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 : <u>Learning Representations over Crystal Material Graphs.</u> under supervision of **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 under supervision of 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, <u>CNeRG Group</u>, under supervision of **Prof.**Niloy Ganguly and Prof. Pawan Goyal.
 - Developing explainable property predictor for crystalline material using limited training data

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, 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%) [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

- o 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.