

## Triggering reactions on metal surfaces with femtosecond laser pulses

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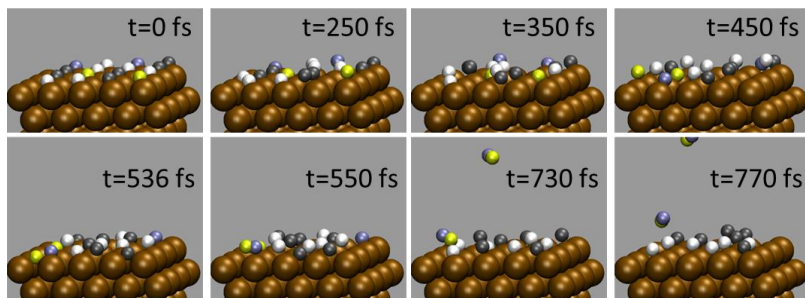
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Femtosecond laser pulses have proven to be very efficient in promoting reactions at metal surfaces that cannot be initiated by thermal activation [1,2]. The wavelength and intensity of the laser pulse determine if a reaction starts as a direct excitation of the adsorbate or, on the contrary, if it is an indirect mechanism in which the substrate efficiently absorbs the laser energy to subsequently release it on the adsorbates. The latter is precisely the mechanism that better accounts for reactions induced by UV/vis lasers on metal surfaces. In this talk I will focus on such kind of photodesorption processes and present recent results on the desorption of molecular O<sub>2</sub> from Ag(110) [3] as well as on the recombinative desorption of H<sub>2</sub>, D<sub>2</sub> and HD from Ru(0001) [4]. These two systems will allow us to extract information on how the desorption yields and dynamics are affected by the chemisorption properties and by the presence of additional adsorbates. In this respect, our newly developed *ab initio molecular dynamics with electronic friction* (AIMDEF) [5,6] method, which is based on the *local density approximation* (LDF) [7] and recently extended to account for the hot electrons created by the laser pulse through a time-dependent electronic temperature [4], constitutes a powerful tool to get insight in the nanoscale dynamics of the reaction.

### References

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### Figures



**Figure 1:** Snapshots of one of the AIMDEF simulations for an equal (8:8) H:D isotope mixture on Ru(0001) that ends with two HD desorbing molecules. White and black spheres are respectively the non-desorbing H and D atoms, yellow and blue spheres are the desorbing H and D atoms, and golden spheres are Ru atoms