

# Kishalay Das

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📄 <https://kdmsit.github.io/>

## Research Interest

I am broadly interested in **Graph Representation Learning**, **Geometric Deep Learning**, and **Generative Modeling**, with a particular focus on their applications in **AI for Science** and **AI for Medicine**.

## Education

- 2022 - 2025 **Ph.D. in Computer Science**, *Indian Institute of Technology(IIT)*, Kharagpur, India, **GPA: 9.5/10**.  
◦ **Research Objective :** *AI for Scalable Material Generation and Property Prediction*.  
Advisors: **Prof. Niloy Ganguly** and **Prof. Pawan Goyal**
- 2018 - 2020 **M.Tech. in Computer Science**, *Indian Institute of Science(IISc)*, Bangalore, India, **GPA: 8.8/10**.  
◦ **Thesis:** *Graph Neural Network on Hypergraphs by Learning Line Graph Expansion*  
Advisor: **Prof. M. Narasimha Murty**
- 2008 - 2012 **B.Tech. in Computer Science**, *West Bengal University of Technology*, Kolkata, India, **GPA: 8.37/10**.

## Publications

- Subhojyoti Khastagir\*, Kishalay Das\*, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **LLM Meets Diffusion: A Hybrid Framework for Crystal Material Generation**. accept in *NeurIPS 2025* [Paper][Code]
- Kishalay Das, Subhojyoti Khastagir, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **CrysLDM: Latent Diffusion Model for Crystal Material Generation**. accept in *AI4MAT-ICLR-2025* [Paper]
- Kishalay Das, Subhojyoti Khastagir, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **Periodic Materials Generation using Text-Guided Joint Diffusion Model**. accept in *ICLR 2025* [Paper][Code]
- Kishalay Das, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **"CrysMMNet: Multimodal Representation for Crystal Property Prediction."** accept in *UAI 2023* [Paper][Code]
- Kishalay Das, Bidisha Samanta, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **"CrysGNN : Distilling pre-trained knowledge to enhance property prediction for crystalline materials"** accept in *AAAI 2023*, *ML4Materials Workshop @ ICLR-2023* [Paper][Code]
- Kishalay Das, Bidisha Samanta, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **"CrysXPP: An Explainable Property Predictor for Crystalline Material"** accept in *NPJ Computational Materials, 2022* [Paper][Code]
- Sambaran Bandyopadhyay, Kishalay Das, M Narasimha Murty, **"Hypergraph Attention Isomorphism Network by Learning Line Graph Expansion"** *2020 IEEE-Big Data* [Paper][Code]
- Sambaran Bandyopadhyay, Kishalay Das, M Narasimha Murty, **"Line Hypergraph Convolution Network: Applying Graph Convolution for Hypergraphs"** *arXiv, 2020* [Paper]

## Research Experiences

Jul,2020 - Dec, 2021 **Research Assistant**, IIT Kharagpur, CNeRG Group.

## Work Experience

- May,2017 - Jul,2018 **Scientist/Engineer-SC**, *Indian Space Research Organisation (ISRO)*, Bangalore.
- Mar,2013 - Apr,2015 **System Engineer**, *Tata Consultancy Services (TCS)*, Kolkata.
- Jul,2012 - Feb,2013 **Associate Software Developer**, *Accenture Pvt. Ltd.*, Hyderabad.

## Academic Services

- PC Member at AAAI 2026, IJCAI 2025, AAAI 2025
- Reviewer at ICLR 2026, LOG 2025, NeurIPS 2025, ICLR 2025, AAAI 2024, LOG 2024, KDD 2024

## Scholastic Achievements

- Received **ICLR Travel Grant** for ICLR 2025
- Received **ACM/IARCS Travel Grant** for ICLR 2025

- Nominated as one of the **Top Reviewers** at LOG 2024.
- **ACM/IARCS Travel Grant** for UAI 2023
- **Google Travel Grant** for UAI 2023
- Rewarded prestigious **Prime Minister’s Research Fellowship (PMRF)** in 2022
- Rewarded Best Grade (A+) on M.Tech Thesis in IISc, 2020.
- Rewarded Outstanding Grade on annual performance evaluation in ISRO, 2018.
- Secured **All India Rank 37** among 96878 candidates in GATE-2017 in Computer Science.
- Secured **All India Rank 38** among around 35000 candidates in ISRO Entrance Exam,2017.

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## References

- **Prof. Niloy Ganguly** Professor, IIT Kharagpur, India
- **Prof. Pawan Goyal** Associate Professor, IIT Kharagpur, India
- **Dr. Satadeep Bhattacharjee** R&D Team Leader, Indo Korea Science and Technolgy Center (IKST)
- **Prof. M. Narasimha Murty** Honorary Professor, Indian Institute of Science, India