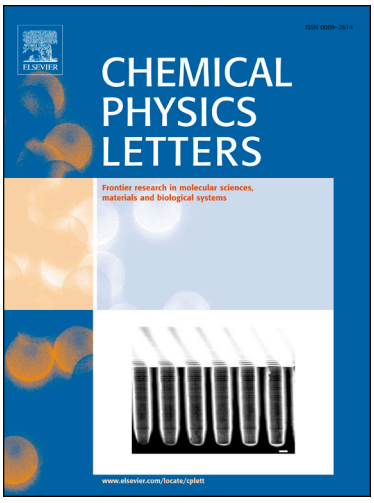

Research paper

Delocalization of frontier orbitals induced red emission for heptazine based thermally activated delayed fluorescence molecule: First-principles study

Yongxiang Kang, Liyun Zhao, Jiancai Leng

PII: S0009-2614(18)30199-4
DOI: https://doi.org/10.1016/j.cplett.2018.03.017
Reference: CPLETT 35498

To appear in: *Chemical Physics Letters*

Received Date: 17 January 2018
Accepted Date: 10 March 2018

Please cite this article as: Y. Kang, L. Zhao, J. Leng, Delocalization of frontier orbitals induced red emission for heptazine based thermally activated delayed fluorescence molecule: First-principles study, *Chemical Physics Letters* (2018), doi: https://doi.org/10.1016/j.cplett.2018.03.017

Delocalization of frontier orbitals induced red emission for heptazine based thermally activated delayed fluorescence molecule: First-principles study

Yongxiang Kang[†], Liyun Zhao[‡], Jiancai Leng[‡*]

[†] *College of Medical Information Engineering, Jining Medical University, Rizhao 276826, China*

[‡] *School of Science, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250353, China*

[*]Corresponding authors: jiancaileng@qlu.edu.cn

Abstract

Design of red organic emitting molecules with characteristic of thermally activated delayed fluorescence (TADF) remains a great challenge. Here, electronic and optical properties of a series of multi-branched TADF molecules have been investigated based on the newly-proposed optimal Hartree–Fock percentage method. Results show that, though enlarging the delocalization of HOMO and LUMO, the emission wavelength is redshift. The designed red TADF molecule possesses smaller reorganization energy than these for reported molecules. This indicates the non-radiative energy consumption of excited state is small and effective luminescence can be expected. Thus, a promising red thermally activated delayed fluorescence molecule is proposed.

Keywords

Thermally activated delayed fluorescence; Red emission; Optimal Hartree–Fock percentage (OHF) method; Delocalization of HOMO and LUMO; Huang-Rhys factor and reorganization energy.