Mohan **Liu**

MATERIALS SCIENTIST · DATA SCIENTIST

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Education

Northwestern University	*Evanston, IL, United States*
PH.D. IN MATERIALS SCIENCE AND ENGINEERING	*Sept. 2013 – June. 2019*
Nanjing University	*Nanjing, Jiangsu, China*
B.S. IN PHYSICS	*Sept. 2009 – June. 2013*
University of California, Los Angeles	*Los Angeles, CA, United States*
EXCHANGE PROGRAM, CROSS-DISCIPLINARY SCHOLARS IN SCIENCE AND TECHNOLOGY (CSST)	*July 2012 – Sept. 2012*
The Data Incubator	*San Fransisco, CA, United States*
DATA SCIENCE	*June 2019 – Aug. 2019*

Skills

Materials Science	Density Functional Theory (DFT), Monte Carlo Simulation, Cluster Expansion, Nudged Elastic Band
Data Science	Data Mining, Data Visualization, Machine and Deep Learning, Time Series, Image Processing, NLP
Data Engineering	SQL, Apache Spark, RESTful API, GUI Programming, Web Scrapping, Web Development
Programming	Python, C/C++, Javascript, Matlab, HTML, CSS, LaTeX
Platform	GCP, AWS, Git, Docker, Heroku

Research Experience

Department of Materials Science and Engineering, Northwestern University *Evanston, IL, US*

GRADUATE RESEARCH ASSISTANT, *Advisor: Professor Chris Wolverton* *Sept. 2013 – June. 2019*

— *Materials informatics: large databases and machine learning for materials design and discovery*
- Managed and maintained a MySQL database that stores computed physical and chemical properties for more than 600,000 materials; created a Docker image to provide the community with an easy access to our database using python API based on Django
- Performed high-throughput hybrid-functional density functional theory (DFT) investigation on materials electronic and thermodynamic properties for over 2000 materials
- Implemented a RESTful API for our database using Django rest-framework that allows stateless data delivery with features including pagination, sorting, filtering and authentication
- Designed a python API wrapper, available in PyPI, aiming to provide a straight-forward and pythonic querying method
- Trained regression machine learning models (LASSO, SVR, random-forest and boosting decision tree) to predict materials band gaps with around 20% relative RMSE using elemental-property-based attributes

— *Predictive modeling of adsorbate coverage and compositional effects on catalytic activity*
- Investigated the interplay of compositional and local atomic ordering on adsorption at the surface bimetallic transition-metal (Pt, Rh and Pd) alloys to search for optimal catalyst with high activity and low cost
- Generated computed materials data for greater than 500 different crystal structures and applied linear regression models to predict adsorbate binding energies at alloyed surfaces with less than 5% relative RMSE
- Predicted the stability of Pt-based multi-component nanoparticles and theoretically proved that ternary PtAuCu catalyst out-preforms the state-of-the-art HER catalyst
- Established a framework to efficiently predict the stability and catalytic activity of bimetallic alloys and utilized our framework to identify the ideal composition of Au-Cu alloys with the optimal ORR reactivity

— *Theoretical investigation on thermodynamically stable structures of polyelemental nanoparticles*
- Developed a model to design the interfaces and heterostructures in polyelemental nanoparticles and performed DFT simulation of the architecture of Au-Co-Pd_3Sn and Ag-Cu-Co triphase nanoparticles
- Studied the effect of trace elements (Sb, Bi, Te and Pb) on stabilizing the high-index facets of Pt nanoparticles in order to enhance the overall catalytical performance

Department of Materials Science and Engineering, UCLA *Los Angeles, CA, US*

VISITING RESEARCH ASSISTANT, *Advisor: Professor Vidvudz Ozolins* *June 2012 – Sept. 2012*
- Improved Heisenberg Model by considering long-range and multi-body (triplets and quadruplets) interaction and computed the Curie Temperature of ferromagnetic materials with increased accuracy
- Applied compressive sensing algorithm to accelerate the model optimization and utilized Markov Chain Monte Carlo to simulate the thermodynamic phase transition

Department of Physics, Nanjing University
Nanjing, Jiangsu, China

UNDERGRADUATE RESEARCH ASSISTANT, *Advisor: Professor Wei Zhong* — *Sept. 2012 – June 2013*

- Synthesized carbon-based nanotubes using chemical vapor deposition and characterized nanostructures using SEM and TEM
- Investigated the reactivity of water-soluble sodium-based catalysts and magnetic properties of produced nanotubes
- Comprehensively reviewed on topological insulators and quantum spin hall effect

Extracurricular Activity

The Data Incubator
San Francisco, CA, US

FELLOW — *June 2019 – Aug. 2019*

- Explored the Divvy bike sharing system in Chicago and deployed an end-to-end product to predict daily bike demand at each Divvy station on a future date
- Applied time series forecasting using historical bike-trip data considering stationarity, seasonality, special events and historical Chicago weather; decreased the error by 50% compared with baseline model
- Developed a Live Station Status Monitor to visualize the trend of available bikes/docks at each station over the past week
- Built an ETL pipeline including extracting real-time data of Divvy bike station status using cron job scheduler, transforming JSON format into PostgreSQL and loading the data into Google Cloud database

Avito Demand Prediction Challenge (Kaggle Data Competition)
Chicago, IL, US

LEADER — *June 2018*

- Applied latent semantic analysis for natural language processing to collect text features from advertisement titles and descriptions; used transfer learning and CNN models to extract image features from images of items provided by each seller
- Stored large pre-processed datasets (more than 15 GB in total) using Hierarchical Data Format (HDF) and Feather format to facilitate data I/O; performed multiprocessing to accelerate feature engineering process
- Trained the dataset with more than 1,500,000 observations and 900 features using gradient boost decision tree model with a predicted RMSE of 0.2236 (ranked top 11% on the Kaggle leaderboard)

Mathematical Contest in Modeling (MCM)
Nanjing, Jiangsu, China

LEADER — *Feb. 2011*

- Won the Meritorious Winner award from Consortium for Mathematics and Its Applications
- Modified half-pipe snowboard course to enable higher and longer jumps for athletes

Publications

1. Peng-Cheng Chen, <u>Mohan Liu</u>, Jingshan Du, Brian Meckes, Shunzhi Wang, Haixin Lin, Vinayak P. Dravid, Chris Wolverton, Chad A. Mirkin, "*Interface and heterostructure design in polyelemental nanoparticles*", **Science 363**, Issue 6430 (2019), pp. 959-964

2. Liliang Huang, <u>Mohan Liu</u>, Haixin Lin, Yaobin Xu, Jinsong Wu, Vinayak P. Dravid, Chris Wolverton, Chad A. Mirkin, "*Shape regulation of high-index facet nanoparticles by dealloying*", **Science 365**, Issue 6458 (2019), pp. 1159-1163

3. Huang, Liliang, Peng-Cheng Chen, <u>Mohan Liu</u>, Xianbiao Fu, Pavlo Gordiichuk, Yanan Yu, Chris Wolverton, Yijin Kang, and Chad A. Mirkin. "*Catalyst design by scanning probe block copolymer lithography.*" **Proceedings of the National Academy of Sciences 115**, no. 15 (2018): 3764-3769

4. Jingshan Du, Yi-Ge Zhou, <u>Mohan Liu</u>, Edward J. Kluender, Andrey Ivankir, Peng-Cheng Chen, James L. Hedrick, Chris Wolverton, Vinayak P. Dravid, Chad A. Mirkin, "*Combinatorial Assessment of Au-Cu Alloy Nanoparticle Electrocatalysts*", (under preparation, 2019)

5. <u>Mohan Liu</u>, William F. Schneider, and Chris Wolverton, "*Configuration-dependent adsorption energy at bimetallic surfaces*", (under preparation, 2019)

6. <u>Mohan Liu</u>, Vinay I. Hegde, and Chris Wolverton, "*High-throughput hybrid-functional DFT investigations on materials band gaps and formation energies*", (under preparation, 2019)

7. <u>Mohan Liu</u>, Vinay I. Hegde, and Chris Wolverton, "*qmpy-rester: A RESTful API for accessing materials properties in the Open Quantum Materials Database*", (under preparation, 2019)

Presentations

APS March Meeting 2018
Los Angeles, CA, United States

ORAL PRESENTER — *Mar. 5 – 9, 2018*

- High-throughput hybrid-functional DFT investigations on materials band gaps and formation energies

25th North American Catalysis Society Meeting
Denver, CO, United States

ORAL PRESENTER — *June 4 – 9, 2017*

- Configuration-dependent adsorption energy modifications at bimetallic surfaces

Honors & Awards

2014	**Hierarchical Materials Cluster Program fellowship**	*Northwestern University*
2011	**Excellent Leader of Student Union**	*Nanjing University*
2011	**Outstanding Student Model of Nanjing University**, awarded to top 0.15%	*Nanjing University*
2010	**National Scholarship**, awarded to top 1.5%	*Nanjing University*