Raymond Yiqun Wang

EDUCATION

Northwestern University, Evanston, IL   09/2016 - 06/2021
Ph.D. in Computational Chemistry   GPA: 3.74/4.0
Predictive Science and Engineering Design Fellow

Fudan University, Shanghai, China   09/2012 - 06/2016
Bachelor of Science in Chemistry   GPA: 3.53/4.0
National Scholarship (top 1%)

WORK EXPERIENCE

ByteDance AI Lab, Mountain View, CA   07/2021 – Present
Research Scientist
- Develop geometric deep learning models for biomolecular systems
- More details to be announced

DOCTORAL RESEARCH PROJECTS

Machine Learning Accelerated Functional Materials Design and Discovery   02/2018 – 06/2021
- Led a team 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

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, computational chemistry
	Familiar with Open Babel, RDKit, AutoDock, protein modelling
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. R.* (under review) *arXiv:2101.01773* (2022)

[2] J. Glenn, J. Cho, **Y. Wang**, *et al.*, "$Cu_4MnGe_2S_7$ and Cu_2MnGeS_4: Two Polar Thiogermanates Exhibiting Second Harmonic Generation in the Infrared and Structures Derived from Hexagonal Diamond", *Dalton Trans.* 50 (47), 17524 (2021)

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

[4] **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)

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

[6] 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 [link]   04/2020 – 04/2022

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

Research funding awarded: **$1,521,898**

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, 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

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 – 06/2021
Committee member, Department of Chemistry

- Represented Chemistry 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 social events