



Figure : charge-transfer excitation from pentacene to F4TCNQ acceptor as given by embedded Bethe-Salpeter calculations. The associated hole-averaged electron density and electron-averaged hole density are given in red and blue, respectively. The skeleton molecules are model polarizable molecules in a QM/MM spirit. From: Li *et al.* Phys. Rev. Mater. **1**, 025602 (2017)