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有機半導体/酸化物界面における分子配向の温度依存性

Temperature dependence of molecular alignment at organic semiconductor/oxide interfaces

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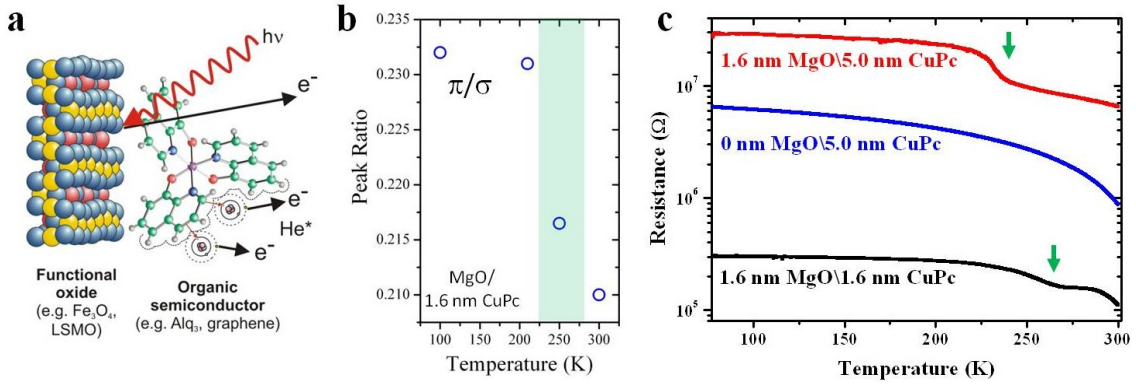
Organic semiconductor (OSC)/oxide interfaces play a critical role in the operation of organic electronic and molecular spintronic devices. For continued progress in these fields, it has recently become clear that a much deeper understanding of surface and interfacial effects is required with spin injection across a 'spinterface' in particular a standout phenomena that is poorly understood [1].

Here, we use the extremely surface sensitive technique of metastable de-excitation spectroscopy (MDS) to study the changes in surface electronic structure that occur when OSCs adsorb on oxide substrates relevant to device technologies. In particular, we focus on copper phthalocyanine (CuPc) deposited on MgO(001) and Fe_3O_4(001) investigating the coverage and temperature dependence of adsorption. The metastable helium (2^3S) atoms used in MDS only interact with the molecular orbitals of the OSC that protrude furthest into the surface vacuum allowing information on molecular orientation to be obtained [2]. Additionally, when the He 2^3S atoms are spin-polarized, the magnetic interaction at OSC/ferromagnetic (FM) oxide interfaces can be probed allowing, for example, induced spin polarization and exchange coupling to be determined [3].

By comparison with MDS spectra obtained from CuPc deposited on Fe, we determine a weak molecule-oxide interaction which leads to a more ordered interfacial layer. We also measure a strong change in the relative contribution to the MDS spectra of π- and σ-derived molecular states as the temperature reduces indicating an evolving adsorption geometry that has significant implications for spin injection from a FM oxide substrate into the π-conjugated network of the OSC layer, as will be discussed. This temperature-dependent transition correlates well with an unusual and abrupt change in the junction resistance observed for CuPc-based magnetic tunnel junctions (see figure). As well as providing insight into device behaviour, our results reveal the importance of studying surface effects at OSC/oxide interfaces and highlight the applicability of MDS for this task.



(a) MDS provides an extremely surface sensitive probe of OSC/oxide interfaces allowing information on, for example, molecular orientation as a function of temperature to be obtained, (b). This then provides understanding of the performance of molecular spintronic devices such as magnetic tunnel junctions (c).

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