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研究论文

含氯不对称配体**8**-羟基喹啉铝配合物电子和光谱性质的**TDDFT**研究

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摘要 以含时密度泛函理论(TDDFT) B3LYP方法通过电子结构计算研究了含氯不对称配体8-羟基喹啉铝配合物$AlQ(ClQ)_2$的吸收和发射光谱性质. 计算表明, 第一激发态与基态结构变化主要集中在单一含氯配体中, 与*mer*-AlQ_3相比, 前线占有轨道离域程度变大而未占据轨道则定域化程度提高. 最大吸收主要来自配体内电荷转移跃迁, 电荷从苯酚环和氯向含氮的吡啶环跃迁. 电子陷入态计算表明, 抽取电子能量比AlQ_3相应值略大, 与实验结果一致.

关键词 8-羟基喹啉铝衍生物 电子光谱 激发态 含时密度泛函

分类号

Electronic Structure and Optical Spectra of Tris(8-hydroxyquinolinato)aluminum Derivative with Mixed Ligand Containing Chlorine: A TDDFT Study

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Abstract Absorption and emission properties of novel mixed ligand complex, $AlQ(ClQ)_2$ (Q＝8-quinolinolate, ClQ＝5,7-dichloro-8-quinolinolate) were investigated with electronic structure calculations by time-dependant density functional theory (TDDFT) B3LYP method. The optimized lowest excited state structure has an interesting feature in that only one 5,7-dichloro-8-quinolinolate ligand distorts appreciably, while the others keep their ground state structures. It is more evident that the delocalization in HOMO and localization in LUMO compared with AlQ_3. The maximal absorption band could be assigned mainly to intra-ligand charge transfer transition character. It mostly originated from transitions starting from the phenoxide side containing chlorine to pyridyl side. The calculation of anion state showed that it has a higher electron extraction potential than AlQ_3, which agreed with experimental result.

Key words tris(8-hydroxyquinolinato)aluminum derivative electronic spectrum excited state TDDFT

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