

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

- Subhojoyoti 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, Subhojoyoti 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, Subhojoyoti 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.

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 Technology Center (IKST)
- [Prof. M. Narasimha Murty](#) Honorary Professor, Indian Institute of Science, India