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Molecular-scale Structure of Pentacene at Functionalized Electronic Interfaces

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A dipolar interlayer can cause dramatic changes in the device characteristics of organic field-effect transistors (OFETs) or photovoltaics. A shift in the threshold voltage, for example, has been observed in an OFET where the organic semiconductor active layer is deposited on SiO2 modified with a dipolar monolayer. Dipolar molecules can similarly be used to change the current-voltage characteristics of organic-inorganic heterojunctions. We have conducted a series of experiments in which different molecular linkages are placed between a pentacene thin film and a silicon substrate. Interface modifications with different linkages allow us to predict and examine the nature of tunneling through pentacene on modified Si surfaces with different dipole moment. The molecular-scale structure and the tunneling properties of pentacene thin films on modified Si (001) with nitrobenzene and styrene were examined using scanning tunneling spectroscopy. Electronic interfaces using organic surface dipoles can be used to control the band lineups of a semiconductor at organic/inorganic interfaces. Our results can provide insights into the charge transport characteristics of organic thin films at electronic interfaces.

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