Renormalization of magnetic anisotropy in adatoms by exchange coupling

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The coupling of a magnetic adatom to the conduction electrons of the underlying substrate can lead to the screening of its spin by formation of a Kondo singlet state if the coupling is strong enough. The Kondo effect is signaled by the appearance of a sharp and strongly renormalized peak in the spectral density right at the Fermi level, the so-called Kondo resonance. On the other hand for weak coupling, magnetic anisotropy (MA) induced by the local environment of the adatom leads to inelastic spin flip excitations visible as steps at the corresponding excitation energies in the STM spectra. Recently, it we have shown experimentally and theoretically [1] that the exchange coupling of a Co adatom to the conduction electrons of the substrate also leads to the renormalization of MA and the corresponding spin flip excitations. Hence the effective MA of a single ion can be tuned by tailoring its coupling to the substrate. Here we extend our theory presented in [1] to the case of Fe and Mn adatoms. We calculate the spectra of Co, Fe and Mn adatoms in dependence of the coupling to the substrate, by solving the generalized multi-orbital Anderson impurity model including MA in the One-Crossing Approximation. This allows us to treat the strong electronic correlations leading to the Kondo effect and the MA leading to inelastic spin-flip excitations on the same footing. We find that the spectra evolve from purely inelastic spin-flip at weak coupling, via the coexistence of Kondo effect and inelastic spin flips at intermediate coupling, to pure Kondo effect at strong coupling. As the coupling increases, the inelastic spin flip steps broaden and shift to lower energies, and finally merge into a single Kondo peak at strong coupling. Hence Kondo effect and inelastic spin-flip excitations are really two sides of the same coin.

[1] J. C. Oberg et al., Nature Nanotech. 9, 64 (2014)