Reactivity of LuPc2 thin films towards oxygen

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Abstract

Lutetium bis-Phthalocyanine thin films are gaining attention as candidate for efficient gas sensing applications [1]. Their peculiar electronic structure, and in particular the presence of a Single Occupied Molecular Orbital (SOMO) makes them ideal candidates for different gas sensing, as they are available for both oxidation and reduction. However no fundamental studies exist yet about how the bonding takes place at the molecular level. In this work we studied the low temperature reactivity towards molecular oxygen of a thick film of LuPc2 deposited on Au(111) single crystal in ultra-high vacuum (UHV). We characterized the reaction via X-Ray Photoelectron spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy. We showed a weak interaction, as oxygen desorbs as the sample is heated up to around 100K. We also showed that the reaction mostly affects the isoindole N atom, and only slightly the C atoms and the π system. We also show that the adsorption geometry is almost vertical. Also quantitavie analysis showed that more than a ML was adsorbed, showing the possibility for the oxygen to diffuse inside the layer.

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