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EMPLOYMENT

Google, Mountain View, CA/Los Angeles, CA
Senior Research Engineer, Google DeepMind — 2022 - Now
AI Residency, Google Brain — 2020 - 2022

Staples, Framingham, MA
Senior Associate Scientist — 2018 - 2020

EDUCATION

Massachusetts Institute of Technology, Cambridge, MA
Ph.D. in Computational Chemistry and ML, Advisor: William Green — 2012 - 2018

Tsinghua University, Beijing, China
B.Sc. in Chemical Engineering and Industrial Engineering — 2008 - 2012

PUBLICATIONS

- J. Shi, **K. Han**, Z. Wang, A. Doucet, M.K. Titsias, *Simplified and Generalized Masked Diffusion for Discrete Data*, arXiv
- **K. Han**, K. Kenealy, A. Barua, N. Fiedel, N. Constant, *Transfer learning for text diffusion models*, arXiv
- ..., **K. Han**, ..., *Gemini: a family of highly capable multimodal models*
- ..., **K. Han**, ..., *Scaling up models and data with t5x and seqio*, Journal of Machine Learning Research
- ..., **K. Han**, ..., *Rt-2: Vision-language-action models transfer web knowledge to robotic control*, Conference on Robot Learning
- ..., **K. Han**, ..., *Plex: Towards reliability using pretrained large model extensions*, ICML
- **K. Han**, B. Lakshminarayanan, J. Liu, *Reliable graph neural networks for drug discovery under distributional shift*, NeurIPS
- Y.P. Li, **K. Han**, C.A. Grambow, W.H. Green, *Self-evolving machine: A continuously improving model for molecular thermochemistry*, The Journal of Physical Chemistry A
- **K. Han**, W.H. Green, *A Fragment-Based Mechanistic Kinetic Modeling Framework for Complex Systems*, Industrial & Engineering Chemistry Research
- **K. Han**, A. Jamal, C.A. Grambow, Z.J. Buras, W.H. Green, *An Extended Group Additivity Method for Polycyclic Thermochemistry Estimation*, International Journal of Chemical Kinetics
- **K. Han**, W.H. Green, and R.H. West, *On-the-fly pruning for rate-based reaction mechanism generation*, Computers & Chemical Engineering
- X. Huang, **K. Han**, and Y. Zhu, *Systematic optimization model and algorithm for binding sequence selection in computational enzyme design*, Protein Science
- Y. Zhang, **K. Han**, D. Lu, and Z. Liu, *Reversible encapsulation of lysozyme within mPEG-b-PMAA: experimental observation and molecular dynamics simulation*, Soft Matter
- Y. Hong, K. Sun, **K. Han**, G. Liu, B. Xu, *Comparison of catalytic combustion of carbon monoxide and formaldehyde over Au/ZrO2 catalysts*, Catalysis Today

TALKS

- **K. Han**, S. Kearnes, J. Xu, W. Torng, J.W. Feng, *Improving Hit-finding: Multilabel Neural Architecture with DEL Data*, NeurIPS 2022

- **K. Han**, B. Lakshminarayanan, J. Liu, *Reliable graph neural networks for drug discovery under distributional shift*, NeurIPS 2022

- ..., **K. Han**, ..., *Towards Reliability using Plex*, 2022 ICML

- M. Liu, M.J. Goldman, A.G. Dana, M.S. Johnson, **K. Han**, W.H. Green, *Advances in predictive kinetic modeling using Reaction Mechanism Generator*, 37th International Symposium on Combustion

- **K. Han**, W.H. Green, *Adaptive Organic Molecular Property Estimator using Convolutional Neural Networks*, 255th ACS National Meeting & Exposition

- **K. Han**, W.H. Green, *Predictive Modeling of Thermal Decomposition of Hydrocarbon Mixtures*, 2016 AIChE Annual Conference

- A. Payne, **K. Han**, W.H. Green, *Predicting the chemistry of a surrogate mixture for heavy oil pyrolysis using the reaction mechanism generator (RMG)*, 254th ACS National Meeting & Exposition

- N. Vandewiele, **K. Han**, W.H. Green, *Scalable algorithms in automatic mechanism generation for complex fuel systems*, 251st ACS National Meeting & Exposition