Ravinder

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RESEARCH INTERESTS

Machine learning aided material design, physics informed machine learning, graph neural networks, material modelling, dynamic fracture and crack propagation on ballistic impact, molecular dynamics and peridynamics.

EDUCATION

PhD, Civil Engineering 2017–2023
Indian Institute of Technology Delhi, Delhi
CGPA: 9.50/10

B. Tech., Civil Engineering 2011–2015
Indian Institute of Technology Roorkee, Roorkee
CGPA: 7.92/10

Ph.D. THESIS

Title: Data-driven Modeling and Physics-informed Machine Learning for Glass Discovery
Description: The research work explores the use of machine learning methods in modeling inorganic glass properties, revealing composition–property relationships through explainable ML, understanding mechanisms at the atomic scale, and up-scaling of material properties using MD and DFT simulation trajectory. The research work uses the graph neural network-based interatomic potential for reproducing features at the atomic scale for complex systems and uses ML material models (peridynamics nonlocal operators) for reproducing material behavior at mesoscale with MD and DFT simulation trajectories.

RESEARCH ACHIEVEMENTS AND AWARDS

PyGGi (Python for Glass Genomics)
It is an indigenous industry-relevant software package that uses trained Machine Learning algorithms to predict/optimize composition-property relationships in inorganic glasses. It will make the tedious process of designing tailored glasses economical in terms of time, effort, and money.
The software package is launched through FITT IITD and is available at www.pyggi.iitd.ac.in.

Awards:

- ICG-GOMD 2019 registration grant (2019).
- Prime Ministers Research Fellowship (PMRF) (2020)
- SITARE/SRISTI Gandhian Young Technological Innovation (GYTI) Awards/Appreciations (2020)
- SERB Travel grant (2022)

SOFTWARE AND PROGRAMMING LANGUAGES

- **Packages Developed:**

  Peridynamics: **PeriDyn.jl, PDMesh.jl and PDBenchmark.jl**

  Molecular Dynamics: **MDSimulator.jl and MDBase.jl**

  Others: **GlassConversionPy, MLPipeline, MixModelsPytorch**

  Contribution to other packages: **jax-md**

  All packages can be accessed at the github repository.

- **Operating Systems:** Linux, MacOS and Windows
- **Softwares:** LAMMPS, NAMD, Peridigm, R.I.N.G.S, Ovito, VMD, Abaqus and STAADPRO
- **Languages:** Julia, Python, C++ and Matlab

PUBLICATIONS

1. Bhattoo, Ravinder; Ranu, Sayan; Krishnan, NM; Learning the dynamics of particle-based systems with lagrangian graph neural networks, Machine Learning: Science and Technology, 2023
2. Ravinder, R; Bishnoi, Suresh; Zaki, Mohd; Krishnan, NM; Understanding the Compositional Control on Electrical, Mechanical, Optical, and Physical Properties of Inorganic Glasses with Interpretable Machine Learning, Acta Materialia, 118439, 2022

3. Bhattoo, Ravinder; Ranu, Sayan; Krishnan, NM; Learning Articulated Rigid Body Dynamics with Lagrangian Graph Neural Network, NeurIPS 2022 Conference, 2022

4. Zaki, Mohd; Venugopal, Vineeth; Bhattoo, Ravinder; Bishnoi, Suresh; Singh, Sourabh Kumar; Allu, Amarnath R; Krishnan, NM Anoop; Interpreting the optical properties of oxide glasses with machine learning and Shapely additive explanations, Journal of the American Ceramic Society, 105, 6, 4046-4057, 2022

5. Thangamuthu, Abishek; Kumar, Gunjan; Bishnoi, Suresh; Bhattoo, Ravinder; Krishnan, NM Anoop; Ranu, Sayan; Unravelling the Performance of Physics-informed Graph Neural Networks for Dynamical Systems, NeurIPS 2022 Conference, 2022

6. Ravinder, R; Venugopal, Vineeth; Bishnoi, Suresh; Singh, Sourabh; Zaki, Mohd; Grover, Hargun Singh; Bauchy, Mathieu; Agarwal, Manish; Krishnan, NM Anoop; Artificial intelligence and machine learning in glass science and technology: 21 challenges for the 21st century, International Journal of Applied Glass Science, 2021

7. Bishnoi, Suresh; Ravinder, R; Grover, Hargun Singh; Kodamana, Hariprasad; Krishnan, NM Anoop; Scalable Gaussian processes for predicting the optical, physical, thermal, and mechanical properties of inorganic glasses with large datasets, Materials Advances, 2, 1, 477-487, 2021, Royal Society of Chemistry

8. Ravinder, R; Sridhara, Karthikeya H; Bishnoi, Suresh; Grover, Hargun Singh; Bauchy, Mathieu; Jayadeva, J; Kodamana, Hariprasad; Krishnan, NM Anoop; Deep Learning Aided Rational Design of Oxide Glasses, Materials Horizons, 2020, Royal Society of Chemistry

9. Ravinder, R; Kumar, Abhishek; Kumar, Rajesh; Vangla, Prashanth; Krishnan, NM Anoop; Irradiation-induced brittle-to-ductile transition in α-quartz, Journal of the American Ceramic Society, 103, 7, 3962-3970, 2020

10. Ravinder, R; Singh, Sourabh; Bishnoi, Suresh; Jan, Amreen; Sharma, Amit; Kodamana, Hariprasad; Krishnan, NM Anoop; An adaptive, interacting, cluster-based model for predicting the transmission dynamics of COVID-19, Heliyon, 6, 12, e05722, 2020, Elsevier

11. Nayak, Sumeru; Ravinder, R; Krishnan, NM; Das, Sumanta; A Peridynamics-Based Micromechanical Modeling Approach for Random Heterogeneous Structural Materials, Materials, 13, 6, 1298, 2020, Multidisciplinary Digital Publishing Institute

12. Bhaskar, Pratik; Kumar, Rajesh; Maurya, Yashasvi; Ravinder, R; Allu, Amarnath R; Das, Sumanta; Gosvami, Nitya Nand; Youngman, Randall E; Bødker, Mikkel S; Mascaraque, Nerea; Cooling rate effects on the structure of 45S5 bioglass: Insights from experiments and simulations, Journal of Non-Crystalline Solids, 534, 119952, 2020, Elsevier

13. Krishnan, NM Anoop; Ravinder, R; Kumar, Rajesh; Le Pape, Yann; Sant, Gaurav; Bauchy, Mathieu; Density-stiffness scaling in minerals upon disordering: Irradiation vs. vitrification, Acta Materialia, 166, 611-617, 2019, Pergamon

14. Bishnoi, Suresh; Singh, Sourabh; Ravinder, R; Bauchy, Mathieu; Gosvami, Nitya Nand; Kodamana, Hariprasad; Krishnan, NM Anoop; Predicting Young's modulus of oxide glasses with sparse datasets using machine learning, Journal of Non-Crystalline Solids, 524, 119643, 2019, North-Holland

15. Dhawan, Sameer; Ghosh, Sukanya; Ravinder, R; Bais, Sachendra S; Basak, Soumen; Krishnan, NM Anoop; Agarwal, Manish; Banerjee, Manidipa; Haridas, V; Redox sensitive self-assembling dipeptide for sustained intracellular drug delivery, Bioconjugate chemistry, 30, 9, 2458-2468, 2019, American Chemical Society

16. Rivera, Jared; Berjikian, Jonathan; Ravinder, R; Kodamana, Hariprasad; Das, Sumanta; Bhatnagar, Naresh; Bauchy, Mathieu; Krishnan, NM Anoop; Glass fracture upon ballistic impact: new insights from peridynamics simulations, Frontiers in Materials, 6, 239, 2019, Frontiers Media SA

17. Ravinder, R; Kumar, Rajesh; Agarwal, Manish; Krishnan, NM; Evidence of a two-dimensional glass transition in graphene: Insights from molecular simulations, Scientific reports, 9, 1, 1-9, 2019, Nature Publishing Group

18. Ravinder, R; Garg, Prateet; Krishnan, NM Anoop; Glass Transition and Crystallization in Hexagonal Boron Nitride: Crucial Role of Orientational Order, Advanced Theory and Simulations, 1900174, 2019

19. Bhattoo, Ravinder; Ranu, Sayan; Krishnan, NM; Lagrangian neural network with differentiable symmetries and relational inductive bias, arXiv preprint arXiv:2110.03266, 2021 (**pre-print**)

20. Bishnoi, Suresh; Bhattoo, Ravinder; Krishnan, Ranu, Sayan; NM Anoop; Enhancing the Inductive Biases of Graph Neural ODE for Modeling Dynamical Systems (**submitted**)

Please go to https://scholar.google.com/citations?user=lPTdGRMAAAAJ&hl=en for an updated list of publications.

RESEARCH CONFERENCE AND WORKSHOP

1. **Talk: Understanding the Compositional Control on Electrical, Mechanical, Optical, And Physical Properties of Inorganic Glasses with Interpretable Machine Learning**
   August 2022
   XXX International Materials Research Congress (IMRC2022) and International Conference on Advanced Materials (ICAM2021)
   Cancun, Mexico

2. **Talk: Lagrangian and Hamiltonian Graph Neural Networks for Robust Molecular Simulations**
   August 2022

XXX International Materials Research Congress (IMRC2022) and International Conference on Advanced Materials (ICAM2021)
Cancun, Mexico

3. **Talk: PeriDyn: A Peridynamics Package Written in Julia Programming Language**
   July 2022
   11th European Solid Mechanics Conference
   NUI, Galway, Ireland

4. **Talk: Learning Quantum-accuracy Interatomic Potential for Silica Using Lagrangian Graph Neural Networks**
   May 2022
   2022 Glass and Optical Materials Division Annual Meeting
   Hyatt Regency Baltimore, Baltimore, MD, United States

5. **Talk: Learning interaction laws in atomistic system using Lagrangian Graph Neural Networks**
   May 2022
   2022 Glass and Optical Materials Division Annual Meeting
   Hyatt Regency Baltimore, Baltimore, MD, United States

6. **Talk: Decoding the Genome of Inorganic Glasses using Interpretable Machine Learning**
   December 2021
   14th Pacific Rim Conference on Ceramic and Glass Technology and GOMD 2021 Division Meeting
   Vancouver, British Columbia, Canada (Virtual)

7. **Talk: Molecular Dynamics Simulation Using Graph Neural Networks**
   December 2021
   MRS Fall Meeting 2021
   Boston, Massachusetts, USA (Virtual)

8. **Talk: Understanding the Composition-property Relationship of Glasses Using Interpretable Machine Learning**
   October 2021
   Materials Science and Technology (MS&T) 2021
   Columbus, Ohio, USA (Virtual)

9. **Talk: Machine learning to predict the elastic properties of glasses.**
   October 2019
   Material Science and Technology (MS&T) 2019
   Oregon Convocation Center, Portland, USA

10. **Tutor: Introduction to Machine Learning Tools.**
    September 2019

Artificial Intelligence Concepts and Multidisciplinary Applications in Modern Biology
International Center for Genetic Engineering and Biotechnology, New Delhi

11. **Poster: Designing Functional Glasses using Machine Learning.**
September 2019
IIT Delhi Industry Day 2019
Indian Institute of Technology Delhi, New Delhi

12. **Tutor: Introduction to Machine Learning.**
June 2019
Machine Learning For Engineering Applications (TEQIP Course)
Indian Institute of Technology Delhi, New Delhi

13. **Tutor: Molecular dynamics workshop 2**
March 2019
Advanced Simulation Methods: DFT, MD and Beyond
Indian Institute of Technology Delhi, New Delhi

14. **Poster: Two-dimensional glass transition in graphene: Insights from molecular simulations.**
March 2019
Advanced Simulation Methods: DFT, MD and Beyond
Indian Institute of Technology Delhi, New Delhi

15. **Poster: Role of topological defects on the rigidity of glassy graphene.**
December 2018
COMPFLU-2018: 12th International Conference on Complex Fluids and Soft Matter
Indian Institute of Technology Roorkee, Roorkee

REFERENCES

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Relationship: Student Review Committee member

WORK EXPERIENCE

Trainee Structural Design Engineer 2015–2016
ASC Infratech Pvt Ltd
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