高等学校化学学报 2006 , 27 (11): 2156-2159 ISSN: 0251-0790 CN: 22-1131/O6

研究论文

氟取代三(8-羟基喹啉)铝衍生物电子结构、电子光谱的量子化学研究: 实现蓝色发光的途径

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收稿日期 2006-1-9 修回日期 网络版发布日期 2006-11-7 接受日期

摘要 采用Gaussian 03程序包和密度泛函理论(DFT)B3LYP/6-31G方法, 研究了三(8-羟基喹啉)铝(Alq_3)的3种氟代衍生物的电子结构与电子光谱, 讨论了氟原子在不同位置取代对Alq_3的前线轨道、HOMO-LUMO能隙以及电子光谱的影响, 发现氟取代使Alq_3的前线轨道能级降低, 在6位碳上氟代的Alq_3的HOMO-LUMO能隙变大, 吸收和发射光谱发生蓝移, 而在5和7位碳上氟代的Alq_3能隙变小, 吸收和发射光谱发生红移. 理论模拟结果与实验事实基本吻合, 证明在Alq_3分子的合适位置进行化学修饰可实现蓝色发光.

关键词 三(8-羟基喹啉)铝 氟代作用 基态构型 分子轨道分析 能级调控 电子光谱

分类号 0641

Quantum Chemical Investigation for Electronic Structure and Spectrum of F-substituted Alq_3 Derivatives: An Approach to Blue Luminescence of Alq_3 Derivatives

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Abstract The ground state and electronic spectra in F-substituted Alq_3 derivatives [q=8-hydroxyquinoline], an important electroluminescent material, are studied by using density functional theory(DFT) B3LYP/6-31G in programme Gaussian 03. The effect of substituted position in Alq_3 on their energies, HOMO-LUMO gap and the electronic spectrum are discussed. It is found that F-substitutions in Alq_3 resulted in the decrease of both HOMO and LUMO energies, and the degree of such decrease in energy of HOMO and LUMO levels is dependent on the F-substituted position. Significantly, the HOMO-LUMO bandgap of 6-FAlq_3 is found to be increased, as a result, its absorption and emission spectra are greatly blue-shifted. The results obtained from t

he theoretical investigation was in agreement with the experimental ones, providing an appro
ach to obtain the important blue luminescence Alq_3 derivatives.

Key words Alq_3 Effect of F-substitution Ground state configuration Molecular orbital analysis En
ergy control Electronic spectra

DOI:

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