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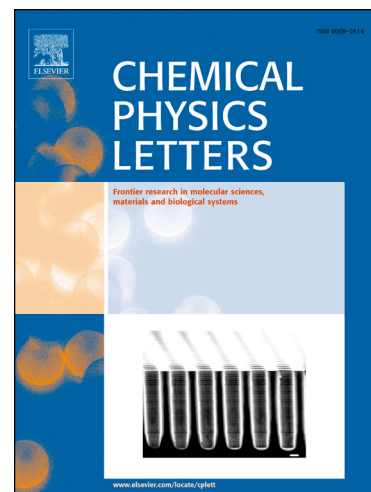
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Delocalization of frontier orbitals induced red emission for heptazine based thermally activated delayed fluorescence molecule: First-principles study

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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.

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