

# Kishalay Das

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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 Machine Learning. My current research is focused on representation learning over molecules and crystal materials using Graph Neural Networks for property prediction and generation.

## Education

- 2022 - **Ph.D. in Computer Science**, *Indian Institute of Technology(IIT), Kharagpur, India*, GPA: 9.5/10.  
◦ **Research Objective** : *Learning Representations over Crystal Material Graphs*.  
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, 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](#)] [[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](#)] [[Code](#)]

## 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

- Nominated as one of the top reviewers at LOG 2024.
- Google travel grants to present at UAI 2023
- Rewarded prestigious Prime Minister's Research Fellowship (PMRF) December cycle 2021
- 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