

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Molecular and electronic structure at C₆₀:pentacene interfaces

S.W. ROBEY, D.B. DOUGHERTY, NIST-Gaithersburg, W. JIN, W.G. CULLEN, G.J. DUTTON, J.E. REUTT-ROBEY, University of Maryland — Successful utilization of organic donor-acceptor systems for photovoltaic applications requires understanding factors controlling molecular and electronic structure at interfaces. We have used STM, STS, and photoemission to study the donor- acceptor system C₆₀:pentacene. At low coverage, C₆₀ deposited on a well-ordered pentacene bilayer structure on Ag (111) adsorbs in between two adjacent pentacene rows. Isolated C₆₀ molecules are easily observed at room temperature indicating that the mobility of C₆₀ on pentacene is significantly smaller than on metal surfaces. Some images of C₆₀ reveal structure that may indicate a preferred C₆₀ orientation. Electrostatic contributions to intermolecular interactions are discussed to help explain C₆₀ adsorption between pentacene molecules. With increasing coverage, C₆₀ forms linear chains, still locked to underlying pentacene rows. A further increase in coverage results in domains of disordered C₆₀ that we propose result from competing C₆₀-C₆₀ and C₆₀-pentacene interactions. Information on nanoscale transport gaps and band alignment was obtained using constant-current distance-voltage spectroscopy. A gap of 4.5 eV is found over the linear C₆₀ chains compared with a gap of 3.6 eV for the surrounding pentacene bilayer.

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Date submitted: 24 Jan 2008

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