

Kehang Han

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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

**AWARDS
HONORS** MIT Energy Initiative (MITEI) Fellowship in 2016
3rd Prize (3/30 teams) of MIT Energy Hackathon in 2015
3rd/300+ in “Mitsui Chemicals Cup” Process Design Contest in 2011
2nd Prize in American Mathematical Contest in Modeling in 2011
1st Prize in Chinese National Mathematical Contest in Modeling in 2010
1st Prize in Beijing Physics Contest in 2009
1st Prize in Chinese National Olympic Chemistry Competition in 2007

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