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DFT based modeling of C60/Dichloropentacene on stepped Au surfaces JUN WANG, JIAN-MING TANG, KARSTEN POHL, Department of Physics, 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 [1]. Our previous STM experimental results show C_{60} to form molecular chains on an intact single-domain, brick-wall structured 6,13-dichloropentacene (DCP) monolayer adsorbed on stepped Au(788) [2]. Here, we have included a stepped gold substrate in DFT calculations for the geometric and electronic structure of this interacting three-component system. Our calculations show that C_{60} molecular chain prefer to absorb on top of the DCP molecules on the upper step edge. We calculate the dipole moments for various C_{60} configurations. The stepped gold substrate interaction shows a major influence on this unique molecular chain formation. [1] J. Wang, I. Kaur, B. Diaconescu, J.-M. Tang, G. P. Miller, and K. Pohl, ACS Nano 5 (2011) 1792. [2] J. Wang, J.-M. Tang, G. P. Miller, and K. Pohl, in preparation.

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