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Density of occupied and unoccupied states monitored during metal deposition onto phthalocyanine layers

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Abstract
Phthalocyanine (Pc) materials find applications in electronic devices such as organic light emitting devices (OLEDs), solar cells, thin film transistors or gas sensors. The electronic properties at interfaces with different materials e.g. inorganic semiconductors or metals, usually dominate the device performance. Therefore the knowledge of the interface electronic properties is required. In the present work valence band photoemission spectroscopy (VB-PES) and inverse photoemission spectroscopy (IPES) were employed to determine the density of occupied and unoccupied states upon silver deposition onto layers of two phthalocyanines (H_2Pc and CuPc). The two different Pc molecules give rise to very distinct behaviour already in the initial stage of silver deposition. While in the CuPc case no shift occurs in the energy levels, the H_2Pc 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-PES spectra the H_2Pc and CuPc characteristic features 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.

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