Guillaume Lamoureux

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Computational Chemistry and Biochemistry

Research Interests

Molecular modeling and computer simulations of enzymatic reactions and membrane transport

We are interested in enzyme catalysis, phase segregation, molecular recognition, and membrane transport. Understanding these processes—and how they can be inhibited or enhanced—is at the core of many pressing issues in physiology, cell biology, and pharmacology. Our research covers three areas: (1) catalysis in metalloenzymes, (2) gas transport across membrane proteins, and (3) the effects of complex solvents on biological molecules. We tackle these questions with computer simulations based on the principles of quantum chemistry and molecular mechanics. Our long-term goal is to develop computational methods to decode the function of proteins from their three-dimensional structures: to find which motions of an enzyme are important for its catalytic activity, to design new enzyme inhibitors or reduce the side effects of existing ones, to understand how proteins carry small molecules across lipid membranes, and to predict how solvent affects the conformation of proteins and drug molecules.

Selected Publications

J. Blumberger*, G. Lamoureux*, and M. L. Klein. 2007. Peptide hydrolysis in thermolysin: Ab initio QM/MM investigation of the Glu143-assisted water addition mechanism. J. Chem. Theory Comput. 3, 1837-1850.

G. Lamoureux, M. L. Klein, and S. Bernèche. 2007. A stable water chain in the hydrophobic pore of the AmtB ammonium transporter. Biophys. J. 92, L82-L84

G. Lamoureux and B. Roux. 2006. Absolute hydration free energy scale for alkali and halide ions established from simulations with a polarizable force field. J. Phys. Chem. B 110, 3308-3322.

S. Yu. Noskov,* G. Lamoureux,* and B. Roux. 2005. Molecular Dynamics Study of Hydration in Ethanol-Water Mixtures Using a Polarizable Force Field. J. Phys. Chem. B 109, 6705-6713.

G. Lamoureux, A. D. MacKerell, Jr., and B. Roux. 2003. A simple polarizable model of water based on classical Drude oscillators. J. Chem. Phys. 119, 5185-5197.