Quanpeng Yang

Postdoctoral Researcher, Ph.D., U.S. Permanent Resident

🌐 www.samtari.com
⚷ samtari1
in quanpengyang
✉ samtariyang@gmail.com
🏴 United States

QUALIFICATIONS SUMMARY

- Ph.D. and post-doc with emphasis on computational simulations and AI for science and engineering
- 10+ years experience with full-stack web development
- 7+ years experience with Python programming and data manipulation libraries such as numpy, pandas
- Extensive experience in full-stack web application development, with a focus on data collection, annotation, and management tools for large-scale deep learning systems
- Proficient in JavaScript and React for building interactive and user-friendly interfaces
- Strong background in Linux, command line tools, and managing cloud infrastructure (e.g., AWS)
- Skilled in using various databases (MySQL, Neo4j, Chroma, etc.)
- Excellent collaboration and communication skills with the ability to work effectively in a team environment
- **Technical Skills:** Python, Django, React, HTML/CSS, SQL, Neo4j, PyTorch, Scikit-learn, AWS, Linux, Bash, Slurm, Cloud High-performance Computing, Schrödinger, LAMMPS, AutoCAD, SolidWorks, MATLAB
- **Certificates:** Machine Learning (Stanford University), Linux and Bash for Data Engineering (Duke University), Neural Networks and Deep Learning, (DeepLearning.AI), Deep Neural Networks with PyTorch (IBM), Introduction to Machine Learning (Duke University), C for Everyone: Programming Fundamentals (UC Santa Cruz)

WORK EXPERIENCE

North Carolina State University
Postdoctoral Researcher
Jan. 2024 – Present
Raleigh, NC, USA

- Developed a customizable AI-powered chatbot web platform enabling users to create their customized chatbots and to convert text, image, or tables to knowledge in vector database and knowledge graph for retrieval-augmented generation (RAG) applications.
- Developed the STEPS Knowledge Hub, a web platform to facilitate STEPS research center's cross-communication, data management, and data analysis using advanced AI techniques such as data mining, large language models (LLMs), RAG, and natural language processing.
- Member of the Science and Technologies for Phosphorus Sustainability (STEPS) Center.
- Performed molecular dynamics simulations to study phosphorus adsorption for promoting phosphorus sustainability in groundwater and soil.

Duke University
Postdoctoral Associate
Nov. 2022 – Nov. 2023
Durham, NC, USA

- Developed a machine learning (ML) force field to accurately model interactions between nanoparticles, enhancing simulation accuracy and predictive capabilities.
- Created a Python package for Monte Carlo simulations with ML and van der Waals force fields for precise and efficient calculations.

University of California, Merced
Graduate Student Researcher
Jan. 2019 – Oct. 2022
Merced, CA, USA

- Collaborated with scientists at ExxonMobil to develop atomistic models and conducted molecular dynamics simulations to understand the stress-strain behaviors of high-performance polymers.
- Created PyL3dMD, a Python package capable of calculating 2000+ molecular descriptors for ML, providing valuable tools for advanced material analysis and research.

- Developed a ML model for hydrocarbon molecules and accurately predicted their densities and viscosities.

George Washington University   *Sep. 2017 – Dec. 2018*
Graduate Student Researcher   *Washington D.C., USA*

- Developed a control system and user interface for an experimental instrument called Ultra-low Temperature Chamber that can be operated as low as -30°C.
- Built a software control system for a pin-on-disk friction testing instrument with a 3-dimensional movement platform and force sensors for research.

South China University of Technology   *Sep. 2014 - Jul. 2017*
Graduate Student Researcher   *Guangzhou, Guangdong, China*

- Developed a web application with features of homework/exam submission and auto-grading, which has been acquired by a company for commercialization.
- Built a physical model and developed a computer software for a pin-on-disk contact mechanism for fast and precise calculations in different experimental conditions.

EDUCATION

🎓 **Ph.D. Degree**   *University of California, Merced*
Mechanical Engineering   *Jan. 2019 – Oct. 2022*
Computational Physics | Machine Learning

🎓 **Master's Degree**   *South China University of Technology*
Mechanical Design and Theory   *Sep. 2014 – Jun. 2017*
Software Development | Numerical Computation

🎓 **Bachelor's Degree**   *Guangdong University of Technology*
Mechanical Design, Manufacturing, and Automation (Microelectronic Track)   *Sep. 2009 – Jun. 2013*
Mechanical Design and Manufacturing, Electronics, Automation, Robotics

PUBLICATIONS

Selected Journal Papers

*Full publication record on **Google Scholar** 𝕏 (published: 15, under review: 2, in preparation: 1)*

* **Q. Yang**, S. Changlani, N. Zaid, A. Conerly, C. Williams, A. Gulyuk, R. Chirkova, Y. Yingling. **Using Data Science and AI Approaches toward Science and Technology Convergence Research** (In preparation)

* **Q. Yang**, S. Callioglu, and G. Arya. **A Machine Learning van der Waals Potential and Monte Carlo Simulation Python Package** (Under review)

* **Q. Yang**, S. Callioglu, J. Laforet, Y. Shao, and G. Arya. Cluster-Move Monte Carlo Simulation with Analytical van der Waals Potential (Under review)

* Y. Wang†, Y. Zhou†, **Q. Yang**, R. Basak, Y. Xie, D. Le, W. Shipley, A. Frano, G. Arya, and A. Tao. **A Multiphysics Approach for Self-Assembly of Nanocrystal Checkerboards via Non-Specific Interactions**. *Nature Communications. 2024*, 15, 3913

* J. Cobena-Reyes, **Q. Yang**, and A. Martini. **Probabilistic Approach to Low Strain Rate Atomistic Simulations of Ultimate Tensile Strength of Polymer Cystals**. *Journal of Chemical Theory and Computation*. 2023, 19, 18, 6326–6331

* P. Panwar, **Q. Yang**, and A. Martini. **Temperature-Dependent Density and Viscosity Prediction of Hydrocarbons: Machine Learning and Molecular Dynamics Simulations**. *Journal of Chemical Information and Modeling. 2023*, 64, 7, 2760–2774

* P. Panwar, **Q. Yang**, and A. Martini. **PyL3dMD: Python LAMMPS 3D Molecular Descriptors**. *Journal of Cheminformatics. 2023*, 15, 1, 1-13.

* A. Pietrangelo, A. Burns, R. Charlton, M. DeRocco, M. Gopinadhan, T. Sun, L. Wang, P. Wright, S. Stober, **Q. Yang**, and A. Martini. Methanol-Assisted ADMET Polymerization of Semiaromatic Amides. *ACS Macro Letters. 2023*, 12, 605-611.

* **Q. Yang**, P. Grützmacher, S. Eder, and A. Martini. Effect of Surface Termination on the Balance between Friction and Failure of $Ti_3C_2T_x$ MXenes. *npj Materials Degradation.* 2023, 7, 1, 6.

* **Q. Yang**, W. Li, S. Stober, A. Burns, M. Gopinadhan, and A. Martini. Effect of Aliphatic Chain Length on the Stress-strain Response of Semi-aromatic Polyamide Crystals. *Macromolecules.* 2022, 55, 12, 5071-5079.

* K. Ahmad, **Q. Yang**, and A. Martini. Analysis of Friction Anisotropy on Self-assembled Monolayers Immersed in Water. *Langmuir.* 2022, 38, 20, 6273-6280.

* **Q. Yang**, W. Li, S. Stober, A. Burns, M. Gopinadhan, and A. Martini. Molecular Dynamics Simulation of the Stress–Strain Behavior of Polyamide Crystals. *Macromolecules.* 2021, 54, 18, 8289-8302.

* X. Hu, **Q. Yang**, W. Nanney, T. Ye, and A. Martini. Simulation of Subnanometer Contrast in Dynamic Atomic Force Microscopy of Hydrophilic Alkanethiol Self-Assembled Monolayers in Water. *Langmuir.* 2020, 36, 9, 2240-2246.

* **Q. Yang**, X. Hu, W. Nanney, T. Ye, and A. Martini. Nanoscale Friction of Hydrophilic and Hydrophobic Self-Assembled Monolayers in Water. *Tribology Letters.* 2020, 68, 1-9.

* T. Lai, Y. Meng, **Q. Yang**, and P. Huang. Evolution and Level Behavior of Adhesion Force by Repeated Contacts of an AFM Colloid Probe in Dry Environment. *The Journal of Adhesion.* 2018, 94, 4, 313-333.

* **Q. Yang** and P. Huang. Friction and Wear Property of Glass Fiber Filled Polytetrafluoroethylene under Sea Water Lubrication. *Hydromechatronics Engineering.* 2016, 44, 18, 12-18.

* **Q. Yang** and P. Huang. **Numerical Calculation of Wear Behavior of Pin and Disk**. *Lubrication Engineering.* 2016, 42, 2, 22-28.

* **Q. Yang** and P. Huang. **Online Homework System of Fundamentals of Mechanical Design Based on ASP**. *Journal of Guangxi University (Nat Sci Ed).* 2015, 40, 2, 226-231.

Software Copyright

* P. Huang and **Q. Yang**. **Online Homework System for Mechanical Curriculum**. December 12, P. Huang and Q. Yang. Online Homework System for Mechanical Engineering. 2016SR366930.

* P. Huang, W. Zhan, and **Q. Yang**. **Exam Paper Generation System for Mechanical Engineering (Online Version)**. 2015SR158368.

* P. Huang, **Q. Yang**, and W. Zhan. **Exam Paper Generation System for Mechanical Engineering (Local Version)**. 2015SR158433.

Patent

* X. Liu, **Q. Yang**. A handheld wall cleaner. (No. ZL 2015 2 1040425.1)

ACTIVITIES AND SERVICES

Conference Session Chair
Biotribology Session | *STLE Tribology Frontier Conference (Chicago, 2019)*
Chemical-mechanical Tribology Session | *STLE Tribology Frontier Conference (Chicago, 2019)*

Organizations
Triangle Molecular Simulation Society (TriMolS) | *Web Master and Social Media Chair*
Society of Tribologist and Lubrication Engineers (STLE) | *Member*
Materials Research Society (MRS) | *Member*

Conferences & Presentations
STEPS NSF Site Visit | *Greensboro, NC, USA. Jun. 2024*
Triangle Molecular Simulation Society | *Durham, NC, USA. May 2024*
Triangle Soft Matter Workshop | *Raleigh, NC, USA. May 2024*
Gordon Research Conference | *Newry, ME, USA. Jul. 2022*
The Web Seminar Series on Tribology (WeSST) | *Online. Jun. 2020*
STLE Tribology Frontier Conference | *Chicago, Illinois, USA. Oct. 2019*
STLE Annual Meeting & Exhibition | *Minneapolis, Minnesota, USA. May 2018*
National Conference on Tribology | *Chengdu, Sichuan, China. Oct. 2015*

National Conference of Mechanical Engineering | *Nanning, Guangxi, China. Jul. 2015*

Outreach and Teaching
Mentor | *Research Experiences for Undergraduates (REU) 2024*
Judge | *The Nano Innavation Challenge 2024*
Interpreter | *Early Family Math (EFM) 2020–2021*
Developer | *Online Homework/Exam System for Engineering Students 2014–2017*
Summer Intern Mentor | *Ohio State University SEEDs Program*

Journal Reviewer
Langmuir | Tribology International | Tribology Letters | Carbon Skeletonl | Sustainability | Polymers | Carbon Skeleton | Applied Sciences | Industrial Lubrication and Tribology | Biophysica

AWARDS

Faculty Mentor Program Fellowship	University of California, Merced	*2022*
Bobcat Fellowship	University of California, Merced	*2019, 2020, 2021, 2022*
Travel Fellowship	University of California, Merced	*2019, 2020*
Summer Fellowship	MACES (sponsored by NASA)	*2019, 2020*
First-tier Annual Scholarship	South China University of Technology	*2016*
Second-tier Annual Scholarship	South China University of Technology	*2015*
Championship in 6th World Choir Games	Interkultur	*2010*
Second-tier Annual Scholarship	Guangdong University of Technology	*2010*