

# Kishalay Das

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## Research Interest

I am a Prime Minister Research Fellow at the Indian Institute of Technology, Kharagpur, and working as a part of CNeRG Group. I am broadly interested in Graph Representation Learning and Generative Modeling. My doctoral research focuses on AI for 3D Material Generation and Property Prediction

## 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

- Kishalay Das\*, Subhojyoti Khastagir\*, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **LLM Meets Diffusion: A Hybrid Framework for Crystal Material Generation.** accept in *NeurIPS 2025*
- 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* (Acceptance Rate of 32.08%) [Paper][Code]
- Kishalay Das, Pawan Goyal, Seung-Cheol Lee, Satadeep Bhattacharjee, Niloy Ganguly, **"CrysMMNet: Multimodal Representation for Crystal Property Prediction."** accept in *UAI 2023* (Acceptance Rate of 31%) [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* (Acceptance Rate of 19.6%), 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* (Impact Factor: 13.2) [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.

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