# Lei Wang

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## SUMMARY OF QUALIFICATIONS

Ph.D. researcher specializing in computational chemistry, data science, ML/AI, and statistics. She excels in project-oriented programming to develop advanced analysis methods for material design and structure prediction. Her latest 10 publications have showcased her ability to deliver cutting-edge solutions for complex projects.

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

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

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

***Simulation Software***: GROMACS, VASP, VMD, VESTA.

## 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, Advanced Statistics Model Project* *2021-2023*

- Spearheaded and implemented a Bayesian-Markov decision-making model using C and Python for forecasting gas hydrates formation pathway at the molecular level with 900K+ samples. The novel method has bridged the gap of time scale between simulation and experimentation.
- Adapted ML algorithms (e.g., hierarchical clustering, Kernel Density Estimation, K-means, and PCA) for data mining and structural motif identification.
- Employed network science to visualize the transition 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 ETL data pipelines for data extraction, transformation, analysis, and visualization across 30+ systems using Python, and Unix shell scripts from structured and semi-structured datasets

*Project Lead, Hydrate Formation within Water Nanodroplets Project* *2018 –2019*

- Investigated gas hydrate formation mechanisms within water droplets, to interpret flow assurance issues caused by hydrate blockages in multiphase fluids in pipelines.
- Explored the radial distribution of density of hydrate crystal, to identify the impacts of water droplet sizes and temperature on the crystal formation.

*Project Lead, Mixed Gas Hydrate Formation Mechanisms Project* *2017 –2018*

- Investigated the roles of different guest species as gas hydrates form, to optimally control formation processes in a desirable direction.
- 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* *2019 – 2023*

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

***M.Sc. Researcher, Chemical Engineering, China University of Petroleum, Beijing, China***

*Project Lead, Thiophene Desulfurization Mechanisms Project* *2013 - 2016*

- Utilized quantum chemistry (DFT) to explore efficiency of catalysts for Thiophene desulfurization, considering Co, Mo, Cr, Ni, Cu, Ag, and Au.
- Elucidated the adsorption desulfurization mechanism via investigation of the free energy landscape for desulfurization of thiophene on Ni13@ZnO by quantum mechanical calculations.

## OTHER EXPERIENCE

***Teaching Assistant, Department of Chemistry, University of Calgary, Canada*** ***2017 - 2023***

- Assisted in creating teaching materials and facilitating discussions for lab sessions with over 1000 undergraduates.
- Worked collaboratively with over 50 teaching assistants and instructors to support students.

***Undergraduate, China University of Petroleum Beijing, China***

*Team number, Canadian Oil Sands Bitumen Project* *2013*

- Explored optimal conditions for viscosity-breaking bitumen to explore the economic feasibility of oils and mining.

*Technician Assistant Intern, SINOPEC, China* *Aug 2011 – Sep 2011*

- Addressed routine chemical processing issues and provided troubleshooting in an oil refinery.

## EDUCATION

**Ph.D.**, Computational Chemistry, University of Calgary, Canada 2023

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

**M.Sc**., Chemical Engineering, China University of Petroleum, Beijing, China 2016

- Thesis title: 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

## CERTIFICATION, TRAINING AND RELEVANT COURSE

Deep Learning Specialization, *Coursera Certificate* 2024

Physics-informed Neural Networks - Developer level, *University of Alberta micro-credential course* 2024

Machine Learning Specialization, *Coursera Certificate* 2023

Molecular Driving Forces: (A+), *University of Calgary enrolled course* 2020

Biology Python: Machine Learning: (A-), *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)

## REFERENCES

**Dr. Peter Kusalik –** [Ph.D. supervisor]

Professor in Department of Chemistry, University of Calgary

*Email: pkusalik@ucalgary.ca*

**Dr. Peter Tieleman –** [Ph.D. supervisor committee member]

Professor in Department of Biochemistry, University of Calgary

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**Dr. Grenfell Pate –** [Ph.D. defense committee member]

Professor in Department of Chemistry, University of British Columbia

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**Dr. Matthew Clarke** – [Ph.D. defense committee member]

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