications, experience required, etc)
***The candidate will be shortlisted based on common shortlisting criteria decided by ScRC (SIRe)**

- B.Tech. with a valid GATE score or M.Tech. in Civil/Mechanical/Electrical/Materials Science/Computer Science or allied disciplines or M.Sc. in physics with CSIR/JRF or MCA or any other equivalent degree.
- Candidates with prior experience in machine learning related projects is preferred.
- Candidates with background in materials/physics is preferred.

Source of fellowship/funding
(CSIR/UGC/DBT/ICMR/ICAR/NEET-PG/DST-INSPIRE/IRD/FITT Project details, if any)

Candidate with his/her own fellowship/ Project fellowship

Role of Faculty Members involved:	
Supervisor-1	Physics-based modeling and materials modeling.
Supervisor-2	Development of ML and GNN algorithms.