Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Sorting Category: 01.1.8 (C)

Investigation of Interfaces between Sub-Phthalocyanine and C60 using First-Principles Calculations[1] HOSSEIN HASHEMI, XIAO MA, JOHN KIEFFER, STEVEN E. MORRIS, MAX SHTEIN, Materials Science and Engineering Department, University of Michigan, Ann Arbor, Michigan 48109, USA, SHAOHUI ZHENG, EITAN GEVA, BARRY DUNIETZ, Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA — The structure and electronic properties of a boron subphthalocyanine (SubPc) adsorbed on buckminsterfullerene (C60) and of C60 on SubPc surfaces, mimicking reverse orders of deposition, have been studied using density-functional theory (DFT) including long-van der Waals. Total-energy calculations are used to elucidate the initial adsorption of SubPc on C60 low index surfaces and also C60 on SubPc surfaces. The energetics of crystalline substrates with different surface terminations were mapped out using a single molecule of the partnering species. Accordingly, the interfacial structure and properties are different depending on whether the substrate is SubPc or C60, due to the incongruency between lattices and the disorder that develops in the contact layers of C60 and SubPc, respectively. The dependence of the charge transfer energies on the interface morphology is studied using range separated hybrid functionals. The stabilization of charge transfer states to below the absorbing state, needed to optimize the fill factor, also depends on the order of layer deposition. These results are discussed in the context of experiments performed on organic solar cells, showing trade-offs in the short circuit current and open circuit voltage with varying deposition order of the organic layers.

Hossein Hashemi
hashemi@umich.edu
Materials Science and Engineering Department,
University of Michigan, Ann Arbor, Michigan 48109, USA

[X] Prefer Oral Session
[ ] Prefer Poster Session

[1]DoE-BES Award # DE-SC0000957

Date submitted: 12 Jan 2012 Electronic form version 1.4