

# **Chemical Reactions at Aqueous Surfaces, in Ionic Liquids, and within Catalytic Antibodies from QM/MM Simulations**

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An “on water” environment, defined by the absence of water solubility of the reactants, has been reported to provide increased rate accelerations, yields, and specificity for several types of organic reaction classes compared to organic solvents. New computational tools were developed to reproduce these effects and to formulate a detailed conception of how the aqueous boundary affects rates. Ionic liquids (room temperature molten salts) also have the potential to control chemical reactivity in an environmentally favorable manner; however, few systematic studies have been conducted to address microscopic details. Mixed quantum and molecular mechanical (QM/MM) calculations featuring our recently developed ionic liquid force field are used to elucidate the intermolecular interactions behind their chemical impact.

This seminar details changes along multiple reaction pathways for fundamentally important organic reactions and provides a better understanding of how the immediate molecular environment from solvent to catalytic antibodies affects the rates and selectivity. Representative reactions to be discussed include: aromatic Claisen rearrangements, aldol reactions, Diels-Alder, Kemp eliminations, allylic isomerizations, aromatic nucleophilic substitutions, and base-induced  $\beta$ -eliminations.