Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Phosphorescence from organic metal-free materials: Simulation and experimental studies[1] HOSSEIN HASHEMI, JAEHUN JUNG, JINSANG KIM, JOHN KIEFFER, Univ of Michigan - Ann Arbor, KIEFFER TEAM, KIM TEAM — The desire for green technology has touched all aspects of our lives, including the way we light our homes. Using density functional theory (DFT) and time-dependent DFT (TDDDFT) calculations, we have investigated the photophysical properties of a series of bromofluorene (BrFl) derivatives as potential candidates for a new generation of OLEDS. The calculated absorption and emission properties of the series as well as phosphorescence quantum yield are in good agreement with the available experimental data. The underlying phosphorescence mechanisms are explored through calculations of the spin orbit coupling values, the S $\rightarrow$ T intersystem-crossing matrix elements and the crossing rate constants. In addition, we calculate both the radiative and non-radiative decay rates of the lowest triplet state (T_1) for all the BrFl derivatives. Our studies suggest that functional group modification can control not only phosphorescence properties and emission color but also brightness. Our findings demonstrate how computation can be effectively used for the predictive design of organic materials in lighting devices.

[1]Acknowledgement: National Science Foundation, grant no. DMR-1435965

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Date submitted: 11 Nov 2016 Electronic form version 1.4