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Molecular Self-assembly for Organic Electronics JUN WANG, IRVINDER KAUR, BOGDAN DIACONESCU, MIKAEL JAZDZYK, GLEN P. MILLER, KARSTEN POHL, University of New Hampshire — Self-assembled thin films of novel organic molecules hold the promise of emerging technologies and applications ranging from sensors for biological applications to organic electronics and more efficient organic photovoltaics. Self-assembled monolayers (SAMs) form as a result of a delicate balance between competing molecule-substrate and intermolecular interactions. To control such self-assembly processes, it is mandatory to understand how this balance reflects onto the SAM's final structure. Here we present an ultra-high vacuum scanning tunneling microscopy (STM) study of the self-assembly of novel pentacene derivatives and functionalized fullerenes (F-C60) on metal surfaces. Pentacene is known to exhibit large carrier mobility and has been studied extensively as a semiconductor in organic thin film devices. However, it is subject to facile photo-oxidation that limits device lifetime. We recently synthesized novel pentacene derivatives that show a dramatically increased resistance to photo-oxidation. We identified 6,13-dichloropentacene as a promising candidate for organic electronics. On the compact surface of gold, 6,13-dichloropentacene forms self-assembled domains with various high symmetry orientations. The quality of the SAM is seen to dramatically improve when the 6,13-dichloropentacene are deposited on the (788) vicinal surface of gold where the presence of parallel atomic steps will select only one of the possible SAM orientations due to the molecule-step interaction. Thus we observe the formation of very large self-assembled 6,13-dichloropentacene monolayers with perfect single domain orientation. We have also studied the self-assembly of C60 functionalized with alkyl chains of various lengths (F-C60) on Ag(111). We find that as a function of the alkyl chain length various structures are forming, ranging from zigzag like to linear arrays of C60 fullerene cages. The symmetry and unit cell size of the F-C60 SAMs is dictated by the alkyl-surface and the intermolecular interactions. These results show that C60 molecules can be assembled in 2D and non-compact molecular arrays with a surface density controllable via appropriate chemical functionalization. Those structures show promise as candidates for self-assembled molecular junctions.

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