Kondo effects in magnetic molecules on metal surfaces

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The Kondo effect is one of the intriguing phenomena arising from the interaction between magnetic molecules and metal surfaces. The Kondo singlet state resulting from the Kondo effect changes the magnetic state and the conductivity drastically. Therefore, the Kondo effect is a fundamental problem to solve toward application of the magnetic molecules to electronic and/or spintronic devices.

To elucidate several kinds of Kondo effects emerging in single molecules on metal surfaces, I have carried out theoretical studies by density functional theory (DFT) and numerical renormalization group (NRG) in collaboration with experimental groups. In this talk, I will introduce recent studies on two molecular systems; Fe-phthalocyanine (FePc) on Au(111), and Mn-phthalocyanine (MnPc) on Pb(111).

In the first system, the scanning tunneling spectroscopy (STS) spectrum taken at the Fe atom in FePc adsorbed at ontop site of Au(111) shows characteristic peak structure. The DFT+NRG studies reveal that the peak structure is attributed to the Kondo effect arising from the combination of the spin and orbital degrees of freedom due to the orbital degeneracy in Fe d-orbitals in the ontop configuration [1]. Such characteristic enables the orbital-selective controlling of the Kondo effect [2]. In addition, we recently find that the competition between such multi-orbital Kondo effect and the spin-orbit interaction enables us to control the conductivity through the single molecule mechanical manipulation [3].

In the second system, the coupling between the Mn center and molecular ligand in combination with the interafacial charge transfer forms unique collective S=1 spin state. The Kondo screening of this collective spin state results in the spatially extended and underscreened Kondo state [4].

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