

Li, Yi-Pei (李奕霽)

Assistant Professor

B.S. in Chemical Engineering
National Taiwan University, 2009

Ph.D. in Chemical Engineering
University of California at Berkeley, 2016

Research and Professional Interests

Reaction Engineering
Computational Chemistry
Machine Learning

Journal Papers

1. C. A. Grambow, **Y.-P. Li** and W. H. Green, "Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach", *The Journal of Physical Chemistry A*, 123(27), 5826–5835, 2019(Jun)
2. M. Keçeli, S. N. Elliott, **Y.-P. Li**, M. S. Johnson, C. Cavallotti, Y. Georgievskii, W. H. Green, M. Pelucchi, J. M. Wozniak and A. W. Jasper, "Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics", *Proceedings of the Combustion Institute*, 37(1), 363-371, 2019(Aug)
3. **Y.-P. Li**, K. Han, C. A. Grambow and W. H. Green, "Self-evolving machine: A continuously improving model for molecular thermochemistry", *The Journal of Physical Chemistry A*, 123(10), 2142-2152, 2019(Feb)
4. C. A. Grambow, A. Jamal, **Y.-P. Li**, W. H. Green, J. Zador and Y. V. Suleimanov, "Unimolecular reaction pathways of a γ -keto hydroperoxide from combined application of automated reaction discovery methods", *Journal of the American Chemical Society*, 140(3), 1035-1048, 2018(Dec)
5. J. G. Howell, **Y.-P. Li** and A. T. Bell, "Propene metathesis over supported tungsten oxide catalysts: A study of active site formation", *ACS Catalysis*, 6(11), 7728-7738, 2016(Oct)
6. **Y.-P. Li**, A. T. Bell and M. Head-Gordon, "Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules", *Journal of chemical theory and computation*, 12(6), 2861–2870, 2016(May)
7. **Y.-P. Li**, M. Head-Gordon and A. T. Bell, "Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid Catalyzed by Sn-BEA", *ACS Catalysis*, 6(8), 5052–5061, 2016(Jun)
8. **Y.-P. Li**, J. Gomes, S. Mallikarjun Sharada, A. T. Bell and M. Head-Gordon, "Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies", *The Journal of Physical Chemistry C*, 119(4), 1840–1850, 2015(Dec)

Conference Papers

1. **Yi-Pei Li**, "Towards High Fidelity Reaction Modeling by Combining Quantum Mechanics and Machine Learning", 第八屆海峽兩岸理論計算化學研討會, Taipei, Taiwan, 2019(Dec), **Invited Speaker and Session Chair**
2. **Yi-Pei Li**, Kehang Han, Colin A. Grambow and William H. Green, "Towards High Fidelity Reaction Modeling by Combining Quantum Mechanics and Machine Learning",

2019 台灣化學工程學會 66 週年年會, Taichung, Taiwan, 2019(Nov), **Invited Speaker**

3. Ting-Wei Hsu, Ke-Yang Dai, Kehang Han, Colin A. Grambow, William H. Green and **Yi-Pei Li**, "Uncertainty Quantification for Machine Learning and a Self-Learning Model for Molecular Property Prediction", 2019 台灣化學工程學會 66 週年年會, Taichung, Taiwan, 2019(Nov)
4. Tsai-Chen Hsiung, Colin A. Grambow, William H. Green and **Yi-Pei Li**, "Machine Learning with Small Data Sets for Molecular Property Prediction", 2019 台灣化學工程學會 66 週年年會, Taichung, Taiwan, 2019(Nov)
5. **Yi-Pei Li**, "Application of Quantum Mechanics and Machine Learning in Reaction Engineering", Seminar at the College of Chemistry and Chemical Engineering, Fuzhou University, Fuzhou, China, 2019(Nov), **Invited Speaker**
6. **Yi-Pei Li**, "Computer-Aided Reaction Mechanism Discovery and Catalysis Engineering", Seminar at the Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, Canada, 2019(Apr), **Invited Speaker**
7. **Yi-Pei Li**, "Engineering Chemical Reactions with Quantum Mechanics and Machine Learning", Seminar at the Department of Mineral and Energy Engineering, Penn State University, University Park, PA, USA, 2019(Apr), **Invited Speaker**
8. **Yi-Pei Li**, Kehang Han, Colin A. Grambow and William H. Green, "Self-Evolving Machine: A Continuously Improved Model for Molecular Thermochemistry", 256th ACS National Meeting, Boston, MA, USA, 2018(Aug)
9. **Yi-Pei Li**, "Computer-Aided Reaction Engineering: Tuning of Catalysts for Biofuel Conversions", Seminar at the Academia Sinica, Taipei, Taiwan, 2018(Apr), **Invited Speaker**
10. Colin A. Grambow, Adeel Jamal, **Yi-Pei Li**, William H. Green, Judit Zádor and Yury V. Suleimanov, "Automated Reaction Discovery from Combined Application of Transition State Search Algorithms", 2018 APS Meeting, Los Angeles, CA, USA, 2018(Mar)
11. **Yi-Pei Li**, "Computer-Aided Reaction Engineering: Tuning of Catalysts for Biofuel Conversions", Seminar at the Department of Chemical Engineering, Texas A&M, College Station, TX, USA, 2018(Feb), **Invited Speaker**
12. **Yi-Pei Li**, Kehang Han and William H. Green, "Estimation of Thermodynamic Properties of Polycyclic Molecules by a Linear Regression Model", 2017 AIChE Annual Meeting, Minneapolis, MN, USA, 2017(Oct)
13. **Yi-Pei Li**, "Theoretical Modeling of Reactions Occurring in Zeolite Catalysts", Chemical and Biomolecular Colloquium at UC Berkeley, Berkeley, CA, USA, 2015(Oct)
14. **Yi-Pei Li**, Martin Head-Gordon and Alexis T. Bell, "Theoretical Study of 4-(Hydroxymethyl)Benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)Furoic Acid Catalyzed By Sn-BEA", 24th North American Catalysis Society Meeting, Pittsburgh, PA, USA, 2015(Jun)

Honors and Others

1. 指導學生李世晟同學，獲得堉璘獎學金 (2019)
2. 論文被美國能源部選為 NERSC Science Highlight (2019)
3. Outstanding Scholar Award, Foundation for the Advancement of Outstanding Scholarship, Taiwan (2019)
4. Graduate Division Conference Travel Grant Award, UC Berkeley (2015)

