Kishalay Das

Kharagpur, West Bengal
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https://kdmsit.github.io/

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 - **Ph.D. in Computer Science**, *Indian Institute of Technology(IIT), Kharagpur, India*, **GPA: 9.5/10**.

- **Research Objective :** *AI for 3D 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, **CrysLDM: Latent Diffusion Model for Crystal Material Generation.** accept in *AI4MAT-ICLR-2025*
- 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]
- 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]
- 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]
- 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]
- Sambaran Bandyopadhyay, Kishalay Das, M Narasimha Murty, **"Hypergraph Attention Isomorphism Network by Learning Line Graph Expansion"** *2020 IEEE-Big Data* [Paper]
- 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

- **ACM/IARCS Travel Grant** to present at ICLR 2025
- Nominated as one of the top reviewers at LOG 2024.
- **ACM/IARCS Travel Grant** to present at UAI 2023
- **Google Travel Grant** to present at 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
- **Prof. M. Narasimha Murty** Honorary Professor, Indian Institute of Science, India