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DFT based modeling of C60/Dichloropentacene/Au OPV heterojunctions JUN WANG, JIAN-MING TANG, KARSTEN POHL, University of New Hampshire — The co-assembly of functionalized pentacenes (electron-donor materials) and fullerenes (electron-acceptor materials) on metal substrates provides a model for studying the structural and electronic properties for novel organic photovoltaic (OPV) heterojunctions. Our previous STM experimental results show C_{60} to form single, double and triple nano chains on an intact single-domain, brick-wall structured 6,13-dichloropentacene (DCP) monolayer adsorbed on stepped Au(788). Here, we present theoretical DFT calculations of the geometric and electronic structure, and the charge transfer in this interacting three-component system. Our calculations show that single C_{60} molecules prefer to either absorb on top of the DCP molecules (slightly shifted off the Cl center) or in between the DCP rows of the brick-wall structure. When adsorbing chains of C_{60} they will align with either the troughs in between the DCP rows or the top of the DCP rows, in agreement with experiment. Compared to the isolated DCP molecules, the HOMO and LUMO levels move up towards the vacuum level by about 1 eV upon monolayer formation, resulting in charge transfer to C_{60}.

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