

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.

EXPERIENCE

Postdoctoral Scholar <i>Civil and Environmental Engineering</i> <i>University of Wisconsin–Madison, Madison</i>	April 2023 – Present
Postdoctoral Scholar <i>Civil Engineering</i> <i>Indian Institute of Technology Delhi, Delhi</i>	January 2023 – March 2023

EDUCATION

Ph.D., Civil Engineering <i>Indian Institute of Technology Delhi, Delhi</i> CGPA: 9.50/10	July 2017 – January 2023
B.Tech., Civil Engineering <i>Indian Institute of Technology Roorkee, Roorkee</i> CGPA: 7.92/10	July 2011 – June 2015

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)

TEACHING EXPERIENCE

Teaching Assistant

- Structural Analysis Lab, Civil Engineering, IIT Delhi, 2018,2019
- Structural Analysis I Course, Civil Engineering, IIT Delhi, 2018
- Finite Element Method Course, Civil Engineering, IIT Delhi, 2018

Workshop Instructor

- Molecular dynamics workshop 2, Advanced Simulation Methods: DFT, MD and Beyond, Delhi, 2019

- Introduction to Machine Learning: Machine Learning For Engineering Applications (TEQIP Course) IIT Delhi, 2019
- Introduction to Machine Learning Tools, Artificial Intelligence Concepts and Multi-disciplinary Applications in Modern Biology, ICGEB, Delhi, 2019

BOOKS AND CONTRIBUTED CHAPTERS

Machine Learning for Materials Discovery: Numerical Recipes and Practical Applications (In Draft)

N. M. Anoop Krishnan, Hariprasad Kodamana and Ravinder Bhattoo

JOURNAL 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. 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
4. **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
5. 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
6. **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

7. **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
8. **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
9. 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
10. Bhaskar, Pratik; Kumar, Rajesh; Maurya, Yashasvi; **Ravinder, R**; Allu, Amarnath R; Das, Sumanta; Gosvami, Nitya Nand; Youngman, Randall E; Bdker, 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
11. 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
12. 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
13. 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
14. 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
15. **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
16. **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

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

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

CONFERENCE PUBLICATIONS

1. Bishnoi, Suresh; **Bhattoo, Ravinder**; Jayadeva, Jayadeva; Ranu, Sayan; Krishnan, NM Anoop; Learning the Dynamics of Physical Systems with Hamiltonian Graph Neural Networks, ICLR 2023 Workshop on Physics for Machine Learning, 2023
2. Bishnoi, Suresh; **Bhattoo, Ravinder**; Krishnan, Ranu, Sayan; NM Anoop; Enhancing the Inductive Biases of Graph Neural ODE for Modeling Dynamical Systems, The Eleventh International Conference on Learning Representations, 2023
3. **Bhattoo, Ravinder**; Ranu, Sayan; Krishnan, NM; Learning Articulated Rigid Body Dynamics with Lagrangian Graph Neural Network, Advances in Neural Information Processing Systems 35, 2022
4. 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, Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track, 2022

CONFERENCE TALKS AND WORKSHOP

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

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

Talk: PeriDyn: A Peridynamics Package Written in Julia Programming Language

July 2022

11th European Solid Mechanics Conference

NUI, Galway, Ireland

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

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

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)

Talk: Molecular Dynamics Simulation Using Graph Neural Networks

December 2021

MRS Fall Meeting 2021

Boston, Massachusetts, USA (Virtual)

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)

Talk: Machine learning to predict the elastic properties of glasses.

October 2019

Material Science and Technology (MS&T) 2019

Oregon Convocation Center, Portland, USA

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

Poster: Designing Functional Glasses using Machine Learning.

September 2019

IIT Delhi Industry Day 2019

Indian Institute of Technology Delhi, New Delhi

Tutor: Introduction to Machine Learning.

June 2019

Machine Learning For Engineering Applications (TEQIP Course)

Indian Institute of Technology Delhi, New Delhi

Tutor: Molecular dynamics workshop 2

March 2019

Advanced Simulation Methods: DFT, MD and Beyond

Indian Institute of Technology Delhi, New Delhi

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

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

MEMBERSHIP AND AFFILIATION

- **Professional Memberships:**

1. [Structural Engineering Institute \(SEI\)](#)
2. [Engineering Mechanics Institute \(EMI\)](#)
3. [The Institution of Engineers \(India\)](#)
4. [The American Ceramic Society](#)

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:** HPC, LAMMPS, NAMD, Peridigm, R.I.N.G.S, Ovito, VMD, Abaqus and STAAD-PRO
- **Languages:** Julia, Python, C++ and Matlab

WORK EXPERIENCE

Trainee Structural Design Engineer

2015–2016

ASC Infratech Pvt Ltd

Noida, Uttarpradesh, India

REFERENCES

Prof. N. M. Anoop Krishnan

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Relationship: Research collaborator