Charge-transfer at silver/phthalocyanines interfaces

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Abstract

Valence band photoemission spectroscopy (VB-PES) and inverse photoemission spectroscopy (IPES) were employed to determine the occupied and unoccupied density of states upon silver deposition onto layers of two phthalocyanines (H$_2$Pc and CuPc). The two different Pc molecules give rise to very distinct behaviour already during the initial stage of silver deposition. While in the CuPc case no shift occurs in the energy levels, the H$_2$Pc highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are shifting simultaneously by 0.3 eV, i.e., the HOMO shifts away from the Fermi level while LUMO shifts towards the Fermi level. As the silver quantity increases the HOMO levels of both Pcs are shifting towards the Fermi level. When the Fermi level is resolved in the VB spectra, the characteristic features of H$_2$Pc and CuPc are smeared out to some extent. Shifts in HOMO and LUMO energy positions as well as changes in line shapes are discussed in terms of charge-transfer and chemical reactions at the interfaces.

Keywords: Metal free phthalocyanine; Copper phthalocyanine; Valence band photoemission; Inverse photoemission; Charge-transfer

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