First-principles calculation of charge transfer times: analysis of the spin dependence in Cs/Fe(011)

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We have recently developed a scheme to compute resonant charge-transfer times from adsorbates on metal surfaces using first-principles density functional calculations [1]. We combine the information from surface calculations using the traditional finite slab approach with bulk calculations of the substrate material, and then compute the surface Green's function using recursive methods with arbitrary energy resolution.

We have applied this scheme to study several systems: i) alkalis on noble-metal surfaces in the low [1] and high coverage limits [2]; ii) the c(4x2)-S/Ru(0001) surface, for which we found, in agreement with core-hole-spectroscopy measurements, charge-transfer times well below the femtosecond scale [3] with a peculiar dependence on the polarization of the excitation light [4]; iii) Ar monolayers on Ru(0001) [5] with charge transfer times in the femtosecond scale.

As a new application, I will present here calculations for Cs adsorbed on Fe(011) [6]. In principle, using light with the appropriate polarization, it is possible to excite electrons with a well defined spin orientation from the spin-orbit-split $5p$ levels onto the $6s$ unoccupied resonance of Cs. At the energy of the $6s$ resonance, the calculated density of electronic state in the substrate is widely different for both spin channels. We analyze in detail if this spin-dependence of the number of available states in the susbtrate also translates into an appreciable spin-dependence of the elastic lifetimes.

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