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研究论文

以喹啉衍生物和乙酰丙酮为配体的Ir配合物的结构和光谱性质的理论研究

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摘要 用密度泛函理论(DFT)B3LYP方法对以喹啉衍生物(C∧N)及乙酰丙酮(acac)为配体的金属Ir(Ⅲ)的三个配合物的电子结构和光谱性质进行了理论研究. 计算结果表明, 当喹啉上的取代基(sub)由苯变为联苯或萘时, 电离能变小, 电子亲和势变大, 尤其是分子3, 可预测其能作为电子传输材料和空穴传输材料. 同时, HOMO和 LUMO之间的能隙变窄, 导致光谱红移. T1态主要为HOMO→LUMO 的跃迁. T1→S0 的磷光发射过程为MLCT和LLCT的混合.

关键词 Ir配合物 基态构型 分子轨道 电子光谱

分类号 0641

Theoretical Studies on Structures and Spectrocopic Properties for Iridium (Ⅲ) Complexes Based on Ligands Quinoline Derivatives and Acetylacetonate

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Abstract Theoretical studies of electronic structures and photochemical properties were performed via DFT/B3LYP method on three Ir(Ⅲ) complexes, each of which contains two quinoline derivatives and a single acetylacetonate. Our calculation results indicate that the substitution of biphenyl and naphthalene instead of benzene can decrease PI and increase EA values, especially for complex 3, which can be used as the electron-transport materials and hole-transport materials. At the same time, this substitution can decrease the energy gap between HOMO and LUMO which leads to the red-shift of absorption spectra. The T1 state transitions are mainly HOMO→LUMO, and the process of phosphorescence emission of T1→S0 is the mixture of MLCT and LLCT.

Key words Iridium complex Ground state configuration Molecular orbital Electronic spectrum

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