Rui Qi Chen

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Education

Georgia Institute of Technology   Atlanta, GA
H. Milton Stewart School of Industrial and Systems Engineering
Ph.D. Student in Machine Learning   2021–Present

Carnegie Mellon University   Pittsburgh, PA
B.S. in Chemical Engineering, University and College Honors   2017–2021

- Minor: Computer Science

Experience

Fritz Haber Institute - Max-Planck-Gesellschaft   Berlin, Germany
Research Internship at Karsten Reuter Group   Summer 2021

- Compared Bayesian and ensemble methods of uncertainty quantification for machine-learned interatomic potentials to improve active learning framework.
- Explored uncertainty recalibration methods to improve the quality of uncertainty measures.

Carnegie Mellon University   Pittsburgh, PA
Undergraduate Research Assistant at Zachary Ulissi Group   Summer 2019–Spring 2021

- Calculated adsorption energies of different adsorbates and surfaces with density functional theory (DFT) to find desirable catalysts for electrochemical processes.
- Trained machine learning models to prioritize high-success calculations and skip futile calculations.
- Developed an active learning framework that learns the correction between first principle theory and simple physics-based potentials to serve as an inexpensive DFT surrogate.

BorsodChem   Kazincbarcika, Hungary
Liaison Internship   Summer 2018

- Oversaw the pipe replacement process in the toluene diisocyanate and methylenediphenyl diisocyanate production plants.
- Supervised the Chinese welders and pipefitters in the Hungarian work environment to comply with local work habits and safety standards.

Publications

[1] M. Shuaibi, S. Sivakumar, R. Q. Chen, and Z. W. Ulissi, "Enabling robust offline active learning for machine learning potentials using simple physics-based priors", *Machine Learning: Science and Technology*, vol. 2, no. 2, p. 025 007, 2020.

Poster Presentations

- "Accelerating Quantum Mechanical Simulations Using Physics-Based Machine Learning Potentials"   2020
  AIChE Annual Meeting (virtual)
- "Enhancing the Workflow Efficiency of High Throughput Surface Calculations"   2019
  Pittsburgh-Cleveland Catalysis Society Annual Symposium

Skills

- **Software:** MATLAB, Aspen Plus, GAMS, Linux, Conda, MongoDB, Google Search
- **Programming:** Python (NumPy, PyTorch, pandas, SciPy, seaborn, OpenCV), C, Standard ML, assembly language, Prolog

Languages

- **English:** fluent
- **Mandarin:** native
- **Hungarian:** native
- **Spanish:** intermediate

Projects

See full list of research projects on ruiqic.github.io/projects/

Active Learning for Machine Learning Potentials
- A software package for active learning to reduce the cost of *ab-initio* atomistic simulations.

Atomistic Machine Learning Package PyTorch
- A machine learning potential package to model atomic interactions

Scholarships

- Chemical Engineering Summer Scholars — 2020
- Summer Undergraduate Research Fellowship — 2019
- Chemical Engineering Summer Scholars — 2019

Academic Awards

- Dean's List — Fall 2017–Spring 2021

Extracurricular Activities

- The Kiltie Band — 2020
  Played clarinet in a large student organized band.
  Performances ranged from classical pieces to marching band music.
- Tartan Wind Ensemble — 2018–2019
  Played clarinet in a young, student-run ensemble of 25 people.
  Performed classical music in a concert every semester.