Raymond Yiqun Wang

raywang.sci@gmail.com | raymond-yiqunwang.github.io

EDUCATION

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

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

WORK EXPERIENCE

ByteDance AI Lab, Mountain View, CA 07/2021 – Present
Research Scientist

- Design novel geometric deep learning models to describe protein-drug interactions
- Apply group theory and equivariant conditions to model 3D molecular systems
- Develop massive biological dataset processing pipelines for statistical analysis

RESEARCH PROJECTS

Machine Learning Accelerated Functional Materials Design and Discovery 02/2019 – 06/2021

- Led a team to build a PointTransformer model on 130k crystalline materials data using 3D Fourier space representations
- Applied novel perturbation and ablation studies to interpret materials physics using deep neural networks as information extractor, pioneered in utilizing statistical learning for structure-based 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 budget
- Constructed self-attention-based graph convolutional network (GCN) to accurately predict molecular properties
- Applied symbolic regression with genetic programming methods to uncover hidden physical laws from materials data
- Scraped 10^4 materials data from unstructured online resources, converted the dataset into machine-readable database format and trained machine learning regression models to find proper descriptors for alloy property predictions

First Principles Computational Simulations for Electronic Materials Platforms 02/2018 – 06/2021

- Employed density functional theory calculations to study the electronic and magnetic phase transitions of multiple materials exhibiting metal-insulator-transitions upon lattice distortions and other external stimuli
- Proposed and demonstrated an effective materials design framework using adaptive learning and structure-based statistical analysis to enable co-design of crystal structural prototype and composition optimization
- Implemented inelastic neutron scattering simulation package for crystal structure phonon dispersion analysis
- Benchmarked the performance of different levels of density functional on simulating electronic properties of a materials family exhibiting Skyrmion lattice states and metal-insulator transitions

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
- Integrated scalar relativistic approximation algorithms (Douglas-Kroll-Hess) into the standard SCF solver
- Realized active space decomposition with orbital optimization to reconstruct total wave function from fragments
- 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}

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)

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

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