无机化学学报
CHINESE JOURNAL OF INORGANIC CHEMISTRY

二(2-苯基-8-羟基喹啉)锌及其衍生物的电子光谱性质的含时密度泛函理论研究

TD-DFT Study on Electronic Spectrum Properties of Bis(2-phenyl-8-hydroxyquinolato)zinc and Its Derivatives

中文关键词：8-羟基喹啉锌衍生物　电子光谱　激发态　含时密度泛函理论

英文关键词：bis(8-hydroxyquinolinolinato)zinc derivatives　electron spectrum　excited state　TDDFT

基金项目：

作者	单位
李志锋	天水师范学院生命科学与化学学院，天水 741001
吕玲玲	天水师范学院生命科学与化学学院，天水 741001
袁焜	天水师范学院生命科学与化学学院，天水 741001
康敬万	西北师范大学化学化工学院，甘肃省高分子材料重点实验室，兰州 730070

中文摘要：

采用从头算(*ab initio*)和密度泛函理论(DFT B3LYP)方法。对二(2-苯基-8-羟基喹啉)锌($Zn(qPh)_2$)及其衍生物的基态结构进行优化，同时用*ab initio* HF单激发组态相互作用(CIS)法在6-31G基组上优化其最低激发单重态几何结构，用含时密度泛函理论(TD-DFT/B3LYP)及6-31G基组计算吸收和发射光谱。计算表明，该类物质电子在基态与激发态间的跃迁，主要是电子云分布由定域化向离域化的转变。吸收及发射光谱的计算值与实验值基本符合。该类化合物的电子亲和能较大，都是优良的电子传输材料，改变中心金属原子对配合物光谱性质影响不大。而羟基氧被硫原子取代后，化合物的吸收光谱产生明显红移。

英文摘要：

The structures of bis(2-phenyl-8-hydorxyquinolato)zinc ($Zn(qPh)_2$) and its derivatives were optimized in the ground states using *ab initio* HF and B3LYP methods. The molecular structure of the first singlet excited state for $Zn(qPh)_2$ and its derivatives were optimized by CIS/6-31G. The absorption and excite spectra based on the above structure were obtained by the time-dependent density functional theory (TD-DFT) by the B3LYP method with the 6-31G basis set. The calculated results of emission spectrum for $Zn(qPh)_2$ and its derivatives have good agreement with the experimental data. All compounds are excellent electrontransporting materials, luminescence wave bands of which can be tuned little by different metals on the ligand of 8-hydroxyquinolinateo anion.