Kishalay Das

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https://kdmsit.github.io/

Research Interest

I am a Prime Minister Research Fellow at Indian Instiiute 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: 9.33/10**.

- **Research Objective :** *Learning Representations over Crystal Material Graphs.* 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, CNeRG Group, 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, Kishalay Das, 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

- 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.