Shaswat Mohanty | STANFORD UNIVERSITY

Department of Mechanical Engineering

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EDUCATION

PROGRAM	INSTITUTION	%/CGPA	COMPLETION
Ph.D: Mechanical Engineering	Stanford University	4/4	09/2019 - ongoing
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			

RESEARCH PROJECTS

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

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

- Formulating a bond-breaking theory for reversible and irreversible crosslinks in polymers to study fracture

- Developed a novel representation of non-local shortest path (SP) distribution as branched random walks (available at PolyBranchX)

- Developed a transfer map proxy to track material evolution to substitute expensive atomistic or coarse-grained simulations

- Formulated empirical laws for the evolution of SP in dynamic polymer networks that explain critical material behavior such as self-healing and stress-relaxation

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

Pricipal Investigator: Prof. Wei Cai

- Experienced with graph neural network (GNN) based force field (GAMD) and interatomic potentials (NequIP), and symmetry function based neural networks (ANI, SANI, QRNN).
- Developed a series of benchmarking tests as a protocol for these force fields and interatomic potentials (available at TB-MLFF)

- Identified material analysis cases that most potentials fail on such as: vacancy diffusion, phonon dispersion and gamma surface predictions, for robust development of machine-learned force fields (MLFF)
- Developed a Companion GNN to predict potential energies for GNN-based force fields that are energy-agnostic

- Currently developing an MLFF to serve as a finite temperature potential energy landscape to explain mismatch between predicted and observed dynamics
- Used convolutional neural networks (CNN) to encode information from a 2D surface roughness map of silicon wafers to estimate contaminant separation force required during fabrication processes

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

Pricipal Investigator: Prof. Wei Cai

- Predicting material dynamics by computing the XPCS and XSVS measurements from molecular dynamics simulations

- Self-implemented open-source code available at C-XPCS actively in use by groups at SLAC and the European XFEL

Using Coarse-Grained Molecular Statics to model Carbon Nanotubes, *Stanford University* — 03/2020 - 09/2021

*Pricipal Investigator: Prof. Wei Cai in collaboration with **Honda Research Institute***

- Understanding mechanical and electrical hysteretic behavior of carbon nanotube (CNT) networks using molecular simulations

- Used network analysis for describing the topological change in the CNT network under deformation

Electro-Chemo-Mechanical Study of Li-ion Battery Electrode Materials, *IIT Madras* — 06/2018 - 03/2019

Pricipal Investigator: Dr. Ratna Kumar Annabattula; Co-Principal Investigator: Dr. Narasimhan Swaminathan

- A coupled analysis of lithium ion battery electrodes using my Finite Element code written on FENiCS

Study of Fracture in Functionally Graded Piezoelectric Ceramics, *IIT Madras* — 01/2019 - 07/2019

Pricipal Investigator: Dr. Ratna Kumar Annabattula

- Implemented a hybrid formulation of the phase-field method in a multiphysical system associated with piezoelectric ceramics

Industrial Internships

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

Tutor: Dr. Atif Afzal (Senior Scientist II)

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

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)

- Improvement in 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

Technical Skills

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

Journal Publications

- **Shaswat Mohanty**, Dimitris Konomis, Youssef Marzouk, Wei Cai, *Conditional Generative Modeling of Shortest Path Statistics in Polymer Systems*, (to be submitted)
- Zhenyuan Zhang, **Shaswat Mohanty**, Jose Blanchet, Wei Cai, *On the First Passage Times of Branching Random Walks in $\mathbb{R}^d$*, (in preparation)
- **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** (to be submitted)
- **Shaswat Mohanty**, Yikai Yin, Christopher Cooper, Zhenan Bao, Wei Cai, *Network evolution controlling strain-induced damage and self-healing of elastomers with dynamic bonds*, **Journal of the Mechanics and Physics of Solids** (to be submitted)
- **Shaswat Mohanty**, Sanghyuk Yoo, Keonwook Kang, Wei Cai, *Evaluating the Transferability of Machine-Learned Force Fields for Material Property Modeling*, **Computer Physics Communications**
- **Shaswat Mohanty**, James Stevenson, Andrea Browning, Leif Jacobson, Karl Leswing, Mathew Halls, Mohammad Atif Faiz Afzal, *Development of Scalable and Generalizable Machine Learned Force Field for Polymers*, **Scientific Reports**
- 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**
- **Shaswat Mohanty**, Anirudh Vijay, Shailesh Deshpande, *Understanding Urban Water Consumption Using Remotely Sensed Data*, **IEEE Xplore**
- **Shaswat Mohanty**, Christopher Cooper, Hui Wang, Mengning Liang, Wei Cai, *Computational Approaches to Model X-ray Photon Correlation Spectroscopy from Molecular Dynamics*, **Modelling and Simulation in Materials Science and Engineering**
- **Shaswat Mohanty**, Anirudh Vijay, Nandagopan Gopakumar, *StockBot: Using LSTMs to Predict Stock Prices*, **Journal of Banking Finance and Technology** (under review)
- **Shaswat Mohanty**, Pramod Kumbhar, Narasimhan Swaminathan, Ratna K Annabattula, *Stress-Electrochemistry Interactions in a Composite Electrode for Li-ion Batteries*, **Solid State Ionics**
- **Shaswat Mohanty**, Pramod Kumbhar, Narasimhan Swaminathan, Ratna K Annabattula, *A Phase-field Model for Crack Growth in Electro-mechanically Coupled Functionally-graded Piezo-ceramics*, **Smart Materials and Structures**
- Jagannadh Boddapati, **Shaswat Mohanty**, Ratna K Annabattula, *An Analytical Model for Shape-morphing hrough Combined Bending and Twisting in Piezo-composites*, **Mechanics of Materials**
- **Shaswat Mohanty**, Pramod Kumbhar, Narasimhan Swaminathan, Ratna K Annabattula, *A Finite Strain based Coupled Chemo-mechanical Study of the Anode Materials in Lithium-ion Batteries*, **Journal of Coupled Systems and Multiscale Dynamics**

Conference Presentations

- **Shaswat Mohanty**, Oleg A. Kuznetsov, Wei Cai, and Avetik R. Harutyunyan, *Stress-strain and Resistance-strain Hysteresis in Single-Wall Carbon Nanotube Films for Stretchable Battery Electrodes*, **ECS Meeting**, Boston, May 28st - June 2nd, 2023

- **Shaswat Mohanty**, SangHyuk Yoo, Keonwook Kang, Wei Cai, *Benchmarking the transferability of machine-learned force fields for material property modeling*, **MRS Spring Meeting**, San Francisco, April 14th - April 14th, 2023

- **Shaswat Mohanty**, James Stevenson, Andrea Browning, Leif Jacobson, Karl Leswing, Mathew Halls, Mohammad Atif Faiz Afzal, *Scalable and Generalizable Machine Learned Force Field for Polymers*, **MRS Spring Meeting**, San Francisco, April 14th - April 14th, 2023

- **Shaswat Mohanty**, Oleg A. Kuznetsov, Wei Cai, and Avetik R. Harutyunyan, *Stress-strain and Resistance-strain Hysteresis in Single-Wall Carbon Nanotube Films for Stretchable Battery Electrodes*, **US National Congress on Theoretical and Applied Mechanics**, UT Austin, July 21st - July 24th, 2022

- **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, May 8th - May 14th

- **Shaswat Mohanty**, Pramod Kumbhar, Narasimhan Swaminathan, Ratna K Annabattula, *Chemo-Mechanical Study of Li-ion Battery Electrode Materials in a Finite Strain Framework*, **International Workshop on Mechanics of Energy Materials**, Indian Institute of technology Madras, 19th-22nd November 2018

- **Shaswat Mohanty**, Pramod Kumbhar, Narasimhan Swaminathan, Ratna K Annabattula, *Electro-Chemo-Mechanics of Si-C Composite Anode Particles Using Cyclic Voltammetry Simulations*, **235th Electrochemical Society Meeting**, Dallas, Texas, 26th-30th 05/2019

- **Shaswat Mohanty**, Pramod Kumbhar, Narasimhan Swaminathan, Ratna K Annabattula, *Modeling Fracture in Functionally Graded Piezoelectric Materials using a Phase-Field Approach*, **4th Indian Conference for Applied Mechanics**, IISc Bangalore, 3rd-5th July 2019

- Pramod Kumbhar, **Shaswat Mohanty**, Narasimhan Swaminathan, Ratna K Annabattula, *A Two-way Stress-diffusion Coupled Study for Core-shell Anode Particles for Li-ion Batteries*, **4th Indian Conference for Applied Mechanics**, IISc Bangalore, 3rd-5th July 2019

Teaching Experience

Teaching Assistant, ME123 Introduction to Comptuational Mechanics, *Stanford University* 09/2020 - 12/2022
Course Instructor: Prof.Wei Cai
- Introduction to Numerical methods and subsequent implementation on COMSOL. (2 offerings)
- Coordinated 16 student-run projects (64 students) to provide engineering solutions.

Teaching Assistant, Materials and Design, *IIT Madras* 01/2019 - 05/2019
Course Instructor: Dr. Ratna Kumar Annabattula
- A course covering dislocation and fracture theories, and fatigue analysis

Teaching Assistant, Kinematics and Dynamics of Machinery, *IIT Madras* 08/2018 - 11/2018
Course Instructor: Dr. Piyush Shakya
- A course covering constrained link motion analysis and design of mechanical linkage systems.

Scholastic Achievements

- **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**