Basic Science

Revealing the Atomic Site-Dependent *g*-Factor within a Single Magnetic Molecule

The Landé g-factor of a free atom determines the effective magnetic moment of an electron or atom with both spin and orbital angular momentum, which can be calculated by Landé formula. For a transition metal ion in the crystal field, the spin-orbital interaction can mix the non-zero orbital angular momentum of excited states with the "pure spin" ground state, resulting in an effective *g*-factor. Thus, the ability to probe the fine structure of the *g*-factor allows us to understand the internal spin properties of a magnetic system, such as the spin-orbital interaction. However, for molecular systems, traditional experimental methods for *g*-factor measurement, like EPR, can only provide averaged information over many molecules. The determination and mapping of *g*-factor within a single molecule at atomic scale has been missing, despite its very critical role in revealing local fine spin interactions.

Recently, LIU Liwei, YANG Kai and their co-workers from Prof. GAO Hongjun's group at the Institute of Physics (IOP), CAS, revealed an inhomogeneous distribution of *g*-factor inside a single molecule for the first time, in collaboration with Prof. OUYANG Min from University of Maryland, USA, Prof. Werner Hofer from Newcastle University, USA and Prof. Antonio Castro Neto from

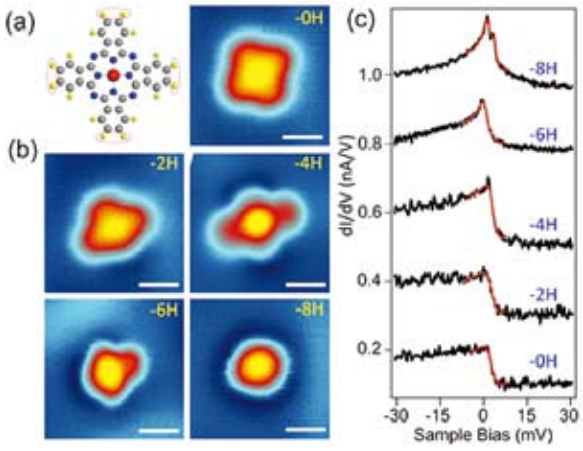

Fig. 1: Manipulation of the molecular Kondo effect by systematic dehydrogenation.

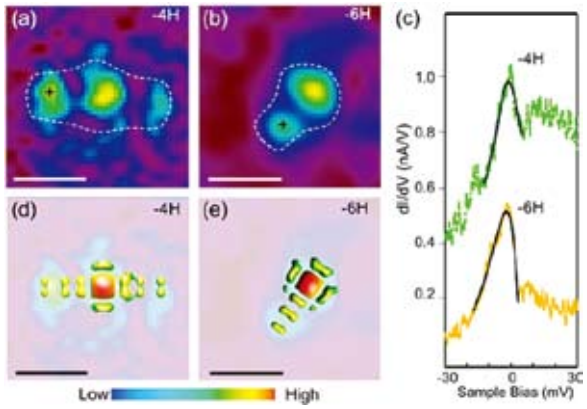

Fig. 2: Spin polarization properties of dehydrogenated MnPc molecules.

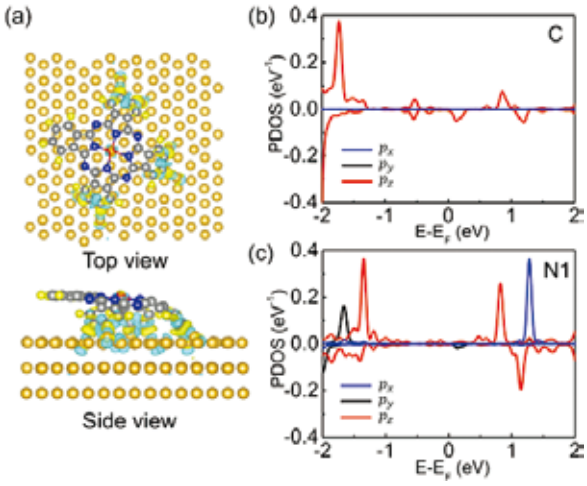

Fig. 3: Mechanism of observed extended Kondo effect.

National University of Singapore, To meet the goal, they first detached single hydrogen atoms of Mn-phthalocyanine (MnPc) by STM manipulation to alter the molecular structure and the electronic properties of the molecule. The dehydrogenated MnPc exhibits extended Kondo effect. This extended Kondo effect is attributed to spin polarizations induced by symmetry breaking of the molecular framework, as confirmed by calculations based on density functional theory. Measuring the evolution of the Kondo splitting with applied magnetic fields at different atomic sites, they found a spatial variation of the *g*-factor within a single molecule. The existence of atomic site-dependent *g*-factors results from different spin-orbit coupling of molecular orbitals within the molecule. As both molecular orbitals and their associated *g*-factor measurements are relevant to the chemical environment, these results provide a new route to explore the internal electronic and spin structure of complex molecules, which would be hard to achieve otherwise.

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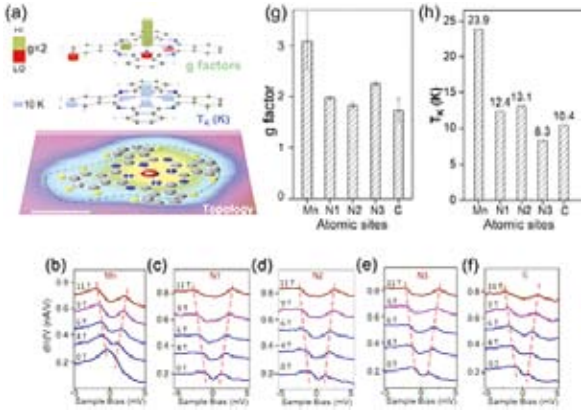

Fig. 4: Site-dependent *g*-factor of a -6H-MnPc molecule.