Kharagpur, West Bengal ⋈ kishalay.msit@gmail.com †† https://kdmsit.github.io/

Kishalay Das

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

- <u>Kishalay Das</u>, 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, <u>Kishalay Das</u>, M Narasimha Murty, "Hypergraph Attention Isomorphism Network by Learning Line Graph Expansion" 2020 IEEE-Big Data [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

- $\circ\,$ 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

- o Prof. Niloy Ganguly Professor, IIT Kharagpur, India
- o Prof. Pawan Goyal Associate Professor, IIT Kharagpur, India
- o Prof. M. Narasimha Murty Honorary Professor, Indian Institute of Science, India