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Transport gap of organic semiconductors in organic modified Schottky contacts

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Abstract

Two different organic molecules with similar structure, 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) and *N*,*N*′-dimethyl-3,4,9,10-perylenetetracarboxylic diimide (DiMe-PTCDI), were used for the modification of Ag Schottky contacts on sulphur passivated GaAs(1 0 0) (S-GaAs). Such diodes were investigated recording in situ current–voltage (*I*–*V*) characteristics. As a function of the PTCDA thickness the effective barrier height of Ag/PTCDA/S-GaAs contacts initially increases from 0.59±0.01 to 0.72±0.01 eV, and then decreases to 0.54±0.01 eV, while only a decrease in barrier height from 0.54±0.01 to 0.45±0.01 eV is observed for DiMe-PTCDI interlayers. The initial increase and decrease in effective barrier height for PTCDA and DiMe-PTCDI respectively, is correlated with the energy level alignment of the lowest unoccupied molecular orbital (LUMO) with respect to the conduction band minimum (CBM) of S-GaAs at the organic/inorganic semiconductor interface. Whilst there is an additional barrier for electrons at the PTCDA/S-GaAs interface of about 150 meV, i.e. the LUMO lies above CBM, the LUMO is aligned or below CBM in the DiMe-PTCDI case. The results also shine light on the important issue of the transport gap in organic semiconductors for which an estimation can be obtained.

Author Keywords: Transport gap; Organic semiconductor; Schottky contacts

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