Lei Wang

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SUMMARY OF QUALIFICATIONS

Ph.D. degree with (6+) years of research experience in data analytics, ML/AI, and statistics.10 publications showcasing advanced problem-solving skills and innovative solutions across multi-disciplinary projects

Programming languages: (Advanced) Python, C, Unix shell scripts, (Intermediate) SQL

Python libraries*:* Pandas, NumPy, Scikit-learn, TensorFlow, Keras, Matplotlib, Seaborn, SciPy

Developer tools and platforms: Git, Linux, Jupyter Notebooks, VS code, Conda, Slurm, High Performance Computing

Cloud Tools: Azure ML services

RELEVANT EXPERIENCE

Machine Learning and Deep Learning Projects

Deep Learning Specialization & Machine Learning Specialization Certification, Coursera *2023*- Present

- Implemented Deep Q-Learning (RL) for training a lunar lander simulator.
- Developed and applied pre-trained CNNs (U-net, YOLO, MobileNetV2) for object detection in images.
- Created an LSTM (RNN) network for improvising a Jazz solo.

Kaggle Project *2023*- Present

- Conducted data cleaning, exploratory data analysis (EDA), and implemented regression models (linear regression, XGBRegressor, random forests) for product price prediction.

Ph.D. Researcher, University of Calgary, Calgary, AB

Project Lead, Markov-State Model Project *2021-2023*

- Spearheaded and implemented a Bayesian-Markov decision-making model using C and Python for forecasting gas hydrates formation pathway with 900K+ samples. The novel method has bridged the gap of time scale between simulation and experimentation.
- Adapted ML algorithms (logistic regression, hierarchical clustering, Kernel Density Estimation, K-means, PCA) for data mining and structural motif identification.
- Employed network science to visualize transitions in structural building blocks from liquids to solids

Project Lead, Computational Algorithm Project *2019 - 2021*

- Investigated the impact of computational algorithms for temperature control on crystal formation to enhance the numerical accuracy.
- Developed data pipelines for data extraction, transformation, analysis, and visualization across 30+ systems using Python, C, and Unix shell scripts from structured and semi-structured datasets

Research Assistant, Molecular Simulation and Theoretical Studies *2019 – 2023*

- Mentored and trained over 10 students and junior scientists in ML/AI techniques.
- Collaborated with multi-disciplinary scientists to test and implement in-house programs for molecular simulations

EDUCATION

Ph.D., Computational Chemistry, University of Calgary, Calgary, AB 2023
M.Sc., Chemical Engineering, China University of Petroleum, Beijing, China 2016
B.Eng., Chemical Engineering, China University of Petroleum, Beijing, China 2013

CERTIFICATIONS

Deep Learning Specialization, Coursera, 2024
Physics-informed Neural Networks (PINN) - Developer level, University of Alberta, 2024
Machine Learning Specialization, Coursera, 2023

PUBLICATIONS

Wang, L. (2023). Probing nucleation mechanisms of gas hydrates via molecular simulations (Doctoral thesis, University of Calgary, Calgary, Canada).

Wang, L.; Kusalik, P. G. Understanding Why Constant Energy or Constant Temperature May Affect Nucleation Behavior in MD Simulations: A Study of Gas Hydrate Nucleation. *J. Chem. Phys.* **2023**, *159* (18), 184501.

Wang, L.; Zhang, Z.; Kusalik, P. G. Hydrate Nucleation in Water Nanodroplets: Key Factors and Molecular Mechanisms. *Energy & Fuels* **2023**, *37* (2), 1044–1056.

Wang, L.; Hall, K.; Zhang, Z.; Kusalik, P. Mixed Hydrate Nucleation: Molecular Mechanisms and Cage Structures. *J. Phys. Chem. B* **2022**, *126* (36), 7015–7026.

Wang, L.; Zhao, L.; Xu, C.; Wang, Y.; Gao, J. Screening of Active Metals for Reactive Adsorption Desulfurization Adsorbent Using Density Functional Theory. *Appl. Surf. Sci.* **2017**, *399*, 440–450.

Zhao, L.; Zhai, D.; Zheng, H.; Ji, J.; **Wang, L.**; Li, S.; Yang, Q.; Xu, C. Molecular Modeling for Petroleum-Related Applications BT - Structure and Modeling of Complex Petroleum Mixtures; Xu, C., Shi, Q., Eds.; Springer International Publishing: Cham, 2016; pp 121–177.

Wang, L., Kusalik, P. (2022). Hydrate Nucleation in Water Nanodroplets: Key Factors and Molecular Mechanisms. 29th *Canadian Symposium on Theoretical and Computational Chemistry 2022*.- (Poster)

Wang, L., Kusalik, P. (2022). Hydrate Nucleation in Water Nanodroplets: Key Factors and Molecular Mechanisms. *Canadian Chemistry Conference and Exhibition 2022.* - (Poster)

Wang, L., Zhao, L, Kusalik, P. (2018). Screening of Active Metals for Reactive Adsorption Desulfurization Adsorbent Using Density Functional Theory. Canadian *Chemistry Conference and Exhibition 2018.* - (Poster)