Abstract Submitted
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Ab initio studies of the optoelectronic properties of biphenyl derivatives in OLEDs[1] HOSSEIN HASHEMI, AVI BREGMAN, JAEHUN JUNG, MINSANG KWON , JINSANG KIM, JOHN KIEFFER, Univ of Michigan - Ann Arbor, KIEFFER GROUP TEAM, KIM GROUP TEAM — The influence of molecular conformation on electron relaxation and photophysical properties of a series of biphenyl derivatives have been investigated using density functional theory (DFT) and time-dependent DFT(TDDFT). 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 spin orbit coupling values and the S $\rightarrow$ T intersystem-crossing matrix elements and crossing rate constants are also explored as a function of the twist angle between the rings. The T $\rightarrow$ S_0 radiative and non-radiative transition rates are calculated and discussed for each member of the series. In addition, the T $\rightarrow$ S_0 radiative transition rate constant is calculated for twisted biphenyls and compared to those for planar molecules.

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