

Kishalay Das

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📄 <https://kdmsit.github.io/>

Research Interest

I am a Prime Minister Research Fellow at 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 solid materials using Graph Neural Network (GNN).

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.

Research Experiences

Jul,2020 - Dec, 2021 **Research Assistant**, IIT Kharagpur, [CNeRG Group](#).

Work Experience

- May,2017 - Jul,2018 **Scientist/Engineer-SC**, *ISRO Telemetry Tracking and Command Network*, 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.

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%)
- [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](#)]

Relevant Courses

- Topics in Pattern Recognition, Machine Learning, Deep Learning, Natural Language Processing, AI and Ethics, Linear Algebra and Probability, Computational Method of Optimization, Data Analytic,

Accomplishments

- 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