Lei Wang

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SUMMARY OF QUALIFICATIONS

A Ph.D. researcher specializing in computational chemistry and data analytics with a proven track record in 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

Simulation Software: GROMACS, VASP, VMD, VESTA.

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

RELEVANT EXPERIENCE

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

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

- Brought novel techniques to bridge the gap of time scale between simulation and experimentation.
- 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.
- 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.

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

Email: tieleman@ucalgary.ca

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

Professor in Department of Chemistry, University of British Columbia

Email: patey@chem.ubc.ca

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

Professor in Department of Chemical and Petroleum Engineering, University of Calgary

Email: maclarke@ucalgary.ca