**RAJNI CHAHAL**

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**EDUCATION**

August 2015 - December 2020 **Ph.D. in Aerospace Engineering,** The University of Texas at Arlington Advisor: Dr. Ashfaq Adnan

Dissertation Title: Mechanics of Nanoscale Fiber Networks & Their Composites: A Three-dimensional Multiscale Stochastic Modeling Study

August 2011 - July 2015 **Bachelor of Technology in Mechanical Engineering**, Dr. B.R. Ambedkar National Institute of Technology (NIT), Jalandhar

**APPOINTMENTS**

December 5, 2022 – Present **Postdoctoral Research Associate,** Oak Ridge National Laboratory, Carbon & Composites Group, Physical Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN

March 2021 – 4th Dec, 2022 **Postdoctoral Research Associate,** University of Massachusetts Lowell, Chemical Engineering, Lowell, MA

Principal Investigator (PI): Dr. Stephen T Lam

February 2021 – March 2021 **Research Assistant,** UTA Research Institute (UTARI), Institute for Predictive Performance Methodologies, Fort Worth, TX

January 2020 - December 2020 **Research Assistant,** Idaho National Laboratory, Material Science & Engineering, Idaho Falls, ID

January 2016 - May 2020 **Enhanced Graduate Teaching Assistant,** The University of Texas at Arlington (UTA), Mechanical & Aerospace Engineering, Arlington, TX. Courses: Aerospace Structures Statics, Mechanical Design, Thermodynamics, Finite Element Methods

June 2019 - December 2019 **Graduate Research Intern,** Idaho National Laboratory, Material Science & Engineering, Idaho Falls, ID

June 2017 - Dec 2017 **Research Assistant,** UTARI, Institute for Predictive Performance Methodologies, Fort Worth, TX

May 2014 - July 2014 **Research Intern,** National Institute of Science & Technology, Odisha, India

**RELEVANT TECHNICAL SKILLS**

Languages: C/C++ (Proficient) | MATLAB (Expert) | Python (Expert) | Bash (Proficient)

OS/Office Software: Windows (Expert) | Linux (Expert) | Microsoft Office Suite (Expert)

High-Performance computing: MPI | CPU | GPU | Linux Bash shell script | Job schedulers (PBS, LSF, Slurm)

Simulation Tools: Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Expert) | Quantum Espresso (Proficient) | Vienna Ab-initio Simulation Package (VASP) (Expert) | CP2K (Expert) | Abaqus (Expert) | SPSS Statistics (Proficient) | DL-POLY (Proficient) |DeePMD-kit for Neural Network interatomic potential training (Expert)

Machine-learning Libraries: Tensorflow/Keras (Expert) | Scikit-learn (Expert)

Post-processing/Analysis Tools: Atomic Simulation Environment (Proficient) | Pymatgen (Proficient) | OVITO (Expert) | Avogadro (Proficient) | VESTA (Expert) | Packmol (Expert)

Image Analysis Tools: ImageJ (Expert) | CT-FIRE (Proficient) | WebPlotDigitizer (Expert)

Material Characterization: Scanning Electron Microscope (Expert) | Energy-dispersive X-ray Spectroscopy (Expert) | X-ray diffraction (Proficient) | Instron/MTS Machine (Expert) | Dielectric Spectroscopy (Proficient)

Manufacturing: Vacuum Assisted Resin Transfer Moulding (Proficient) | Compression Moulding (Basic) | 3D Printing (Basic) | Ultra-Sonication (Proficient) | Sputter Coater (Expert) | Grinder/Polisher (Expert) | Precision Saw (Expert)

**RESEARCH EXPERIENCE**

1. **Development of Reliable and Robust Machine Learning Potentials for Polyacrylonitrile (PAN) Cyclization and Molten Salts,** Oak Ridge National Laboratory 2022-Present
* Performing Born-Oppenheimer ab-initio molecular dynamics calculations to generate training data for PAN polymers, LiCl, AlCl3, AlCl3-KCl molten salts.
* Validating and understanding limitations of already existing classical and reactive interatomic potentials for modeling polymers and AlCl3-based molten salts in LAMMPS and CP2K, respectively.
* Using DeePMD-kit to train **reactive Neural network interatomic potential (rNNIP)** to perform computationally efficient Neural Network molecular dynamics (NNMD) calculations for understanding cyclization reactions in PAN polymers. Enhanced sampling techniques, such as metadynamics and umbrella sampling are employed to train the rNNIP.
* Validating polymer structure and properties obtained from simulations using experimental data for X-ray structure factor, Hermans orientation factor, densities, and elastic properties.
* Using DeePMD-kit to train NNIP to perform computationally efficient NNMD simulations for LiCl, AlCl3, AlCl3-KCl molten salts. The structure and properties obtained from simulations are validated using experimental data for Raman spectra, X-ray and Neutron structure factors, and experimental values for densities, vapor pressures, conductivities, viscosities, etc.
* Collaborating with computational and experimental groups from University of Massachusetts Lowell, Massachusetts Institute of Technology (MIT), Boston University, and Worcester Polytechnic Institute.
1. **Accelerating the Development of Reliable and Robust Machine Learning-Based Interatomic Potentials for the Prediction of Molten Salt Structure and Properties,** University of Massachusetts Lowell 2021-2022
* Performed Born-Oppenheimer ab-initio molecular dynamics calculations to evaluate thermophysical properties of multicomponent molten salts.
* Validated and understood limitations of already existing classical interatomic potentials, such as Rigid ion model, Polarizable ion model, etc. in LAMMPS and CP2K.
* Used DeePMD-kit to train Neural network interatomic potential (NNIP) to perform computationally efficient Neural Network molecular dynamics (NNMD) calculations.
* Mentoring graduate students to develop a model to evaluate the solubility of corrosion products (Chromium, Iron, Cobalt, Nickel) and gaseous species (xenon, krypton, tritium, oxygen, etc.) in molten salt systems.
* Investigated Ensemble learning methods for NNIP uncertainty quantification to help improve transferability of NNIPs across wider phase space.
* Collaborated with computational and experimental groups from Oak Ridge National Laboratory (ORNL), Brookhaven National Laboratory (BNL), State University of New York at Stony Brook, University of South Carolina, Massachusetts Institute of Technology (MIT), and Electrified Thermal Solutions (ETS) at Medford, MA.
1. **Multiscale Stochastic Analysis of Aligned/Random Carbon nanotube (CNT)/Polymer Nanocomposites**, Multiscale Mechanics & Physics Lab, UTA 2015-2020
* Used ReaxFF force-field parameters to obtain cross-linked epoxy structure using LAMMPS.
* Performed Molecular Dynamics Simulations of CNT/Epoxy composites to obtain interface failure properties using ReaxFF force-field utilizing resources at Texas Advanced Computing Center (TACC).
* Contributed to a Python and MATLAB script to generate a two and three-dimensional representative volume element by incorporating statistical distributions of morphological parameters, such as CNT length, diameter, waviness, inter-spacing, and agglomeration.
* Used Embedded Element Method in Abaqus to predict elastic properties from the above-generated composite models and studied the effect of morphological parameters on elastic constants.
* Developed a three-phase (Phases: CNT, epoxy, interphase region) CNT/ polymer composite model to study the effect of hard (polymer crystallinity and CNT surface enhancement) and soft (voids and impurities) interphase on their elastic properties.
1. **Mechanical & Thermal Properties of Silica nanofibers (NFs) and their Electrospun Network/Mats,** Idaho National Laboratory (INL) 2019-2020
* Used reactive molecular dynamics simulations to study the size-dependent thermal stability and mechanical properties of NFs using LAMMPS.
* Studied the effect of hydroxylation/silanol formation on mechanical properties of the NFs.
* Used in-house developed Python script to generate stochastic models of nanofiber network and studied the effect of inter-fiber interactions on overall network mechanics using Abaqus.
* Collaborated with an experimental team to validate the melting behavior of silica NF.
1. **Battery Development using Reactive Force Field Molecular Dynamics Simulations,** Idaho National Laboratory (INL) 2019
* Generated Python scripts to develop molecular models of different State of Charge (SOC) of battery
* Evaluated Self-diffusion coefficient at varied SOC using ReaxFF force-field in LAMMPS
* Studied the effect of charging/lithiation on mechanical properties of graphite anode
1. **Molecular Simulations for Predicting Mechanical and Electrical Properties of Carbon Fiber/Epoxy Composites,** UTARI 2017
* Quantified the change in Mechanical & Electrical properties with the presence of 0.53% w/w moisture content in the CFRP composite material using ReaxFF force-field in LAMMPS.
* Verified the simulation findings with the available experimental evidence.

**MATLAB/PYTHON SCRIPT PUBLICATION**

* **Chahal R.** (2024): Generating Three-dimensional Stochastic RVEs for Finite Element Analysis of Wavy and Aligned/Random Fiber Networks and their Composites using Python (In progress).
* **Chahal R.**, Adnan A., and Roy A. (2017): Generating Representative Volume Element (RVE) for Finite Element Analysis of Random Fiber Composites/Nanocomposites (<https://cdmhub.org/resources/1398>). As of October 1, 2023, the open-source script has been accessed 2564 times.

**ACCEPTED/PUBLISHED RESEARCH**

* Barra J., **Chahal R.**, Audesse S., Zhang J., Zhong, Y., Kabel J., and Lam S. T. (2024): “Chemistry Informed Machine Learning-Based Heat Capacity Prediction of Solid Mixed Oxides,” *J. Phys. Chem. Lett.*, pp. 4721–4728, Apr. 2024, doi: 10.1021/acs.jpclett.4c00506.
* Gibson L., Roy S., Khanal R., **Chahal R.**, Sedova A., and Bryantsev V. (2024): “Tracing mechanistic pathways and reaction kinetics toward equilibrium in reactive molten salts,” *Chemical Science*, 15, pp.3116-3129, Jan. 2024, doi: 10.1039/D3SC06587A.
* Fayfar S., **Chahal R**., Williams H., Gardner D.N., Zheng G., Sprouster D., Neuefeind J., Olds D., Hwang A., Mcfarlane J., Gallagher R.C., Asta M., Lam S., Scarlat R.O., and Khaykovich B. (2024): Complex Structure of Molten FLiBe (2 Li F – Be F 2 ) Examined by Experimental Neutron Scattering, X-Ray Scattering, and Deep-Neural-Network Based Molecular Dynamics, *PRX Energy*, vol. 3, no. 1, p. 013001, Jan. 2024, doi: 10.1103/PRXEnergy.3.013001.
* Lam S. T., Marcella N., **Chahal R.**, and Frenkel A. (2023): Studying Solvation Structure of Metallic Impurities with Machine Learning Molecular Dynamics Enhanced EXAFS, in *Transactions of the American Nuclear Society*, Materials in Nuclear Energy Systems (MiNES) (December 2023). https://www.ans.org/meetings/mines2023/session/view-2253/.
* Zhang Y., **Chahal R.**, Gao M., Ludwig K., Pal U., Powell A.C., Lam S., and Zhong Yu (2023): MD Simulation and Transport Property Analysis of Silicon in High-Temperature Molten Fluoride Salts Electrolyte, in *Transactions of the Electrochemical Society Meeting Abstracts,* vol. 243, no. 21, pp. 1541-1541.
* Coletti M., Sedova A., **Chahal R.**, Gibson L., Roy S., and Bryantsev V. (2023): Multiobjective Hyperparameter Optimization for Deep Learning Interatomic Potential Training Using NSGA-II, in *Proceedings of the 52nd International Conference on Parallel Processing Workshops,* August 2023, pp. 172–179, link: https://doi.org/10.1145/3605731.3608931.
* Lam S. T., Banerjee S., and **Chahal R.** (2023): Uncertainty and Exploration of Deep Learning-based Atomistic Models for Screening Molten Salt Properties and Compositions, in *Proceedings of International Conference on Advances in Nuclear Power Plants (ICAPP’23),* Gyeongju, South Korea (April 23–27, 2023).
* **Chahal R.**, Roy S., Banerjee S., Bryantsev V., and Lam S. (2022): Transferable Deep Learning Potential Reveals Intermediate-Range Ordering Effects in LiF–NaF–ZrF4 Molten Salt. JACS Au 2022, 2, 12, 2693–2702. doi: 10.1021/jacsau.2c00526.
* **Chahal R.**, Banerjee S., and Lam S. T. (2022): Ensemble Learning for Uncertainty Estimation in Molten Salt Atomistic Simulations, in *Transactions of the American Nuclear Society*, vol. 127, no. 1, pp. 483–486.
* Banerjee S., **Chahal R.**, and Lam S. T. (2022): First-Principles Study of Correlated Structures, Dynamics and Transport in Molten MgCl2, in *Transactions of the American Nuclear Society*, vol. 127, no. 1, pp. 487–490.
* Sadeghi, B., Cavaliere P., Pruncu C.I., Balog M., M.M., and **Chahal R.** (2022):Architectural design of advanced aluminum matrix composites: A review of recent developments, Critical Reviews in Solid State and Materials Sciences, pp. 1-71. doi: 10.1080/10408436.2022.2078277.
* Lam S., Banerjee S., and **Chahal R.** (2022): Density Functional Theory van der Waals Corrections for Simulating Fluoride and Chloride Molten Salts, in *Transactions of the American Nuclear Society*, vol. 126, no. 1, pp. 385-386.
* **Chahal R.** and Lam S. (2022): Structure Analysis of LiF-NaF-ZrF4 Molten Salts with Deep Learning Potentials, in *Transactions of the American Nuclear Society*, , vol. 126, no. 1, pp. 113-116.
* **Chahal R.**, Banerjee S., and Lam S. (2022): Short to Intermediate-Range Structure, Transport, and Thermophysical Properties of LiF–NaF–ZrF4 Molten Salts. Front. Phys. 10:830468. doi: 10.3389/fphy.2022.830468.
* **Chahal R.** and Lam S. (2021): Ab-initio Molecular Dynamics Study of LiF-NaF-ZrF4 Molten Salt System, in *Transactions of the American Nuclear Society*, vol. 125, no. 1, pp. 549–553.
* Lam S. and **Chahal R.** (2021): Molecular Analysis of Tritium Solvation in Flibe and Flinak: Effect of Fluoroacidity, Oxidation State, and Impurities, vol. 125, no. 1, pp. 128–130.
* **Chahal R.** and Adnan A. (2021): Three-Dimensional Stochastic Modeling of Wavy Carbon Nanotube/Epoxy Nanocomposites, Multiscale Sci. Eng. 3, 51–61. doi: 10.1007/s42493-020-00052-3.
* **Chahal R.** and Adnan A. (2019): Effect of Carbon Nanotube (CNT) Waviness on Elastic Modulus of CNT/Epoxy Nanocomposites, in *Transactions of the American Society of Composites 34th Technical Conference.*
* **Chahal R.**, Adnan A., Reifsnider K., Raihan R., Wu Y.T., Vadlamudi V., and Elenchezhian M.R.P. (2018): Molecular Dynamics for Prediction of Interfacial Shear Stress & Dielectric Properties of Carbon Fiber/ Epoxy Composites, in *Transactions of the American Society of Composites 33rd Technical Conference.*
* **Chahal R.**, Adnan A., and Roy A. (2017): Elastic Constants of Carbon Nanotube Reinforced Polymer Nanocomposites, in *Transactions of the American Society of Composites 32nd Technical Conference.*
* **Chahal R.**, Adnan A., and Roy A. (2017): Molecular Dynamics Study of Carbon Nanotube/Epoxy Interfaces using ReaxFF, in *Transactions of the American Society of Composites 32nd Technical Conference.*
* Reza M., **Chahal R.,** and Sharma N. (2016): Radiation effect on MHD casson fluid flow over a power-law stretching sheet with chemical reaction. World Academy of Science, Engineering and Technology International Journal of Chemical, Molecular, Nuclear, Materials and Metallurgical Engineering, vol. 10, no. 5.

**RESEARCH PUBLICATIONS IN PREPARATION/UNDER REVIEW**

* **Chahal R.**, Kearney L., Toomey M., Sedova A., Damron J., Naskar A., and Roy S (2024): Deep Learning Potentials for studying Structure, Thermophysical, and Mechanical Properties of Polyacrylonitrile (PAN) (Under Review at ACS Applied Materials & Interfaces).
* **Chahal R.**, Kearney L., Toomey M., Gao Y., Damron J., Naskar A., and Roy S (2024): Reactive Deep Learning Potentials Enabled Rate Theory Analysis for Cyclization Reactions in Polyacrylonitrile (PAN) (In Preparation).
* **Chahal R.**, Gibson L., Roy S., and Bryantsev V. (2024): Modeling AlCl3 Liquid-Vapor Phase Equilibrium using Machine Learning Potentials (In Preparation).
* Gibson L., **Chahal R.**, Roy S., and Bryantsev V. (2024): Solvation free energies of LiCl Molten Salt using Thermodynamic Integration Enabled by Machine Learning Potentials (In Preparation).
* Zhang Y., **Chahal R.**, Azeem M.M., Lam S., Ludwig K., Pal U., Gao M.C., Powell A., Yu Zhong Y. (2024): Computational insights into the structural, thermodynamic and transport properties of CaF2-MgF2 binary fluoride system at high temperatures (Under Review at Journal of Molecular Liquids)
* Wadehra A., **Chahal R.**, Banerjee S., Levy A., Zhang Y., Yan H., Olds D., Zhong Y., Pal U., Lam S. T., Ludwig K. (2024): X-ray and molecular dynamics study of the temperature-dependent structure of molten NaF-ZrF4 (Under Review at Physical Review Materials).
* Banerjee S., **Chahal R.**, and Lam S. T. (2024): Ab initio informed inelastic neutron scattering for time-resolved local dynamics in molten MgCl2 (Under Review at Journal of Molecular Liquids).

**RESEARCH PROPOSAL WRITING EXPERIENCE**

* PI for **‘Uncertainty-Guided Toolkit for Interatomic Potential Foundational Models’** for consideration at AI Initiative at ORNL Director’s Research & Development (DRD) Call FY2025. The team included 12 members in total spanning 4 Divisions across the ORNL. (Concept Paper Recommended for Seed Funding Submission Instead)
* Finalist for ORNL DRD Call FY2024 for Enzyme Engineering Initiative for the project **‘Understanding Nylon-Hydrolase Interaction to Enable Efficient Nylon Deconstruction’** as co-Investigator. (Not Awarded)
* Proposed concept paper as PI on ‘**Predicting Microstructure and Properties of Carbon Fiber using Machine Learning Potentials’** for Vehicle Technology Office (VTO) Lab Call 2023. (Not Awarded)

**TECHNICAL PRESENTATIONS/TALKS**

* **Chahal R.**, Gibson L., Roy S., and Bryantsev V. (2024): Speciation Analysis and Properties of AlCl3 and AlCl3-KCl Molten Salts using Deep Learning Potentials, at Molten salt Symposium at ACS Fall 2024 (**Invited Talk**)
* **Chahal R.**, Kearney L, Toomey M., Damron J.T., Naskar A., and Roy S. (2024): Deep Learning Potentials for Studying Structure, Properties, and Cyclization Reactions in Polyacrylonitrile, at Polymeric Materials: Science and Engineering at ACS Fall 2024.
* Sedova A., Smith M., Coletti M., **Chahal R.**, and Roy S. (2024): Deep learning potentials for hydration and protonation in biomolecular simulations: bond breaking is the goal and the problem, American Physical Society (APS) March Meeting 2024.
* **Chahal R.**, Kearney L, Toomey M., Naskar A., and Roy S. (2023): Deep Learning Potentials for Polyacrylonitrile (PAN) Cyclization, at Symposium on Application of Machine Learning in Polymers: Molecular Structure, Properties, Formulations, and Processing at American Chemical Society conference, San Francisco, California (August 2023).
* Banerjee S., **Chahal R.**, and Lam S. T. (2023): Ab initio informed inelastic neutron scattering for time-resolved local dynamics in molten MgCl2, at Molten Salts Symposium at American Chemical Society conference (**Invited talk** in August 2023).
* **Chahal R.**, Roy S., Banerjee S., Bryantsev V., and Lam S. (2022): Structure-Property Relation in LiF-NaF-ZrF4 Molten salt using Transferable Deep Learning Potentials, at Symposium on Integrating Machine Learning with Simulations for Accelerated Materials Modeling at Materials Research Society conference. (November 2022).
* **Chahal R.**, Banerjee S., and Lam S. T. (2021): Ensemble Learning for Uncertainty Estimation in Molten Salt Atomistic Simulations, American Chemical Society, Phoenix, AZ (November 2022).
* Banerjee S., **Chahal R.**, and Lam S. T. (2021): First-Principles Study of Correlated Structures, Dynamics and Transport in Molten MgCl2, American Chemical Society, Phoenix, AZ (November 2022).
* **Chahal R.** and Lam S. T. (2021): Structure Analysis and Properties of LiF-NaF-ZrF4 Molten Salts with Deep Learning Potentials, Molten Salt Symposium, American Chemical Society, Chicago, IL (**Invited talk** in August 2022).
* **Chahal R.** and Lam S. T. (2021): Ab-initio Molecular Dynamics-trained Deep Neural Network Interatomic Potentials for Multicomponent Molten Salts, American Nuclear Society Winter Meeting and Technical Expo, Washington, DC (December 2021).
* **Chahal R.** and Lam S. T. (2021): Structure and Transport properties of LiF-NaF-ZrF4 Molten salt using DFT-accurate Neural Network interatomic potential, Presentation at Chemical Engineering Departmental Seminar, University of Massachusetts Lowell (**Invited talk** on November 18, 2021).
* Lam S. T., **Chahal R.** (2021): Structure and Transport properties prediction of Multicomponent Molten salts using DFT-accurate Neural Network interatomic potential, Presentation at Workshop on Molten Salt Thermal Properties, University of South Carolina, Columbia, SC (November 17, 2021).
* **Chahal R.** (2020): Multiscale Modeling of Carbon Nanotube Reinforced Polymer Nanocomposites, Battery Group, Idaho National Laboratory.
* **Chahal R.**, Pawar G. (2019): Self-diffusion and Phase Transformation of Lithium in Graphite Anode in Li-ion Batteries, Idaho National Laboratory (Poster Presentation at INL).
* **Chahal R.** and Adnan A. (2019): Three-Dimensional Stochastic Modeling of Wavy Carbon Nanotube/Epoxy Nanocomposites, Women in Aerospace Symposium organized by Massachusetts Institute of Technology (MIT)-Stanford University-University of Colorado Boulder.
* **Chahal R.**, Adnan A., and Roy A. (2017): Interface-Driven Failure Properties of Carbon Nanotube/Epoxy Nanocomposites, International Mechanical Engineering Congress and Exposition, American Society of Mechanical Engineers (ASME).
* **Chahal R.**, Adnan A., and Roy A. (2017): Elastic Constants of Carbon Nanotube Reinforced Polymer Nanocomposites, American Society of Composites 32nd Technical Conference.
* **Chahal R.**, Adnan A., and Roy A. (2017): Molecular Dynamics Study of Carbon Nanotube/Epoxy Interfaces using ReaxFF, American Society of Composites 32nd Technical Conference.
* **Chahal R.** and Adnan A. (2017): Stochastic Modeling of Carbon Nanotube/Epoxy Nanocomposites for Rugged Electronics, in Graduate Seminar, Department of Mechanical & Aerospace Engineering, UTA.
* **Chahal R.** and Adnan A. (2016): Predicting Mechanical Properties of Short Fiber Nanocomposites, in Graduate Seminar, Department of Mechanical & Aerospace Engineering, UTA.

**LEADERSHIP COMPUTING RESOURCES AWARDED**

* SummitPLUS 2024 Allocation Award received as Contributor for the project, ‘Revealing Promethium Aqua Ion Chemistry Using Relativistic Calculations and Machine Learning Approaches’ (100,000 computing hours awarded).
* SummitPLUS 2024 Allocation Award received as Contributor for the project, ‘Reactive, Generalizable Machine Learning Potentials for Molten Salts Modeling at Scale (150,000 computing hours awarded).
* DOE Mission Science Allocation Award received as PI under 2022 ERCAP for the project, ‘Development of Reliable and Robust Neural Network Interatomic Potentials for ZrF4 salts using Ensemble Learning Methods’ (31,875 computing hours awarded).
* DOE Mission Science Allocation Award received as Senior Investigator under 2021 ERCAP for the project, ‘Uncertainty-informed neural network interatomic potentials for many-component molten salts’ (5,000 computing hours).
* Computational Resources awarded by Extreme Science and Engineering Discovery Environment (XSEDE) as PI under 2021 Start-up Allocations category for the project, ‘Solute Solvation in Molten Salts’.

**LIST OF ACHIEVEMENTS/AWARDS**

* **Co-Presider** for “Molten Salt Thermodynamics and Properties” Session at Molten Salt Symposium, ACS Fall 2024.
* Selected for a presentation at Symposium on Integrating Machine Learning with Simulations for Accelerated Materials Modeling at Materials Research Society conference to be held in November 2022. The presenters were selected among a large pool of international researchers through a competitive review process.
* Offered third highest salary during my second year as a Postdoctoral Research Associate at UMass Lowell based on outstanding performance. Based on yearly experience among other Postdoctoral researchers, my offered salary was the highest.
* Received funding from Idaho National Laboratory to be appointed Graduate Reaching Funding from January 2020-December 2020.
* Professor Wen Chan Endowed Scholarship for academic year 2020, The University of Texas at Arlington.
* Kalpana Chawla Endowed Aerospace Scholarship from 2019-2020, The University of Texas at Arlington.
* Selected for participation in **Women in Aerospace (WIA) Symposium 2019** organized & sponsored by MIT-Stanford University-University of Colorado Boulder held at MIT from May 28-29, 2019. Nearly 20 researchers were selected through a competitive process among a large pool of international applicants.
* Travel Scholarship from the American Society for Composites 32nd Technical Conference (2017) at Purdue University in recognition of the publication of MATLAB script for random fiber generation model.
* DNE Lawrence Stephens Endowment Scholarship from 2017-2018, The University of Texas at Arlington.
* Awarded Enhanced Graduate Teaching Assistant funding from 2016-2021 from Department of Mechanical and Aerospace Engineering at The University of Texas at Arlington. Only 1% of Ph.D. students were offered this position, which included 25% higher salary among other tuition benefits.

**MENTORSHIP EXPERIENCE**

* Shubhojit Banerjee (Ph.D. Candidate), Chemical & Nuclear Engineering, UMass Lowell
* Julian Barra Otondo (Ph.D. Candidate), Chemical & Nuclear Engineering, UMass Lowell
* Andrew Duckworth (Undergraduate), Chemical & Nuclear Engineering, UMass Lowell
* Elio Kanaan (Undergraduate), Chemical & Nuclear Engineering, UMass Lowell

**PEER REVIEW EXPERIENCE**

* Nature Scientific Reports
* The Journal of Chemical Physics
* The Journal of Physical Chemistry
* Journal of Nuclear Materials
* Frontiers in Physics
* Material Science & Engineering A
* American Nuclear Society Conference
* Journal of Molecular Liquids

**MEDIA COVERAGE FOR FUNDED RESEARCH PROJECT**

* Research work highlighted on ACS Axial blog for celebrating National Science Day 2023 under the title “Honoring the Legacy of Professor C. V. Raman” (<https://axial.acs.org/cross-disciplinary-concepts/celebrating-national-science-day-2023>).
* An article by UMass Lowell highlights the funding received for the research: ‘UML-led Research on Molten Salt for Energy Generation Wins DOE Funding’ (<https://www.uml.edu/News/stories/2021/Stephen-Lam-DOE-grant.aspx>).

**THEORETICAL BACKGROUND/ RELEVANT TRAINING**

* **Machine Learning for Materials Research Bootcamp** by University of Maryland (To be held online on July 22-24, 2024).
* **Artificial Intelligence for Materials Science (AIMS) Workshop** held on July 12-14, 2022.
* **PRACE Spring School on Modeling Materials using AI/ML** organized by University of Viennafrom June 15 – June 18, 2021.
* **Introduction to Molecular Modeling Concepts for Polymers:** Online paid courseby Schrödinger.
* **LAMMPS Workshop and Symposium (2019)** held in New Mexico, USA.
* **Introduction to Computational Material Sciences:** Random Walk Models, Molecular Dynamics, Coarse-Grained Molecular Dynamics (CGMD), Phase-field Simulations, Density Functional Theory (DFT) Calculations.
* **Fracture Mechanics:** Effect of temperature, geometric parameters & strain rate on Stress Concentration Factors and Failure strength, Elasticity & Plasticity, ASTM Standards to perform Fracture Testing.
* **Failure Analysis & Reliability Engineering:** Mechanical, Electrical, & Corrosion Material Failure, Failure by Reaction: Electromigration & Ion-migration, Weibull, Normal, and Log-Normal Distributions to predict failure & reliability.
* **Advanced Non-traditional Manufacturing Processes:** Diffusion Processes, Integrated Circuits (IC) Fabrication & Packaging, Chemical Etching, Powder Bed Technology, Physical Vapor Deposition, Chemical Vapor Deposition.
* **Advanced Mechanics of Materials:** Polymer physics,Theory of Elasticity, Plasticity, Viscoelasticity, and Piezoelectricity.
* **Advanced Finite Element Methods:** Buckling simulations,Non-linear Geometric and Material Analysis, Cohesive Zone Modeling.
* **Fundamentals of Composites:** Micromechanics, Classical Lamination Theory and its implementation, short fiber composite Analysis (Shear-lag Theory).
* **High-Rate High-Temperature Composites Material Systems:** Change in composite material properties with Temperature and High strain rate/impact loadings, Weibull Distributions to predict Failure.
* **Thermodynamics:** Laws of Thermodynamics, Entropy, Equilibrium, Reaction Kinetics, Introduction to Statistical Mechanics.
* **Heat Transfer:** Conduction, Convection, Thermal Radiation, conjugate heat transfer problems.
* **Introduction to machine learning with Python** (Online course): Neural networks, Regression analysis.
* **Technical Writing in English:** Object Description,Summaries/Analysis,Literature Review & Source Synthesis, Dissertation writing, Research & Funding Proposal writing.

**SELECT SYNERGISTIC ACTIVITIES**

* Women in Physical Sciences (WiPhy) Social Chair at ORNL February 2023-Present
* Student Pilot - Federal Aviation Administration (FAA) Glider Plane Rating June 2018 – Present
* Served as a Judge for the Fort Worth Regional Science and Engineering Fair to intrigue interest in STEM field among school students February 2018 & 2019
* Student Volunteer Captain at 12th International Conference on Durability of Composite Systems 2016

**REFERENCES**

1. **Dr. Santanu Roy (Mentor for current Postdoctoral Appointment at ORNL)**

Research & Development (R&D) Associate, Chemical Science Division

Oak Ridge National Laboratory

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1. **Dr. Vyacheslav Bryantsev (Molten Salts Project lead at current Postdoctoral Appointment at ORNL)**

Group Leader, Chemical Separations Group, Chemical Science Division

Oak Ridge National Laboratory

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1. **Dr. Amit Naskar (Carbon Project lead at current Postdoctoral Appointment at ORNL)**

Group Leader, Carbon & Composites Group, Chemical Science Division

Oak Ridge National Laboratory

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Phone: (865) 576-0309

1. **Dr. Stephen T. Lam (Mentor for Postdoctoral Appointment at UMass Lowell)**

Assistant Professor, Chemical and Nuclear Engineering

University of Massachusetts Lowell

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Phone: (857) 999-7436

1. **Dr. Ashfaq Adnan (Ph.D. Supervisor)**

Professor, Fellow ASME, Mechanical and Aerospace Engineering

The University of Texas at Arlington

Email: aadnan@uta.edu

Phone: (817) 272-2006

1. **Dr. Stephan Irle (Advisor for DRD FY25 Proposal at ORNL)**

Group Leader, Computational Chemistry and Nanomaterial, Chemical Science Division

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