Energy dissipation in abstraction processes from metallic surfaces

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The rationalization of elementary processes at surfaces is of prime importance for numerous natural and technological areas. From a fundamental point of view, the way the energy concomitant to any chemical reaction is distributed among the desorbing molecules degrees-of-freedom and the surface is not entirely pictured. Over the last few years, we have been developing molecular dynamics simulations to investigate this issue for the recombination of H_2 and N_2 resulting from atomic adsorbate abstraction by atom scattering off the W(100) and W(110) covered surfaces. Potential energy surfaces, built from density functional (DFT) theory calculations, have been used to simulate, within the framework of classical dynamics (including semi-classical corrections), the subpicosecond Eley- Rideal and Hot-Atom processes. The implementation of effective models to account for energy dissipation to surface phonons and electron-hole pair excitations, have allowed to rationalize the non-adidabatic dynamics of atom abstraction at metal surfaces. Some examples of this ongoing research will be here shown.

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