



Project Proposal for Ph.D.

Project Details (The research problem must clearly indicate the need for an interdisciplinary approach)

Project Title	Knowledge distillation for atomistic simulations
Project Summary (Minimum 500 and maximum 2000 characters)	This project aims to develop high-fidelity interatomic potentials for atomistic simulations through knowledge distillation techniques that transfer learned representations from large-scale foundation models to specialized, computationally efficient domain-specific models. By leveraging the comprehensive chemical and physical understanding encoded in foundation models trained on vast datasets of atomic structures and properties, we will distill this knowledge into smaller, targeted models optimized for specific material systems or simulation tasks. This approach promises to combine the accuracy and generalizability of foundation models with the computational efficiency required for large-scale atomistic simulations, enabling researchers to perform extensive molecular dynamics studies, property predictions, and materials discovery workflows that would otherwise be computationally prohibitive. The resulting domain-specific interatomic potentials will maintain the predictive power of their foundation model teachers while achieving the speed and scalability necessary for practical applications in materials science, chemistry, and engineering.

Ph.D. Supervisors*
(Supervisor 1 and Supervisor 2 cannot be from the same department of IITD)

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

*Supervisor 1 must be from IIT, Delhi.
+All cells in this table are mandatory fields that need to be filled by faculty for consideration of proposal.
\$The date of superannuation of supervisors should be at least three years from the date of registration of selected candidates.

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. Part-time candidates may also be considered.
- Candidates with prior experience in machine learning related projects is preferred.

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

Candidates with his/her own fellowship/ Project Fellowship/Part-time

Role of Faculty Members involved:

Supervisor-1	Atomistic modeling
Supervisor-2	Graph neural networks and knowledge distillation

Note :-

- 1. Approval from the respective DRC/CRC/ScRC of your Department/Centre/School will be required for using the "Full-time Institute Assistantship (Category-wise) (FIA)" for selecting the students in SRe.**
- 2. Declaration:- Faculty members, please ensure that you have at least 3 years of service left before superannuation along with adequate sitting space & lab facilities for the SRe student.**
- 3. PI/s are also encouraged to submit joint proposals with AIIMS, NII, JNU and institutes with which IITD has an existing MoU. If the Co-PI (Supervisor 2) is from outside IITD, kindly share his/her detailed CV.**
- 4. If a research scholar is to be considered for selection under the project fellowship, then the project should have a minimum of two-year duration remaining.**
- 5. A candidate applying with a valid JRF/INSPIRE/any national level fellowship should have at least two-year validity from the date of joining the Ph.D. program.**
- 6. The third supervisor's name (if required) can be added only after the formation of Student Research Committee (SRC) subject to a strong recommendation of SRC and subsequent approval from the competent authority.**
- 7. If Institute fellowship is being sought, then DRC approval of the parent department of Supervisor 1 is required at the time of selection.**