

START AT	SUBJECT	View All	NUM.	ADD
16:00	<p>Importance of Carrier Delocalization and Disorder for Incoherent Charge Separation at Organic Bilayers</p> <p>Authors : Veljko Jankovic, Nenad Vukmirovic Affiliations : Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia; Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia</p> <p>Resume : Recent studies [1,2,3] have challenged the view that free-charge generation in all-organic blends predominantly occurs on ultrafast time scales via delocalized hot charge transfer states. However, the mechanisms behind very efficient and weakly electric field-dependent charge separation on longer time scales remain highly debated. We investigate field-dependent charge separation in a one-dimensional lattice model of an all-organic bilayer. Charge separation is considered as a sequence of phonon-assisted transitions among eigenstates of an electron-hole pair supported by the interface. We find that the yield of charge separation starting from the strongly bound charge transfer state is weakly field-dependent and above 50% even at zero electric field. Moderate diagonal static disorder and good charge delocalization increase the yield by strengthening the transitions from the initial state toward long-lived states with increased electron-hole separation, from which further separation proceeds without kinetic obstacles. We also observe almost field-independent (at low to moderate fields) charge separation starting from a donor exciton state, while the yield varies from around 40% (from the lowest-energy donor state) to around 80% (from states energetically well above the lowest-energy donor state). [1] Vandewal et al., Nat. Mater. 13, 63 (2013). [2] Jankovic and Vukmirovic, Phys. Rev. B 95, 075308 (2017). [3] Grupp et al., J. Phys. Chem. Lett. 8, 4858 (2017).</p>		J.12.7	