Lei Wang

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SUMMARY OF QUALIFICATIONS

Ph.D. researcher specializing in computational chemistry and data analytics with a proven track record of delivering high-quality research and insights for material design and structure prediction.

Programming Languages: Advanced: Python, C, Unix shell scripts, Intermediate: SQL

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

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

Simulation Software: GROMACS, VASP, VMD, VESTA.

EDUCATION

Ph.D. Computational Chemistry

University of Calgary, Canada | 2024

- Thesis: *Probing nucleation mechanisms of gas hydrates via molecular simulations*
- Supervisor: Peter Kusalik

M.Sc. Chemical Engineering

China University of Petroleum, Beijing, China | 2016

- Thesis: *Study mechanisms of adsorption desulfurization of thiophene: density functional theory*
- Supervisor: Chun-Ming Xu

B.Eng. Chemical Engineering

China University of Petroleum, Beijing, China | 2013

RESEARCH EXPERIENCE

Ph.D. Researcher & Principal Researcher - Advanced Statistics Model Project

University of Calgary, Calgary, AB | 2021-2023

- Develop novel techniques bridging the gap of time scale between simulation and experimentation, meeting the project milestones with two papers in submission.
- Spearheaded a Bayesian-Markov decision-making model using C and Python for forecasting gas hydrate building blocks formation at the molecular level with collecting 900K+ samples.
- Applied machine learning algorithms to data mining and structural motif identification, to group hundreds of thousands of individual blocks into a limited number of clusters.
- Employed network science to visualize and prove the stepped transition nature from liquids to solids.

Ph.D. Researcher & Principal Researcher - Temperature Control Project

University of Calgary, Calgary, AB | 2019 - 2021

- Examined the effect of temperature control algorithms on the molecular simulation of crystal formation, to support the accelerated design materials,
- Developed ETL pipelines for (semi)-structured datasets across 30+ systems to automatedly manipulate, analyze, data and visualize pattern using Python, and Unix shell scripts.

Ph.D. Researcher & Principal Researcher - Hydrate Formation within Water Nanodroplets Project

University of Calgary, Calgary, AB | 2018 –2019

- Investigated gas hydrate formation mechanisms within water droplets, to solve flow assurance issues caused by hydrate blockages in multiphase fluids in pipelines.
- Explored the impacts of spatial constraints and the altered thermodynamic and kinetic properties on hydrate formation.

Ph.D. Researcher & Principal researcher, Mixed Gas Hydrate Formation Mechanisms Project

University of Calgary, Calgary, AB | *2017 –2018*

- Investigated the roles of different guest species as gas hydrates form, to quantitatively provide technical support for controlling hydrate formation processes.
- Applied logistic regression to specific descriptors for crystallization processes, to achieve direct a comparison of stochastic behaviors across diverse conditions using Python.

Research Assistant, Molecular Simulation and Theoretical Studies

University of Calgary, Calgary, AB | *2019 – 2023*

- Mentored over 10 junior staffs in data analytics and molecular modelling, simulations techniques.
- Collaborated with multi-disciplinary scientists to implement in-house molecular simulations programs for data analytics

M.Sc. Researcher & Project Lead – Thiophene Desulfurization Mechanisms Project

China University of Petroleum, Beijing, China| 2013 - 2016

- Utilized quantum chemistry (DFT) to accelerate material discovery for oil desulfurization.
- Investigated the thiophene desulfurization capability of transition metals. (Co, Mo, Cr, Ni, Cu, Ag, and Au) with a publication in Appl. Surf. Sci.
- Calculated the free energy landscape to reveal the adsorption desulfurization mechanism and rate determining step for desulfurizing thiophene on Ni13@ZnO.

B.Eng. Researcher & Team Number - Canadian Oil Sands Bitumen Project

China University of Petroleum, Beijing, China | 2013

- Investigated the optimal conditions for bitumen that breaks viscosity to determine the economic feasibility of oil and mining.
- Set up, operated and maintained viscosity-breaking experiments for pilot test.
- Tested materials for stability, density, and gas chromatography

Technician Assistant Intern

China University of Petroleum Beijing &SINOPEC, China| Aug 2011 – Sep 2011

- Provide technical support for routine chemical processing issues and troubleshooting procedures and processes in an oil refinery.

OTHER EXPERIENCE

Machine Learning & Deep Learning Projects

Kaggle Competition Project | 2023 - Present

- Conducted data cleaning, exploratory data analysis, and model training, optimization (linear regression, XGBRegressor, random forests) for product price prediction.

Deep Learning Specialization & Machine Learning Specialization

Coursera | 2023 - Present

- Gained hands-on experience in applying reinforcement learning, Deep Neural Networks, CNNs and RNNs models in devious domains.

Teaching Assistant

University of Calgary, Canada | 2017 – 2023

- Assisted in developing teaching materials for tutorial/lab sessions of various courses.
- Presented complex concepts and facilitated discussions for weekly hour-long tutorial/lab sessions for 1000+ undergraduates.
- Worked collaboratively with over 50 teaching assistants and instructors to support students.

CERTIFICATION, TRAINING AND RELEVANT COURSE

Deep Learning Specialization, Coursera | 2024

Physics-informed Neural Networks - Developer level, University of Alberta | 2024

Machine Learning Specialization, Coursera | 2023

Molecular Driving Forces, University of Calgary | 2020

Biology Python: Machine Learning, University of Calgary enrolled courses | 2020

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)