Raymond Y. Wang

833 N Clark St, Unit 2814, Chicago, IL, 60610
raywang.sci@gmail.com | (224) 714-8582 | raymond931118@github

EDUCATION

Northwestern University, Evanston, IL — 06/2021 (Expected)
Ph.D. in Computational Chemistry — GPA: 3.74/4.0
Predictive Science and Engineering Design Fellow

Fudan University, Shanghai, China — 06/2016
Bachelor of Science in Physical Chemistry — GPA: 3.53/4.0
National Scholarship (top 1%)

PROFESSIONAL EXPERIENCE

Northwestern Research Computing Services, Evanston, IL — 02/2019 – Present
High Performance Computing Consultant

- Developed and open-sourced a library of distributed machine learning regression and classification model templates on multiple code platforms including PyTorch, scikit-learn, and Spark MLlib for in-house supercomputer users
- Hosted quarterly data science workshops on cloud computing (AWS), Apache Spark/Hadoop, and parallel programming
- Realized distributed in-memory processing of large Linux system files by deploying a standalone Spark cluster

LLamasoft Inc., Ann Arbor, MI — 06/2020 – 09/2020
Applied Research Intern (cancelled due to the pandemic)

- Purpose: build deep learning models for effective time series forecasting in supply chain optimization applications

RESEARCH PROJECTS

Project: Machine Learning Accelerated Functional Materials Design and Discovery — 02/2018 – Present

- Led a team of 3 PhDs to build a PointNet-BERT model on 130k materials data using 3D Fourier space representations and achieved state-of-the-art performance; pioneered in learning materials physics using deep neural networks
- Visualized and interpreted the decision-making process of the classification model to facilitate materials design
- Developed multi-objective Bayesian optimization with latent-variable Gaussian processes to realize featureless adaptive optimization, successfully discovered Pareto front electronic-transition materials using 30% of original budget
- Constructed self-attention-based graph convolutional network (GCN) to accurately predict molecular properties
- Applied recurrent neural network (LSTM) to generate candidate drug leads from SMILES molecular fragments
- Scraped 10^4 materials data from unstructured online resources using Python, converted to machine-readable database format and trained machine learning regression models to find proper descriptors for alloy property predictions

Project: Quantum Algorithms Development for Correlated Molecular Systems — 08/2016 – 02/2018

- Developed parallel C++ code and contributed to open-source quantum chemistry software package BAGEL
- Designed object-oriented C++ programs with templates, smart pointers, inheritance, MPI, and multi-threading
- Implemented numerical algorithms: PCA, L-BFGS, Krylov subspace solver, Davidson diagonalization, and tensor contraction for parallel and concurrent data processing, capable of solving matrices of size 10^{18}

TECHNICAL SKILLS

Programming Languages	Proficient in Python, C++; familiar with Bash, R, Matlab
Research Skills	Advanced in PyTorch, scikit-learn, Apache Spark, AWS, computational materials design
Relevant Training	Machine Learning, Deep Learning, Bayesian Optimization, Time Series Analysis, Algorithms, Probability and Statistics, Stochastic Processes, Quantum Mechanics

PUBLICATIONS

[1] **Y. Wang**, X. Zhang, F. Xia, E. A. Olivetti, R. Seshadri, and J. M. Rondinelli, "Learning the Crystal Structure Genome for Property Classifications", *Phys. Rev. X (under revision), arXiv:2101.01773* (2021)

[2] **Y. Wang**, A. Iyer, W. Chen, and J. M. Rondinelli, "Featureless Adaptive Optimization Accelerates Electronic Materials Design", *Appl. Phys. Rev.* 7, 041403 (2020)

[3] **Y. Wang**, D. Puggioni, and J. M. Rondinelli, "Assessing Exchange-correlation Functional Performance in the Chalcogenide Lacunar Spinels GaM_4Q_8 (M = Mo, V, Nb, Ta; Q = S, Se)", *Phys. Rev. B* 100, 115149 (2019)

[4] **Y. Wang**, N. Wagner, and J.M.Rondinelli, "Symbolic Regression in Materials Science", *MRS Commun.*, 9(3), 793 (2019)

[5] M. S. Messina, J. C. Axtell, **Y. Wang**, *et al.*, "Visible-Light-Induced Olefin Activation Using 3D Aromatic Boron-Rich Cluster Photooxidants", *J. Am. Chem. Soc.* 138, 22, 6952 (2016)

GRANTS AWARDED

Adaptive Discovery and Mixed-Variable Optimization of Next Generation Synthesizable Microelectronic Materials 04/2020 – 04/2022

Department of Energy: Advanced Research Projects Agency - Energy (ARPA-E)

Research funding awarded: **$1,624,513**

Award number: DE-AR0001209

Contributions to this grant:

- Developed the original idea of using featureless adaptive optimization in functional electronic materials design through composition optimization with collaborators from mechanical engineering
- Demonstrated the theoretical and technical feasibility of this novel methodology in a family of electronic-transition materials, and successfully identified multiple new materials with superior functionality by design
- Proposed a novel electronic materials discovery workflow which integrates natural language processing (NLP), 3D structure-based convolutional neural network (CNN), and Bayesian optimization with Gaussian processes

HONORS AND AWARDS

2018 Predictive Science and Engineering Design Fellowship, Northwestern University ($10k research funding)

2015 National Scholarship, Fudan University (top 1%)

2015 CSST Best Presenter, University of California, Los Angeles (for outstanding summer research)

2014 Victor & William Fung Scholarship, the University of Hong Kong (for top exchange students)

CONFERENCES ATTENDED

2021 ACerS Electronic Materials and Applications 2021 (Virtual)

2020 American Physical Society March Meeting 2020 (Denver, CO)

2019 Materials Research Society Fall Meeting 2019 (Boston, MA)

2019 American Physical Society March Meeting 2019 (Boston, MA)

2019 ACerS Electronic Materials and Applications 2019 (Orlando, FL)

2019 Data Science Workshop in Materials Science (Houston, TX)

2018 Quantum-Espresso Workshop (University Park, PA)

LEADERSHIP EXPERIENCE

Graduate Liaison Committee, Northwestern University, Evanston, IL 08/2018 – Present

Committee member, Department of Chemistry

- Represented 200+ PhD students to facilitate effective student-faculty communications
- Attended monthly meetings to discuss up-coming events and potential improvements within the department

- Hosted research colloquiums and organized department-wide ChemConnnect social events