





SEMINAIRE ISMO

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Dynamical Insights into Laser-Molecule and Molecule-Metal Surface Interactions

Controlling the dynamics of both electrons and nuclei within molecules by means of attosecond and femtosecond laser pulses is a subject of increasing attention in recent years. In a recent experiment, unexpected bond formation was observed under the influence of ultrashort intense laser pulses. It has been found that irradiation of isolated water molecules by few-cycle pulses of intense infrared laser light can give rise to ultrafast rearrangement resulting in formation of the H₂ + ion. In another interesting experiment, a time-dependent bond hardening was observed when tetramethyl silane (TMS) molecule was exposed to the ultrashort intense laser pulses. In conventional mass spectroscopy, TMS does not exhibit molecular ion (TMS+) as unimolecular dissociation into [Si(CH3)3]+ proceeds very fast. Under a strong field and few-cycle conditions, this dissociation channel is defeated by time-dependent bond hardening. Bond hardening disappears when longer pulse (100 fs) was used. First part of the talk will focus on the quantum dynamical explanations of these two experimental observations.

Second part of the talk will discuss the dynamics of H₂O dissociation on Ni and Cu surfaces. Dissociation of water molecule on metal surfaces is the rate limiting step in the industrially important water gas-shift reaction. Effect of rotational and vibrational state of H₂O on dissociation probability as well as effect of surface temperature on reactivity will be discussed.



Lundi 6 juillet 2015 à 11h Bât. 351 – 2^{ème} étage (Bibliothèque) Université Paris-Sud, 91405 ORSAY cedex