The transport gap of organic semiconductors studied using the combination of direct and inverse photoemission

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Abstract

The combination of valence band photoemission and inverse photoemission spectroscopy is applied to study the densities of occupied and unoccupied states of perylene derivative and phthalocyanine organic layers on inorganic semiconductors. The ionisation energies and electron affinities are determined and it is proposed that the transport gap of the materials can be evaluated from the distance of the HOMO and LUMO edges. The resulting values for the transport gap which are somewhat smaller than other published data are in good agreement with e.g. electrical measurements. The experimental spectra are compared with simulated ones obtained by density functional theory calculations.

Keywords: Organic semiconductors; Phthalocyanine; Perylene derivatives; Photoemission; Inverse photoemission; Transport gap