Ab-initio study of heteromolecular layers: 4,4'-biphenyl dicarboxylic acid with pentacene on Ag(100)

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Heteromolecular films are promising candidates for efficient charge injection layers in organic optoelectronic devices. We show that 4,4'-biphenyl dicarboxylic acid (BDA) fully deprotonated on Ag(100) substrate can be mixed with pentacene (PEN) at two different BDA:PEN ratios, forming donor-acceptor mixtures with their unique structural and electronic properties. Our Density Functional Theory calculations, performed with the Vienna Ab-initio Simulation Package, reveal a BDA:PEN ratio-dependent intermolecular charge transfer from pentacene to BDA, which subsequently modulates the work function of a system. Such heteromolecular structures show increased stability relative to the separated counterparts, due to an attractive interaction between deprotonated carboxylic groups with pentacene hydrogen atoms. Consistent with our previous work [1], such heteromolecular structures can shift energy levels up to 0.5eV in subsequent organic layers, depending on mixing ratio.

[1] Stará, Veronika, et al. "Tunable Energy-Level Alignment in Multilayers of Carboxylic Acids on Silver." Physical Review Applied, 18, 4 (2022), p. 044048