

Manipulation of the Magnetic State of Fe-DPyDBrPP molecules on Gold: From Kondo to Quantum Nanomagnet via the Charge Fluctuation Regime

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Abstract:

We demonstrate how the magnetic state of Fe-porphyrin-based molecules is influenced by surface charge fluctuations using density functional theory (DFT) calculations and scanning tunneling microscopy (STM) measurements. We investigated Fe-DPyDBrPP molecules deposited on Au(111) surface decorated with Br adatoms which produces molecular chains at the surface of gold (Figure 1). When a molecule in the chain is positioned above the Br site, it enters a non-magnetic quantum Kondo regime. In other positions, the molecule remains magnetic and behaves as an $S = 1$ nanomagnet. By using the STM tip to move the molecules, we tracked the transition between the magnetic state and the Kondo effect through several intermediate states. This transition is driven by enhanced charge fluctuations within the molecule, caused by increased hybridization of the molecular orbitals with the conduction electrons as the molecule approaches the Br site. This hybridization is accompanied by a decrease in the magnetic anisotropy. Our findings indicate that strong hybridization and low magnetic anisotropy yield the Kondo effect in the molecule while maintaining $S = 1$ spin state. This study provides valuable insights into the control of molecular spin states, which is critical for advancing spintronics, nanoelectronics, and quantum electronics.

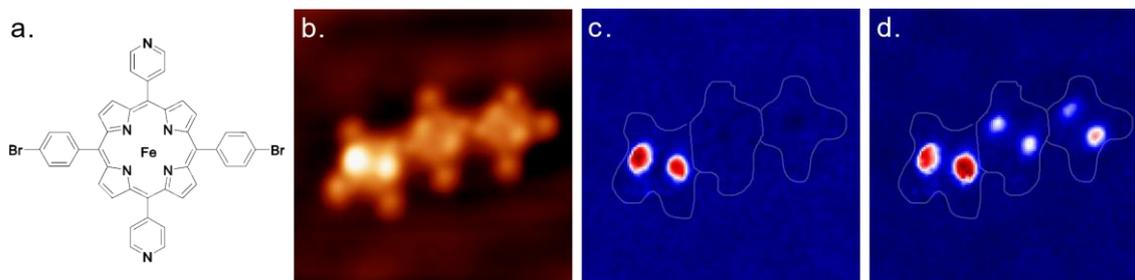


Figure 1. (a) Iron(II) 5,15-(di-4-bromophenyl)-10,20-(di-4-pyridyl)porphyrin molecules chemical composition. (b) STM topography: the molecules group in threes to form a chain. The leftmost molecule in the chain placed by manipulation with the microscope tip above a Br atom. $V=125\text{mV}$, $I=20\text{pA}$. Image size: $7\times 7\text{ nm}^2$. (c & d) Corresponding tunneling conductance maps showing the location of spin-flip excitations at 3 meV and 10 meV, respectively. The presence of a Br atom beneath the left molecule facilitates spin flipping. $V_{\text{stab}}=30\text{mV}$, $I_{\text{stab}}=200\text{pA}$. $V_{\text{mod}}=0.2\text{mV}$, $f=750\text{Hz}$. $T=1.3\text{K}$

References:

Y. Gao, S. Vlaic, T. Gorni, L. de' Medici, S. Clair, D. Roditchev, and S. Pons, ACS Nano 17, 9082–9089 (2023), preprint arXiv:2301.01101