Modification of Molecular Spin Crossover in Ultra-Thin Films

DANIEL DOUGHERTY, ALEX PRONSHINSKE, YIFENG CHEN, Department of Physics, North Carolina State University, ARRIGO CALZOLARI, CNR-NANO, Instituto Nanoscienze, Modena, Italy, GEOFF LEWIS, DAVID SHULTZ, Department of Chemistry, North Carolina State University, MARCO BUONGIORNO-NARDELLI, Department of Physics and Department of Chemistry, University of North Texas — Iron (II) spin crossover compounds exhibit a strong connection between molecular spin state and electronic structure that make them exciting candidates for highly tunable materials for spintronic applications. The spin crossover phenomenon is often extremely sensitive to crystal packing effects that may be modified in device environments compared to bulk materials. We report evidence for dramatic modification of spin crossover in bilayer films of Fe[(H₂Bpz₂)₂bpy] on Au(111) compared to bulk behavior. Scanning Tunneling Microscopy, spectroscopy, and local conductance mapping show spin-state coexistence in bilayer films of Fe[(H₂Bpz₂)₂bpy] on Au(111) that is independent of temperature between 130 K and 300 K due to the unique packing constraints of the bilayer film that promote deviations from bulk behavior. Local density of states measured for different spin states show that high-spin molecules have a smaller transport gap than low-spin molecules in agreement with density functional theory calculations. In addition, aggregation of spin states into “like-spin” domains is observed.

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