Shaswat Mohanty | Stanford University

Postdoctoral Researcher at Department of Mechanical Engineering

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Curriculum Vitae | shaswatm@stanford.edu

Profile Summary

Computational materials simulation experience of over 6 years with modeling expertise covering continuum scale methods such as finite element method and computational fluid dynamics, down to atomistic methods such as molecular dynamics, coarse-grained molecular dynamics, and density functional theory. Experience with scientific code development in Python for over 5 years with numerous open-source projects available from the doctoral dissertation. Over 3 years of experience in integrating machine learning and deep learning techniques to further the understanding of materials science and mechanical engineering problems. Research proficiency is highlighted in a rich publication history with 16 journal publications. I'm currently continuing as a Postdoctoral researcher in my group at Stanford and **currently available to begin work with immediate effect**.

Education

Program	Institution	%/CGPA	Completion
Ph.D: Mechanical Engineering	Stanford University	4/4	09/2019 - 04/2024
Bachelor's: Mechanical Engineering	Indian Institute of Technology, Madras	9.36/10	07/2014 - 05/2019
Master's: Mech. Eng. - Product Design			
Minor: Material Sciences and Technology			

Selected Research Projects (7+ Years)

Analysis of Rare Events in Polymeric Systems, *Stanford University* 09/2022 - ongoing

Pricipal Investigator: Prof. Wei Cai, Co-Pricipal Investigators: Prof. Jose Blanchet, Prof. Youssef Marzouk

- Developed a bond-breaking theory for reversible and irreversible crosslinks in polymers to study fracture
- Created a novel representation of non-local shortest path (SP) distribution as branched random walks (PolyBranchX)
- Developed a transfer map proxy to track material evolution, replacing expensive atomistic or coarse-grained simulations
- Formulated empirical laws for the evolution of SP in dynamic polymer networks to explain self-healing and stress-relaxation

Machine-learned force field and interatomic potentials, *Stanford University* 09/2022 - ongoing

Pricipal Investigator: Prof. Wei Cai

- Worked with graph neural network (GNN) based force fields (GAMD, NequIP) and symmetry function-based neural networks (ANI, SANI, QRNN)
- Developed benchmarking tests to test the generalizability of machine-learned force fields and interatomic potentials (TB-MLFF)
- Identified material analysis cases where many potentials fail, such as vacancy diffusion, phonon dispersion, and gamma surface predictions, for robust MLFF development
- Developing an MLFF for finite temperature energy landscapes to explain mismatches between predicted and observed dynamics
- Implemented convolutional neural networks (CNN) to analyze 2D surface roughness maps of silicon wafers for contaminant separation force estimation during fabrication

Multiphysics Modeling of Smart Materials system, *Stanford University* 09/2020 - ongoing

Pricipal Investigator: Prof. Wei Cai

- Implemented a coupled chemo-mechanical finite element model (FEM) on FEniCS and COMSOL to predict expansion and deformation in patterned polymer systems
- Extended FEM (X-FEM) model on ABAQUS to simulate biological tissue rupture under ballistic loading
- Developed a multiphysics model to estimate mechanical evolution in stretchable battery electrodes

Computational Modeling of XPCS and XSVS Experiments, *Stanford University* 09/2020 - 09/2022

Pricipal Investigator: Prof. Wei Cai

- Predicted material dynamics by computing XPCS and XSVS measurements from molecular dynamics simulations
- Developed and published open-source code for XPCS C-XPCS actively in use by groups at SLAC and the European XFEL

Research Areas

- Material Modeling
- Molecular Dynamics
- Machine Learning

Work Experience (2+ Years)

Multiscale Polymer Fracture Modeling, Postdoctoral Research Scholar, *Stanford University* 04/2024 - Ongoing

Advisor: Prof. Wei Cai

- Developing microstructural evolution-based models using coarse-grained molecular dynamics and network theory to model and explain fracture mechanisms of polymer networks, leading to the design of novel experimental measurement techniques
- Created deep learning tools to estimate finite temperature potential energy landscapes for various materials

Machine-learned Interatomic Potential Development, Polymer Scientist Intern, *Schrodinger* 05/2017 - 07/2017

Tutor: Dr. Atif Afzal (Senior Scientist II)

- Developed a generalizable machine-learned force-field for polyethylene glycol using charge-recursive neural networks
- Developed molecular dynamics descriptors to aid RDKit descriptors in melting point prediction using chemoinformatics

Efficiency Optimization of Gas Generators, Mechanical Engineering Intern, *Hindustan Unilever Limited* 05/2017 - 07/2017

Tutor: Mr. Bernard Conyers (Manufacturing Director, Nigeria); Mentor: Mr. P.Jagadeesh (VP Costing, South Asia)

- Improved generator efficiency by 8% leading to projected annual **savings of up to €220,000-260,000**
- Proposed a Vapour Absorption cooling system to result in a projected savings of €102,000-118,000

Teaching Assistantships, *IIT Madras and Stanford University* 2018 - 2024 (sporadic)

- Developed and delivered coursework and tutorials to 200+ students across four undergraduate courses: *Kinematics and Dynamics of Machinery, Solid Mechanics, and Computational Mechanics*
- Taught course material to 60+ students for two graduate courses: *Statistical Mechanics, and Elasticity, Inelasticty and Fracture*

Technical Skills

- **Molecular Softwares:** LAMMPS, HOOMD-Blue, VASP, Ovito, Paraview, Materials Studio, Jaguar, Psi4
- **Programming Languages (Basic)**: C , C++ , Python; **Analysis Tools**: MATLAB, Octave, SciLab, Simulink (Basic)
- **Continuum Softwares**: Abaqus (User Subroutines), ANSYS Workbench, FEniCS, Creo, Autodesk Inventor, COMSOL
- **Operating Systems**: Windows , Linux, Mac; **Documentation and Reporting**: LaTeX, Microsoft Office Suite, LyX

Selected Journal Publications (16 Total Publications)

- **Shaswat Mohanty**, Zhenyuan Zhang, Jose Blanchet, Wei Cai, *Modeling shortest paths in polymeric networks using spatial branching processes*, **Journal of the Mechanics and Physics of Solids**
- **Shaswat Mohanty**, Yikai Yin, Christopher B Cooper, Zhenan Bao, Wei Cai, *Network evolution controlling strain-induced damage and self-healing of elastomers with dynamic bonds*, **Macromolecules** (under review)
- **Shaswat Mohanty**, Sanghyuk Yoo, Keonwook Kang, Wei Cai, *Evaluating the Transferability of Machine-Learned Force Fields for Material Property Modeling*, **Computer Physics Communications**
- Oleg Kuzentsov, **Shaswat Mohanty**, Elena Pigos, Gugang Chen, Wei Cai, Avetik Harutyunyan, *High Energy Density Flexible and Ecofriendly Lithium-ion Smart Battery*, **Energy Storage Materials**

Selected Conference Presentations (12 Total Presentation)

- **Shaswat Mohanty**, Yikai Yin, Christopher B Cooper, Zhenan Bao, Wei Cai, *Non-local Shortest Paths: Microstructural Evolution controls Macroscopic Response for Dynamic Polymer Networks*, **APS March Meeting**, Minneapolis, 3rd - 4th March 2024
- **Shaswat Mohanty**, Christopher B Cooper, Hui Wang, Mengning Liang, Wei Cai, *Computational X-ray Photon Correlation Spectroscopy from Molecular Dynamics Trajectories* , **Materials Research Society**, Hawaii Convention Center, 8th - 14th May 2022

Honors and Awards

- **Governor's Prize** awardee for **all round proficiency** in extra-curricular and curricular activities (2019)
- **Institute Blues** awardee for **all round proficiency** in co-curricular, extra-curricular and organizational activities (2019)
- **Sri Rajesh Achanta Prize** awardee for the **highest CGPA** in Mechanical Engineering-Product Design (2017-18)
- **All India Rank 798** (top **0.05%**) in IIT-JEE Main; **All India Rank 1092** (top **0.07%**) in IIT-JEE Advanced
- In the **top 1%** in Class X; In the **top 0.3%** in Class XII; Awardee of the **INSPIRE scholarship** by the **Govt. of India**