A time-dependent view of electronic excitations in the nanoscale

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Femtosecond and subfemtosecond time scales typically rule electron dynamics in low-dimensional metallic systems. Recent advance in experimental techniques permits now remarkable precision in the description of these processes. In particular, shorter time scales, smaller system sizes, and spin-dependent effects are current targets of interest. In this lecture, we will review some of the distinct aspects that define electron dynamics in the nanoscale, focusing into confinement effects [1]. Using density functional theory and its time-dependent extension, we will show that the screening of localized charges in metal clusters and surfaces is created locally in the attosecond time scale, while collective excitations transfer the perturbation to larger distances in longer time scales. We will also briefly discuss the elastic width of resonances in excited alkali adsorbates on surfaces and the electron – electron scattering in several metallic systems of nanometer size. In addition, we will discuss the role of electron excitations in a different context, namely the elementary reactive processes that take place at metal surfaces [2]. Over the last years, the combination of experimental molecular-beam techniques and refined theoretical calculations based on ab-initio methods have led research on this field to a new stage, in which detailed investigations of the kinetics and dynamics of molecular reactivity at surfaces are possible. The possible relevance of non-adiabatic effects in these processes, as well as the time scale in which the different energy dissipation channels play a role will be discussed.

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References

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