Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

How Number of Layers and Relative Position Modulate the Interlayer Electron Transfer in π-Staked 2D Materials MARCO CARICATO, ALESSANDRO BIANCARDI, University of Kansas — Understanding the photoinduced electron transfer (ET) between 2D layers, e.g. from π-stacked molecular films to few-layers graphene, is central to both technological and biological applications. While electron transfer has been extensively studied in the case of isolated molecules, its description in the case of extended solids is still unsatisfying. Here, using our recent extension of the Fock/Kohn-Sham matrix reconstruction within periodic boundary conditions, we describe the ET as a function of both number of layers and relative positions. Specifically, we consider the photoinduced ET from a zinc phthalocyanine film deposited over few-layer graphene with number of layers ranging from one to four. We find the ET critically dependent on both number of layers, staking of layers and relative position between donor and acceptor layers. In agreement with experiment, we show that the ET to a single-layer graphene is faster than to a double-layer graphene due to interference effects between layers in the latter arrangement. These results shed light on the subtle interplay between 2D structure and interlayer transfer, which may lead to more effective strategies for the bottom up design of these materials.

Marco Caricato
University of Kansas

Date submitted: 11 Nov 2016 Electronic form version 1.4