# Femtosecond laser-induced desorption of CO on metals: hot electrons and phonons at play

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Femtosecond laser pulses within the ultraviolet and near-infrared range constitute an efficient tool to promote reactions, diffusion, and desorption of adsorbates at surfaces [1,2]. With laser fluences exceeding 1 mJ/cm$^2$, reactions start as an indirect mechanism in which the substrate electrons efficiently absorb the laser energy to subsequently release it on the surface lattice and adsorbates. Still, the challenge is to understand the details of these photo-induced surface reactions and identify what factors do actually rule and contribute to initiate the adsorbate dynamics and subsequent reaction: the laser-induced hot electrons, the substrate hot phonons, or the likely interadsorbate energy exchange that may occur at large coverages. In this respect, our ab initio molecular dynamics with electronic friction (AIMDEF) [3-5] method, which has recently been extended to account for the hot electrons and phonons trough time-dependent electronic and lattice temperatures, constitutes a powerful tool to get insight in the nanoscale dynamics of the reaction. Our simulations of photo-induced experiments investigating the desorption of CO from Pd(111) [6] and the desorption and oxidation of CO from Ru(0001) [7] are able to disentangle the role of each of the ingredients involved in such complex scenario.

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