



SEMINAIRE ISMO

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Chemical reactivity at aqueous interfaces

Chemical reactions at liquid water interfaces are essential in many different contexts, including atmospheric processes, engineering applications, and prebiotic chemistry. In organic synthesis, recent experiments have found a 300-fold acceleration in the rate constant of some chemical reactions when performed under heterogeneous aqueous conditions. However, the reasons why reactivity at interfaces is dramatically different from that in the bulk are still not well understood.

In order to determine the origin of the suggested catalytic role played by the interface, we combine molecular dynamics simulations and theoretical modeling to establish the mechanism of 'on-water' catalysis.

Following previous work in the group, we first characterize the structural and dynamical properties of a typical oil-water interface, including the vibrational sum-frequency generation spectrum of interfacial water molecules. We then focus on a paradigm cyclo-addition reaction studied experimentally. We design a coupled valence-bond state model to simulate the reaction and we contrast the mechanisms and reaction rate constants in different environments, including neat solvents and a series of aqueous interfaces. We finally offer a molecular explanation for the observed rate acceleration at aqueous interfaces and the 'on-water' catalytic effect.

Mardi 15 janvier 2018 à 11 h

Amphithéâtre du bât 520 (3^{ème} étage)

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