Abstract Submitted
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Exciton localization and delocalization in phenyl-cored thiophene dendrimers* MUHAMMET ERKAN KOSE, KWISEON KIM, WILL J. MITCHELL, NIKOS KOPIDAKIS, GARRY RUMBLES, SEAN E. SHAHEEN, National Renewable Energy Laboratory — A group of π-conjugated dendrimers, which are soluble organic molecules consisting of a core group to which branched arms (dendrons) are attached, were synthesized and characterized[1]. These dendrimers have a phenyl core with 3 or 4 arms, i.e., 3 or 4 thiophene dendrons. It has been shown that these dendrimers present a viable alternative to polymers in organic photovoltaic devices with PCBM as the acceptor[2]. We studied electronic structure of these dendrimers by density functional theory and restricted CI singles methods. Quantum mechanical calculations aimed at predicting the optical properties as well as the spatial location of excitons upon photoexcitation were performed. In particular, correlated electron-hole probability diagrams and transition density plots, to be presented here, reveal the nature of excitonic behavior in the dendrimers. [1] Mitchell, W. J.; Kopidakis, N.; Rumbles, G.; Ginley, D. S.; Shaheen, S. E., *J. Mater. Chem.* **15**, 4518 (2005). [2] Kopidakis, N.; Mitchell, W. J.; van de Lagemaat, J.; Ginley, D. S.; Rumbles, G.; Shaheen, S. E.; Rance, W. L., *Appl. Phys. Lett.* **89**, 103524 (2006). *This work was supported by the NREL LDRD program and the Xcel Energy Renewable Development Fund, and done in collaboration with the NREL Chemical and Biosciences Center and NCPV.

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