

Quanpeng Yang

Computer Science Educator | AI Researcher | Ph.D.

Work Authorization: U.S. Permanent Resident (no employment sponsorship required)

 samtari1

 quanpengyang

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QUALIFICATIONS SUMMARY

- College-level instructor specializing in programming, artificial intelligence, software development, and database systems
- Ph.D. in Mechanical Engineering with postdoctoral research experience in computational science, machine learning, and scientific computing
- Proficiency with multiple programming languages and applications
- In-depth knowledge of computational techniques, tools, and packages
- Experience with applying machine learning to solve engineering problems
- Good people/communication skills and ability to work as a part of a team
- Strong problem-solving, analytical skills, and desire to find practical solutions to challenging problems
- Hard-working, dedicated, and motivated to achieve goals
- **Programming Languages:** Python, C++, C#, JavaScript, SQL, MATLAB, HTML/CSS
- **AI and Machine Learning:** PyTorch, Scikit-learn, Large Language Models (LLMs), Retrieval-Augmented Generation (RAG), LangChain
- **Software and Web Development:** Django, React, Node.js, Full-stack Development
- **Databases:** MySQL, SQL, Neo4j, Database Design
- **Cloud and Computing:** AWS, Linux, Bash, Slurm, High-performance Computing
- **Scientific and Engineering Tools:** LAMMPS, Schrödinger, AutoCAD, SolidWorks, Arduino, ESP32

WORK EXPERIENCE

Sandhills Community College

Instructor, Computer & Information Technology

Jul. 2025 – Present

Pinehurst, NC, USA

- Teach college-level courses in programming (C++, C#, JavaScript), artificial intelligence, database management (MySQL and SQL), and computer applications.
- Develop course lectures, programming assignments, and hands-on laboratory exercises covering software development, database design, and AI concepts.
- Guide students in applying programming, problem-solving, and software development skills to practical projects.
- Co-developed a graduation name pronunciation application with a colleague to support accurate pronunciation of graduates' names during commencement ceremonies.
- Secured institutional funding for AI-assisted grading and student learning support initiatives.

Labvana

Cofounder & CTO

June. 2025 – Present

Remote, USA

- Develop AI-powered Lab Automation platform

North Carolina State University

Postdoctoral Researcher

Jan. 2024 – Jun. 2025

Raleigh, NC, USA

- Led the development of the STEPS Knowledge Hub, a web platform built with Django and React, to enhance cross-communication, data management, and data analysis for the STEPS research center. Utilized advanced AI techniques, including data mining, large language models (LLMs), retrieval-augmented generation (RAG), and natural language processing (NLP). Gained comprehensive experience in the end-to-end development process, from server setup to product deployment.
- 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-learned force field to accurately model interactions between nanoparticles, enhancing simulation accuracy and predictive capabilities.
- Created a Python package for Monte Carlo simulations, incorporating van der Waals potential for precise and efficient calculations.
- Implemented a cluster-move algorithm into the Monte Carlo simulation, effectively preventing unphysical phenomena and ensuring accurate representation of the system.
- Modeled and simulated self-assembly behaviors of polymer-grafted nanoparticles using coarse-grained interaction models within LAMMPS, providing critical insights into nanostructure formation.
- Authored a proposal to secure high-performance computational resources, optimizing research capabilities and productivity.
- Mentored and supervised 3 graduate students and 3 undergraduate students, fostering their skills in computational materials science and research methodologies.

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, focusing on understanding the stress-strain behaviors of high-performance polymers.
- Created PyL3dMD, a Python package capable of calculating 2000+ molecular descriptors, providing valuable tools for advanced material analysis and research.
- Developed a machine learning model for small hydrocarbon molecules, successfully predicting their densities and viscosities in alignment with experimental data, enhancing predictive accuracy.
- Collaborated with a group at UC Merced to uncover the mechanism behind atomic-resolution atomic force microscopy (AFM), providing crucial insights into material characterization at the atomic level.
- Worked in collaboration with scientists at AC2T Research GmbH and Vienna University of Technology to develop a model exploring MXenes with different surface functional terminations. Studied their frictional behaviors and failure mechanisms, contributing to the understanding of novel materials.

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

- Engineered and developed the "Ultra-low Temperature Chamber," an experimental instrument capable of operating as low as -30°C. Implemented a LabVIEW software user interface to efficiently control three motors and six pumps, enhancing precision and usability.
- Designed and built a pin-on-disk instrument featuring a 3-dimensional movement platform and force sensors for in-depth study of friction and wear phenomena, providing valuable insights into material behavior.

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

- Developed an online-homework system in HTML, ASP and SQL languages, with features of homework/exam submission and auto-grading
- Developed an exam paper auto-generation software with both online and desktop versions
- Built a numerical model for a pin-on-disk contact mechanism and developed accompanying software enabling precise calculations based on user-defined input parameters.

EDUCATION

Ph.D. Degree

Mechanical Engineering

Computational Physics | Machine Learning

University of California, Merced

Jan. 2019 – Oct. 2022

Master's Degree

Electro-Mechanical Engineering

Software Development | Numerical Computation

South China University of Technology

Sep. 2014 – Jun. 2017

Bachelor's Degree

Electro-Mechanical Engineering

Mechanical Design and Manufacturing, Electronics, Automation, Robotics

Guangdong University of Technology

Sep. 2009 – Jun. 2013

GRANTS

Sandhills Community College Foundation Mini-Grant

Project Lead | Awarded \$5,000

2026 – 2027

Sandhills Community College

AI-Assisted Student Learning Support and Faculty Effectiveness System. Funded through the Raymond A. and Rachel H. Stone Grants to Enhance Teaching Excellence.

Teaching Innovation Project (TIPS) Grant

Project Lead | Funded

2025 – 2026

Sandhills Community College

AI-Assisted Grading for Programming Courses. Award confirmed November 2025; proposed project budget: \$500 (final awarded amount not specified in award notification).

XSEDE HPC Computational Resources

Proposal Writing Lead

Jun. 2023 - Jun. 2024

PI: Prof. Gaurav Arya

Molecular Dynamics Simulations of Polymer-Directed Nanoparticle Assembly - DMR160063 (2,070,000 Core-hours)

XSEDE HPC Computational Resources

Proposal Writing Lead

Dec. 2021 - Dec. 2022

PI: Prof. Ashlie Martini

Predicting Atomic-Scale Friction at Experimentally-Accessible Sliding Velocities - MSS130014 (750,000 Core-hours)

PUBLICATIONS

Selected Journal Papers

Full publication record on **Google Scholar** (published: 16, under review: 2, in preparation: 2)

* **Q. Yang**, N. A. Zaid, S. Changlani, A. Conerly, R. Lakshmi-Ratan, C. Williams, A. V. Gulyuk, R. Chirkova, and Y. G. Yingling. Unlocking Phosphorus Sustainability Research Powered by AI: The STEPS Knowledge Hub)

* S. Changlani, N. A. Zaid, **Q. Yang**, R. Chirkova, A. V. Gulyuk, and Y. G. Yingling. Mining Scholarly Data: A Framework for Extracting and Integrating Knowledge from Academic Papers

* **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)

* S. Callioglu, **Q. Yang**, Y. Shao, B. H. Lee, and G. Arya. Efficient Monte Carlo Simulation of Faceted Nanoparticles Using Analytical Interaction Potentials. **The Journal of Physical Chemistry Letters**. **2026**, 17, 7, 2027–2036.

* 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 (Visual Basic Version). 2015SR158433.

Patent

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

ACTIVITIES AND SERVICES

Institutional Service and Leadership

AI Taskforce Member | Sandhills Community College, 2026–Present

AI Roundtable Panelist (Scheduled) | Sandhills Community College, October 2026

Conference Session Chair

Biotribology Session | STLE Tribology Frontier Conference (Chicago, 2019)

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

Member

Society of Tribologist and Lubrication Engineers | STLE

Materials Research Society | MRS

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

Guest Lecturer | Materials Informatics, NC State University, 2024

Judge | The Nano Innvation 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 Skeleton* | *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
Gold Medal in World Choir Games	Interkultur	2010
Second-tier Annual Scholarship	Guangdong University of Technology	2010