Tuning the Magnetic Anisotropy of Organic-Inorganic Interfaces

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Abstract

The adsorption of nonmagnetic organic molecules on ferromagnetic materials offers an opportunity to tune their magnetic properties for promising applications in high-density data storage and spintronic devices. In this work, we report the manipulation of the magnetocrystalline anisotropy (MCA) of Co slabs through the adsorption of small molecules, such as benzene, cot etc. We consider a simple model based on 2nd-order perturbation theory to explain the modification of MCA due to molecular adsorption in a qualitative way. Further, we have used Density Functional Theory and the magnetic force theorem to calculate magnetic anisotropy. The results indicate that molecular adsorption drastically reduces the slabs in-plane MCA. A detailed analysis of various atom-resolved quantities demonstrates that the underlying physical mechanism is the metal-molecule interfacial hybridization, and, in particular, it is related to the chemical bond between the molecular p_z and the surface d_{z^2} orbitals. Generalizing the same argument, we also show that the complex molecules C_{60} and Alq_3 deposited on fcc-Co induce a similar modification of the in-plane MCA, and we related the results to recent experimental observations.