Rui Qi Chen

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Education

Carnegie Mellon University — Pittsburgh, PA
B.S. in Chemical Engineering, QPA: 3.97/4.00 — 2017–2021

- Minor: Computer Science

Experience

Carnegie Mellon University — Pittsburgh, PA
Undergraduate Research Assistant at Ulissi Group — Summer 2019–Current

- Calculated adsorption energies of different adsorbates and surfaces with density functional theory (DFT) to find desirable catalysts for electrochemical processes.
- Organized and analyzed past DFT data to assess efficiency of current high-throughput automated workflow.
- Trained machine learning models to prioritize high-success calculations and skip futile calculations.
- Took part in the development of a flexible machine learning potential to learn from atomic simulations.
- 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.
- Translated between Chinese and Hungarian to facilitate communication between colleagues to ensure daily procedures were efficiently conducted.
- 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*, 2020. arXiv: 2008.10773 [physics.comp-ph].

Poster Presentations

- "Accelerating Quantum Mechanical Simulations Using Physics-Based Machine Learning Potentials" — 2020
  virtual AIChE Annual Meeting
- "Enhancement of Workflow Efficiency for High Throughput Density Functional Theory Calculations" — 2019
  Berg Undergraduate Research Poster Symposium
- "Enhancing the Workflow Efficiency of High Throughput Surface Calculations" — 2019
  Pittsburgh-Cleveland Catalysis Society Annual Symposium

Skills

- **Software:** MATLAB, Aspen Plus
- **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

- Carnegie Institute of Technology, Dean's List Spring 2020
- Carnegie Institute of Technology, Dean's List Fall 2019
- Carnegie Institute of Technology, Dean's List Spring 2019
- Carnegie Institute of Technology, Dean's List Fall 2018
- Carnegie Institute of Technology, Dean's List Spring 2018
- Mellon College of Science, Dean's List - High Honors Fall 2017

Extracurricular Activities

- The Kiltie Band 2020–Current
  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.