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Subphthalocyanine on C_{70} Contact Layer Structure and Properties from First Principles Calculations JOHN KIEFFER, HOSSEIN HASHEMI, XIAO MA, MICHAEL WATERS, STEVEN MORRIS, MAX SHTEIN, University of Michigan — Boron subphthalocyanine (SubPc) is a promising donor material for organic photovoltaics, having one of the highest reported open circuit voltages among bilayer OPVs when coupled with C_{60}. Recently, C_{70} has attracted attention as a substitute for C_{60}, largely due to a broader optical absorption spectrum, which leads to a higher current at relatively high voltages. The structure and electronic properties of SubPc derivatives on C_{70}-fullerene were explored using density functional theory (DFT) calculations with added Van der Waals interactions. Total-energy calculations were used to elucidate the initial adsorption derivatives on low index surfaces of C_{70}. The dependence of the electronic and optical excitations on the interface morphology is studied within the Green's-function GW and Bethe-Salpeter approaches. Insights gained from these calculations, and how they can be used to improve device efficiency, are discussed.

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