Rui Qi Chen

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Education

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, Linux, GAMS
- **Programming:** Python, C, SML, assembly language
- **Laboratory:** titrations, UV/Vis spectrometry, high performance liquid chromatography (HPLC), atomic absorption spectroscopy

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.