Theoretical exploration of the electronic structure and photophysical properties of five cyclometalated Ir(III) complexes bearing different substituted acetylacetone moieties

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Abstract

Using time-dependent density functional theory (TDDFT) approach, the electronic structure and photophysical properties of five cyclometalated Ir(III) complexes bearing different substituted acetylacetone moieties have been calculated and investigated. The calculated geometry structure of complex 2 shows a very good agreement with the available experimental data. The HOMO of complex 1 has the different distribution from those of complexes 2–5, that is, residing on the d-orbital of Ir, π-orbital of acac and L ligands. The S0-S1 transition of complex 1 is from HOMO-LUMO and HOMO–1-LUMO, that is, different from those of complexes 2–5. The lowest energy emissions for these complexes from CAM-B3LYP level are localized at 591, 581, 576, 574, and 571, respectively. Complex 4 might possess the largest kr value among these studied complexes. We anticipate that this study can shine some light on Ir(III) emitters in the fabrication of efficient organic light-emitting diodes (OLEDs).

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