THEORY AND MODELING OF STEREOSELECTIVE ORGANIC, TRANSITION METAL AND ENZYME CATALYSIS

K. N. Houk,* Colin Yu-Hong Lam, Adam Simon, Mareike Holland, Matthew Grayson, Gonzalo Jiménez Osés, Yun-Fang Yang, Song Yang, Jessica Grandner

Departments of Chemistry and Biochemistry, and Chemical and Biomolecular Engineering, University of California, Los Angeles, 607 Charles E. Young Dr. East, Los Angeles, CA 90095-1569 USA
houk@chem.ucla.edu

Organocatalysis with cinchona alkaloids and derivatives, especially chiral vicinal diamines, has been explored with density functional theory. New models to understand selectivity have been created.[1],[2] These models are described for fluorinations, oxidations, aldol reactions, and Michael additions. The second part of this lecture involves transition metal processes involving multiple chiral ligands for hydrohydroxyalkylations.[3] In part three, the control of selectivity of oxidation by the P450 enzymes, PikC and MycG, will be described.[4] The utility of modern density functional theory in modeling and explaining the whole range of catalytic processes will be described.

References:
1) M. C. Holland, R. Gilmour, K. N. Houk, *Angew. Chem.* **2015**, *55*, 2022
2) Y.-H. Lam, K. N. Houk, *J. Am. Chem. Soc.* 2014, 136, 9556; Y.-H. Lam, K. N. Houk, *J. Am. Chem. Soc.* 2015, 137, 2116; A. H. Asari, Y.-H. Lam, M. A. Tius, K. N. Houk, *J. Am. Chem. Soc.* **2015**, *137*, 13191; A. Simon, Y.-H. Lam, K. N. Houk, *J. Am. Chem. Soc.* **2016**, *138*, 503; M. N. Grayson, K. N. Houk, *J. Am. Chem. Soc.* **2016**, *138*, 1170
3) M. N. Grayson, M. J. Krische, K. N. Houk, *J. Am. Chem. Soc.* **2015**, *137*, 8838
4) A. R. H. Narayan, G. Jiménez-Osés, P. Liu, S. Negretti, W. Zhao, M. M. Gilbert, R. O. Ramabhadran, Y.-F. Yang, L. R. Furan, Z. Li, L. M. Podust, J. Montgomery, K. N. Houk, D. H. Sherman, *Nature Chem.* **2015**, *7*, 653