Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Role of electronic localization in the phosphorescence of iridium sensitizing dyes BURAK HIMMETOGLU, ALEX MARCHENKO, University of Minnesota, ISMAILA DABO, CERMICS, Universite Paris-Est, MATTEO COCOCCIONI, University of Minnesota — In this talk we present a recent systematic study[1] of three representative iridium dyes, namely, $Ir(ppy)_3$, FIrpic and PQIr, which are commonly used as sensitizers in organic optoelectronic devices. We show that electronic correlations play a crucial role in determining the excited state energies in these systems, due to localization of electrons on Ir d orbitals in the ground state. Electronic localization is treated by employing hybrid functionals within time-dependent density functional theory (TDDFT) and with Hubbard model based corrections within the Δ-SCF approach. The performance of both methods are studied in a comparative fashion and shown to be in good agreement with experiments (within a few tenths of an electron-volt in predicting singlet-triplet splittings and optical resonances). The Hubbard corrected functionals provide further insights on the charge-transfer character of the excited states. The gained insight allows us to comment on envisioned functionalization strategies to improve the performance of these systems.

[1]B. Himmetoglu, A. Marchenko, I. Dabo and Matteo Cococcioni, J. Chem. Phys. **137**, 154309 (2012)

Burak Himmetoglu
University of Minnesota

Date submitted: 18 Oct 2012 Electronic form version 1.4