

# Ravinder

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## RESEARCH INTERESTS

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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

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<b>PhD, Civil Engineering</b> <i>Indian nstitute of Technology Delhi, Delhi</i> <i>CGPA: 7.92/10</i>	2017–Present
<b>B. Tech., Civil Engineering</b> <i>Indian Institute of Technology Roorkee, Roorkee</i> <i>CGPA: 9.50/10</i>	2011–2015

## Ph.D. THESIS

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**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

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### 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](http://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

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- **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

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1. 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
2. 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

3. Ravinder, R; Kumar, Abhishek; Kumar, Rajesh; Vangla, Prashanth; Krishnan, NM Anoop; Irradiation-induced brittle-to-ductile transition in  $\alpha$ -quartz, *Journal of the American Ceramic Society*, 103, 7, 3962-3970, 2020
4. 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
5. 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
6. 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
7. Ravinder, R; Bishnoi, Suresh; Zaki, Mohd; Krishnan, NM; Revealing the compositional control of electrical, mechanical, optical, and physical properties of inorganic glasses arXiv preprint arXiv:2103.12050, 2021 (**under review**)
8. Bhattoo, Ravinder; Ranu, Sayan; Krishnan, NM; Learning Rigid Body Dynamics with Lagrangian Graph Neural Network (**submitted**)
9. Bhattoo, Ravinder; Ranu, Sayan; Krishnan, NM; Lagrangian neural network with differentiable symmetries and relational inductive bias, arXiv preprint arXiv:2110.03266, 2021 (**pre-print**)
10. Bhattoo, Ravinder; Ranu, Sayan; Krishnan, NM; Lagrangian graph neural network (**submitted**)
11. 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
12. 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
13. 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
14. 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

15. 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
16. 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
17. 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
18. 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
19. Bishnoi, Suresh; Bhattoo, Ravinder; Krishnan, Ranu, Sayan; NM Anoop; Enhancing the Inductive Biases of Graph Neural ODE for Modeling Dynamical Systems (**submitted**)
20. 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 (**submitted**)

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

## RESEARCH CONFERENCE AND WORKSHOP

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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*

## **WORK EXPERIENCE**

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**Trainee Structural Design Engineer**

2015–2016

*ASC Infratech Pvt Ltd*

*Noida, Uttarpradesh, India*