# Séminaire de Chimie Théorique

Salle de Réunion, bat. A10

Mardi 8 Novembre à 16:00

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## CLASSICAL TRAJECTORY STUDY OF METHANE REACTIVE STICKING ON Pt(111) and Ir(111)

In this talk we will discuss about recent results of quasi-classical trajectory (QCT) calculations based on reaction-specific reactive force fields (RFFs) built from Density Functional Theory (DFT) total energy data. First, we will illustrate the possibilities of Tersoff-like RFFs to provide an accurate representation of high dimensional molecule-surface potential energy surfaces (PES), through the comparison of RFF- and DFT-total energies for methane interacting with Pt(111) and Ir(111). Then, we will present QCT results, by focusing on the role of the PES corrugation and anisotropy, ioptopic effects and vibrational-mode- and bond-selectivity for deuterated isotopologues of methane, effects of surface relaxation and surface temperature. Finally, we will briefly discus advantages and limitations of RFF-based QCT calculations as well as perspectives, in the light of the comparison with available experimental data.

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