Peng Liu

Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA 90095, USA
+1-(310)-266-1647 • pengliu@ucla.edu

EDUCATION

- **University of California, Los Angeles** — Los Angeles, California — June 2010 – Present
  Department of Chemistry and Biochemistry — Advisor: Prof. Kendall N. Houk
  Postdoctoral Scholar

- **University of California, Los Angeles** — Los Angeles, California — Sep. 2006 – June 2010
  Department of Chemistry and Biochemistry — Advisor: Prof. Kendall N. Houk
  Ph.D. Degree

- **University of Guelph** — Guelph, Ontario, Canada — Sep. 2004 – Aug. 2006
  Department of Chemistry — Advisor: Prof. John D. Goddard
  M.Sc. Degree

- **Peking University** — Beijing, China — Sep. 1999 – Jul. 2003
  Department of Chemistry — Advisor: Prof. Wenjian Liu
  B. Sc. Degree

RESEARCH EXPERIENCES

- **Postdoctoral Research at UCLA** — July 2010 – Present

  Involved in four areas of research:

  (a) *Computational studies of transition metal-catalyzed reactions.* Rationalized reaction mechanisms, and origins of reactivities, regio- and stereoselectivities of transition metal-catalyzed reactions. Reactions investigated include Ru-catalyzed olefin metathesis, Pd- and Fe-catalyzed C–H activations and functionalizations, and Ni-catalyzed reductive coupling reactions. Collaborated with Grubbs and Stoltz at Caltech, Garg at UCLA, Montgomery at Michigan, Lautens at Toronto, Yu at Scripps, and White at Illinois.

  (b) *Quasiclassical trajectory studies of Diels-Alder reactions.* Investigated the mechanisms, asynchronicity, and timing of bond formations in Diels-Alder reactions with quasiclassical molecular dynamics simulations.

  (c) *Molecular dynamics simulations of polymers and carbon nanotubes*. Performed dynamics simulations to predict the dynamical properties of fullerene-containing polymers in solution. Investigated polymer wrapping with single-walled carbon nanotubes. Collaborated with Zhenan Bao at Stanford.

  (d) *Computational studies of asymmetric organocatalysis.* Established theoretical models to predict stereoselectivities of kinetic resolutions of benzylic alcohols, carboxylic acids, and azlactones with chiral acyl transfer catalyst. This is in collaboration with Birman at the University of Washington at St. Louis.

- **Ph.D. Research at UCLA** — Sep. 2006 – June 2010

  Performed computational investigations on mechanisms, and origins of reactivities, regio- and stereoselectivities of transition metal-catalyzed reactions. Reactions investigated include: Rh-, Ni-, and Cu-catalyzed C–C and C–X coupling reactions and Rh-catalyzed (5+2) cycloadditions. Collaborated with Buchwald and Jamison at MIT, Krische at UT Austin, Nicolas at Oklahoma, Wender at Stanford, and Weiping Tang at Madison.

RESEARCH EXPERIENCES (CONTINUED)

- **M.Sc. Research at the University of Guelph** Sep. 2004 – June 2006
  Performed computational studies on the mechanism, reactivity, and selectivity of Ru-catalyzed [2+2] cycloadditions and conformational analysis and variable temperature ^{19}F NMR studies of perfluorooctane sulfonate (PFOS) and its derivatives. Collaborated with Tam at the University of Guelph.

PUBLICATIONS

1. ***Z*-Selectivity in Olefin Metathesis with Chelated Ru Catalysts: Computational Studies of Mechanism and Selectivity**
   Peng Liu, Xiufang Xu, Xiaofei Dong, Benjamin K. Keitz, Myles B. Herbert, Robert H. Grubbs*, and K. N. Houk* *J. Am. Chem. Soc.* **2012**, *134*, 1464–1467.

2. **Theoretical Study of Pd(0)-Catalyzed Carbohalogenations of Alkenes: Mechanism and Origins of Reactivities and Selectivities in Alkyl Halide Reductive Elimination from Pd(II) Species**
   Yu Lan, Peng Liu, Stephen G. Newman, Mark Lautens*, and K. N. Houk* *Chem. Sci.* **2012**, 3, 1987-1995.

3. **Decomposition Pathways of Z-Selective Ruthenium Metathesis Catalysts**
   Myles B. Herbert, Yu Lan, Benjamin K. Keitz, Peng Liu, Koji Endo, Michael W. Day, K. N. Houk,* and Robert H. Grubbs* *J. Am. Chem. Soc.* **2012**, *134*, 7861-7866.

4. **Dynamics, Transition States, and Timing of Bond Formation in Diels-Alder Reactions**
   Kersey Black, Peng Liu, Lai Xu, Charles Doubleday,* and K. N. Houk* *Proc. Natl. Acad. Sci. U. S. A.* **2012**, in press, DOI: 10.1073/pnas.1209316109.

5. **Origin of Enantioselectivity in Benzotetramisole-Catalyzed Dynamic Kinetic Resolution of Azlactones**
   Peng Liu, Xing Yang, Vladimir B. Birman,* and K. N. Houk* *Org. Lett.* **2012**, *14*, 3288-3291.

6. **Ligand Effects on Rates and Regioselectivities of Rh(I)-Catalyzed (5+2) Cycloadditions: A Computational Study of Cyclooctadiene and Dinaphthocyclooctatetraene as Ligands**
   Xiufang Xu, Peng Liu, Adam Lesser, Lauren E. Sirois, Paul A. Wender*, and K. N. Houk* *J. Am. Chem. Soc.* **2012**, *134*, 11012-11025.

7. **Manifestation of Felkin-Anh Control in Enantioselective Acyl Transfer Catalysis: Kinetic Resolution of Carboxylic Acids**
   Xing Yang, Peng Liu, K. N. Houk*, and Vladimir B. Birman* *Angew. Chem., Int. Ed.* **2012**, accepted.

8. **Understanding Reactivity and Stereoselectivity in Palladium-Catalyzed Diastereoselective sp^3 C–H Bond Activation: Intermediate Characterization and Computational Studies**
   Ramesh Giri, Yu Lan, Peng Liu, K. N. Houk*, and Jin-Quan Yu* *J. Am. Chem. Soc.* **2012**, accepted.

9. **Mechanism of the Cycloaddition of Carbon Dioxide and Epoxides Catalyzed by Co-Substituted 12-Tungstenphosphate**
   Fawang Chen, Xiaofang Li, Bo Wang, Tiegang Xu, Shi-Lu Chen,* Peng Liu,* and Changwen Hu* *Chem. Eur. J.* **2012**, in press, DOI: 10.1002/chem.201201042. (PDF)

10. **Ligand Steric Contours To Understand the Effects of N-Heterocyclic Carbene Ligands on the Reversal of Regioselectivity in Ni-Catalyzed Reductive Couplings of Alkynes and Aldehydes**
    Peng Liu, John Montgomery,* and K. N. Houk* *J. Am. Chem. Soc.* **2011**, *133*, 6956–6959.

PUBLICATIONS (CONTINUED)

11. **Mechanism, Regio- and Stereoselectivities of Rh(I)-Catalyzed Hydrogenative Couplings of 1,3-Diynes and Activated Carbonyl Partners: Intervention of a Novel Cumulene Intermediate**
Peng Liu, Michael J. Krische,* and K. N. Houk*, *Chem. Eur. J.* **2011**, *17*, 4021–4029.

12. **Suzuki–Miyaura Cross-Coupling of Aryl Carbamates and Sulfamates: Experimental and Computational Studies**
Kyle W. Quasdorf, Aurora Antoft-Finch, Peng Liu, Anna Komaromi, Amanda L. Silberstein, Tom Blackburn, Stephen D. Ramgren, K. N. Houk*, Victor Snieckus*, and Neil K. Garg* *J. Am. Chem. Soc.* **2011**, *133*, 6352–6363; Highlighted in *Synfacts* **2011**, *7*, 771.

13. **Nickel-Catalyzed Amination of Aryl Carbamates and Sequential Site-Selective Cross-Couplings**
Tehetena Mesganaw, Amanda L. Silberstein, Stephen D. Ramgren, Noah Fine Nathel, Xin Hong, Peng Liu, and Neil K. Garg* *Chem. Sci.* **2011**, *2*, 1766–1771.

14. **Theoretical Studies of Regioselectivity of Ni- and Rh-Catalyzed C–C Bond Forming Reactions with Unsymmetrical Alkynes**
Peng Liu, and K. N. Houk*, *Inorg. Chim. Acta* (invited review in the special issue honoring Robert G. Bergman), **2011**, *369*, 2–14.

15. **Electronic and Steric Control of Regioselectivities in Rh(I)-Catalyzed (5+2) Cycloadditions: Experiment and Theory**
Peng Liu, Lauren E. Sirois, Paul Ha-Yeon Cheong, Zhi-Xiang Yu, Ingo V. Hartung, Heiko Rieck, Paul A. Wender,* and K. N. Houk,* *J. Am. Chem. Soc.* **2010**, *132*, 10127–10135; Indexed by *ChemInform* **2011**, *42*, DOI: 10.1002/chin.201102071.

16. **On the Mechanism of Ligand-Assisted, Copper-Catalyzed Benzylic Amination by Chloramine-T**
Dipti N. Barman, Peng Liu, Kendall N. Houk,* and Kenneth M. Nicholas**,* *Organometallics*, **2010**, *29*, 3404–3412.

17. **Origins of Regioselectivity and Alkene-Directing Effects in Nickel-Catalyzed Reductive Coupling Reactions**
Peng Liu, P. R. McCarren, Paul Ha-Yeon Cheong, Timothy F. Jamison,* and K. N. Houk,* *J. Am. Chem. Soc.*, **2010**, *132*, 2050–2057.

18. **Computational Exploration of Mechanisms and Ligand-Directed Selectivities of Copper-Catalyzed Ullmann-Type Reactions**
Gavin O. Jones, Peng Liu, K. N. Houk,* and Stephen L. Buchwald,* *J. Am. Chem. Soc.* **2010**, *132*, 6205–6213.

19. **Mechanism and Transition State Structures for Nickel-Catalyzed Reductive Alkyne-Aldehyde Coupling Reactions**
P. R. McCarren, Peng Liu, Paul Ha-Yeon Cheong, Timothy F. Jamison,* and K. N. Houk* *J. Am. Chem. Soc.*, **2009**, *131*, 6654–6655.

20. **Substituent Effects on Reaction Barriers, Reactant Preorganization Energies, and Ligand Exchange Energies Control Reactivities in Rh(I)-Catalyzed (5+2) Cycloadditions of Substituted Vinylcyclopropanes with Alkynes**
Peng Liu, Paul Ha-Yeon Cheong, Zhi-Xiang Yu, Paul A. Wender,* and K. N. Houk* *Angew. Chem., Int. Ed.* **2008**, *47*, 3939–3941; *Angew. Chem.* **2008**, *120*, 4003–4005.

PUBLICATIONS (CONTINUED)

21. **Origins of differences in reactivities of alkenes, alkynes, and allenes in $[Rh(CO)_2CI]_2$-catalyzed (5+2) cycloaddition reactions with vinylcyclopropanes**
Zhi-Xiang Yu, Paul Ha-Yeon Cheong, Peng Liu, Claude Y. Legault, Paul A. Wender,* and K. N. Houk* *J. Am. Chem. Soc.* **2008,** *130*, 2378–2379.

22. **Origin of Enantioselectivity in CF_3-PIP-Catalyzed Kinetic Resolution of Secondary Benzylic Alcohols**
Ximin Li, Peng Liu, K. N. Houk,* and Vladimir B. Birman* *J. Am. Chem. Soc*. **2008**, *130*, 13836–13837.

23. **Theoretical studies of the conformations and ^{19}F NMR spectra of linear and a branched perfluorooctanesulfonamide (PFOSAmide)**
Peng Liu, John D. Goddard, Gilles Arsenault,* Jun Gu, Alan J. McAlees, Robert McCrindle, and Valerie Robertson *Chemosphere* **2007**, *69*, 1213–1220.

24. **Ruthenium-Catalyzed [2+2] Cycloadditions between Substituted Alkynes and Norbornadiene: A Theoretical Study**
Peng Liu, William Tam, and John D. Goddard* *Tetrahedron* **2007**, *63*, 7659–7666.

25. **Remote Substituent Effects in Ruthenium-Catalyzed [2+2] Cycloadditions: An Experimental and Theoretical Study**
Peng Liu, Robert W. Jordan, Steven P. Kibbee, John D. Goddard,* and William Tam* *J. Org. Chem.*, **2006**, *71*, 3793–3803.

AWARDS

➢ Chancellor's Award for Postdoctoral Research	University of California, Los Angeles	2012
➢ MBI Postdoctoral Award for Research Excellence	University of California, Los Angeles	2012
➢ Saul and Sylvia Winstein Award	University of California, Los Angeles	2010
➢ Satyan & Vimala Majeti Fellowship Award	University of California, Los Angeles	2009
➢ Excellence in First Year Academics and Research	University of California, Los Angeles	2007

INVITED SEMINARS AND PRESENTATIONS

- Invited Seminar Presentation at the University of Michigan — November 30, 2011
  Computational Studies of Organic and Organometallic Reaction Mechanisms, Reactivities, and Selectivities

- Invited Seminar Presentation at Louisiana State University at Baton Rouge — January 31, 2011
  Theoretical Investigations of Rh and Ni Catalyzed C-C Bond Formations

- Presentation at the Organic Graduate Symposium, University of California, Los Angeles — May 15, 2010
  Theoretical Investigations of Rh and Ni Catalyzed C-C Bond Formations

- Poster Presentation at ACS 239th National Meeting at San Francisco, California — March 24, 2010
  1. Theoretical Investigations of Rh and Ni Catalyzed C-C Bond Formations
  2. Metal-Catalyzed [5+2] Cycloadditions: Experimental and Theoretical Studies on Regioselectivity and a New Highly Efficient Catalyst

- Invited Seminar Presentation at Nankai University, Tianjin, China March 20, 2009
  Theoretical Investigations of Rh and Ni Catalyzed C-C Bond Formations

- Poster Presentation at ACS 235th National Meeting at New Orleans, Louisiana April 7-9, 2008
  Theoretical Studies on Rhodium(I) Catalyzed (5+2) Cycloadditions

TEACHING EXPERIENCES

- **Teaching Assistant at Department of Chemistry and Biochemistry, UCLA** Sep. 2006 – June 2009
  Taught two graduate courses: *Physical Organic Chemistry*, and *Computational Organic Chemistry*,
  Taught three undergraduate courses: *General Chemistry A and B (discussions)*, *Organic Chemistry Lab B.*

- **Teaching Assistant at Department of Chemistry, University of Guelph** Sep. 2004 – Apr. 2006
  Taught *General Chemistry Labs A and B.*

Last updated: June 2012