Hao-Wei Pang

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Education

Massachusetts Institute of Technology **Sept. 2018 – Dec. 2023 (expected)**
Ph.D. Chemical Engineering | Advisor: William H. Green GPA 4.9/5.0
Minor in Computer Science and Machine Learning

Massachusetts Institute of Technology **Sept. 2018 – Sept. 2021**
M.S. Chemical Engineering Practice

National Taiwan University **Sept. 2014 – Jun. 2018**
B.S. Chemical Engineering | Advisor: Kuo-Chuan Ho GPA 4.0/4.0

Research, Software Development, and Work Experience

Graduate Research Assistant **Dec. 2018 – Present**
Green Research Group, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA

- Serve as a lead developer for two open-source software packages: Reaction Mechanism Generator (Python) and Reaction Mechanism Simulator (Julia), and collaborate with 10+ contributors through GitHub to develop new functions, maintain APIs, fix bugs, refactor and optimize existing codes, write documentation, use version control tools, write automated unit tests, review pull requests, and ensure continuous integrations
- Program a workflow in Python for automatic generation and fast simulation of multi-phase chemical kinetic models by implementing cheminformatics toolkits
- Automate a procedure using Julia with parallel computing for identification and minimization of reduced chemistry-induced uncertainties in reacting flow simulations
- Build group contribution and machine-learning models (MPNNs and decision trees) to predict radical solvation free-energy corrections to aid in investigating the degradation of active pharmaceutical ingredients
- Implement preconditioned sparse solvers, analytic Jacobian, preallocation, and SIMD for RMS to speed up large-scale chemical kinetic model simulation and beat commercial and well-funded open-source software packages by up to 8-fold

Technical Consultant **Mar. 2021 – May 2021**
Corning Inc., Remote

- Performed process design and technical-economic analyses to evaluate the feasibility of NaOH-based and amine-based direct air capture
- Improved design of single-use bioreactor products to accommodate the needs of the biopharma industry

Technical Consultant **Jan. 2020 – Mar. 2020**
National Renewable Energy Laboratory, Golden, CO

- Led a team of three to assess technical risks associated with biochemical refinery pioneer plants and outline a framework for risk management
- Performed process design and technical-economic analysis for electrochemical carbon dioxide conversion to polymer synthesis precursor

Undergraduate Research Assistant **Jul. 2016 – Jun. 2018**
Electro-Optical Materials Laboratory, Dept. of Chemical Engineering, National Taiwan University, Taiwan

- Increased the ionic conductivity of PVDF-HFP by 30% by functionalizing it with ionic liquids
- Improved the long-term stability of dye-sensitized solar cells up to 90% of its initial efficiency after 1560 hours using electrospun polymeric ionic liquid membranes

Technical & Language Skills

Julia, Python, OOP, Bash, version control (Git, GitHub), Slurm (HPC), Jupyter Notebook, MATLAB, Cheminformatics (RDKit), Gaussian, QChem, Aspen Plus, COMSOL, Chemkin-Pro, Cantera, machine learning and data engineering (SciKitLearn, TensorFlow, PyTorch, Numpy, Pandas), software engineering/development, parallel computing, Linux, Docker, Chinese (native)

Publications

Selected Peer-Reviewed Journal Articles

(Google Scholar)

[J.7] M. S. Johnson, X. Dong, A. G. Dana, Y. Chung, D. Farina, Jr., R. J. Gillis, M. Liu, N. W. Yee, K. Blondal, E. Mazeau, C. A. Grambow, A. M. Payne, K. Spiekermann, **H. Pang**, C. F. Goldsmith, R. H. West, W. H. Green, "The RMG Database for Chemical Property Prediction," *Journal of Chemical Information and Modeling* 62(20), 4906-4915 (2022)

[J.6] L. Lai, **H. Pang**, W. H. Green, "Formation of two-ring aromatics in hexylbenzene pyrolysis," *Energy Fuels* 34(2), 1365-1377 (2020)

[J.5] **H. Pang**, H. Yu, Y. Huang, C. Li, K. Ho, "Electrospun membranes of imidazole-grafted polymeric ionic liquids for highly efficient quasi-solid-state dye-sensitized solar cells," *J. Mater. Chem. A* 6 14215-14223 (2018)

[J.4] C. Tseng, C. Lee, Y. Huang, **H. Pang**, K. Ho, Y. Chen, "One-step synthesis of graphene hollow nanoballs with various nitrogen-doped states for electrocatalysis in dye-sensitized solar cells," *Materials Today Energy* 8 15-21 (2018)

[J.3] H. Yu, S. Kao, H. Lu, Y. Lin, H. Feng, **H. Pang**, R. Vittal, J. Lin, K. Ho, "Electrospun nanofibers composed of poly(vinylidene fluoride-co-hexafluoropropylene) and poly(oxyethylene)-imide imidazolium tetrafluoroborate as electrolytes for solid-state electrochromic devices," *Sol. Energy Mater. Sol. Cells* 177 32-43 (2018)

[J.2] Y. Huang, C. Lee, **H. Pang**, C. Li, M. Fan, R. Vittal, K. Ho, "Microemulsion-controlled synthesis of CoSe2 /CoSeO3 composite crystals for electrocatalysis in dye-sensitized solar cells," *Materials Today Energy* 6 189-197 (2017)

[J.1] C. Li, C. Lee, I. Chiu, R. Vittal, Y. Huang, T. Chen, **H. Pang**, J. Lin, K. Ho, "Hierarchical $TiO_{1.1}Se_{0.9}$-wrapped carbon cloth as the TCO-free and Pt-free counter electrode for iodide-based and cobalt-based dye-sensitized solar cells," *J. Mater. Chem. A* 5 14079-14091 (2017)

Selected Journal Articles in Progress

[j.4] **H. Pang**, M. Forsuelo, X. Dong, R. E. Hawtof, D. S. Ranasinghe, W. H. Green, "A detailed multi-phase chemical kinetic model for polymer fouling in distillation column," *submitted*

[j.3] **H. Pang**, X. Dong, W. H. Green, "Extending automated generation of multi-phase kinetic models for polymer fouling towards oxygen chemistry," *in preparation*

[j.2] M. S. Johnson, **H. Pang**, A. M. Payne, W. H. Green, "ReactionMechanismSimulator.jl: A Modern Approach to Chemical Kinetic Mechanism Simulation and Analysis," *in preparation*

[j.1] M. S. Johnson, **H. Pang**, M. Liu, W. H. Green, "Species selection for automatic chemical kinetic mechanism generation," *in preparation*

Selected Conference Presentations

[C.5] Y. Chung, M. S. Johnson, C. J. McGill, E. Heid, **H. Pang**, X. Dong, A. M. Payne, K. Spiekermann, L. Pattanaik, W. H. Green, "The Reaction Mechanism Generator, Chemprop, and the Reaction Mechanism Simulator: open-source methods for predicting reaction rates and equilibria, and constructing, solving, and analyzing kinetic simulations", *Oral Presentation*, American Chemical Society (Aug. 2022)

[C.4] **H. Pang**, M. Hassanaly, M. Day, W. H. Green, Iterative Workflow for Quantification and Minimization of Reduced Chemistry-Induced Uncertainties in Reacting Flow Simulation, *Poster Presentation*, Combustion Symposium (Jul. 2022)

[C.3] W. H. Green, Y. Chung, X. Dong, M. Forsuelo, M. S. Johnson, **H. Pang**, A. M, Payne, Matthew B. P Prendergast, K. Spiekermann, F. H. Vermeire, Y. Wang, O. H. Wu, "Progress Towards Predictive Reaction Engineering". *Oral Presentation*, International Symposium on Chemical Reaction Engineering (Dec. 2021)

[C.2] M. Forsuelo, **H. Pang**, D. Ranasinghe, W. H. Green, "A molecular model for reactive fouling in steam-cracker separation trains". *Oral Presentation*, American Institute of Chemical Engineers (Nov 2020)

[C.1] D. Ranasinghe, M. Forsuelo, **H. Pang**, W. H. Green, "Automated Reaction Mechanism Generation and Automatic Quantum Chemical Calculations: The Initial Stages of Butadiene Oligomerization and Polymerization". *Oral Presentation*, American Chemical Society (Aug. 2020)