Molecular Architecture – Electronic Property Relations across Molecular Semiconductor Interfaces

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Successful utilization of organic donor-acceptor systems for photovoltaic applications requires understanding factors that control molecular and electronic structure at interfaces. We have used STM, STS, and photoemission to study technologically relevant donor-acceptor systems that include C_{60} : pentacene, C_{60}: titanyl phthalocyanine, and C_{60}: zinc pththalocyanine. This poster will focus on the C_{60}:pentacene systems, where we utilize sequential physical vapor deposition to fabricate C_{60}:pentacene interfaces with distinct molecular orientations. Organic interfaces are formed starting with the initial growth of C_{60} or pentacene mono-, bi- and multilayers on Ag(111), followed by deposition of the second organic componnent. For low coverage C_{60} growth on a well-ordered pentacene bilayer structure on Ag(111), C_{60} adsorbs between adjacent pentacene rows, adopting a shifted cofacial arrangement. Isolated C_{60} molecules are observed at room temperature indicating that the mobility of C_{60} on pentacene is smaller than on most metal surfaces. With increasing coverage, C_{60} forms linear chains up to 30 nanometers long, still locked to underlying pentacene rows in the shifted cofacial arrangement. Increasing the coverage further results in additional closely spaced chains but the surface is predominantly covered in domains of disordered C_{60}. The disordered C_{60} region consists of meandering chains and closed loop structures with a relatively small number of three-fold or higher coordinated C_{60} molecules. STM and STS data acquired at specific nanoscale regions indicate that the transport gap correlates directly to C_{60} coordination. Through adjusted growth conditions, we generate C_{60}-Pentacene interfaces with a vertical orientation that serves as a model for bulk C_{60}-Pentacene interfaces. Finally, a novel cocrystalline C_{60}-Pentacene interface is formed by C_{60} deposition on the 2-dimensional pentacene gas that is found at submololayer structures. Both STS and UPS measurements show how HOMO and LUMO levels are shifted from their bulk values due to polarization energies that depend explicitly upon local chemical environment (number of nearest neighbors and orientation-dependent polarizabilities).

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