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论文

二邻苯二胺合镍(Ⅱ)载流子传输性能的理论研究

汤肖丹[1], 高洪泽[2], 耿允[1], 廖奕[1,3], 苏忠民[1]

1. 东北师范大学化学学院, 功能材料化学研究所, 长春 130024;
2. 中国人民武装警察部队学院基础部, 廊坊 065000;
3. 首都师范大学化学系, 北京 100048

摘要:

利用密度泛函理论UB3LYP方法, 对二邻苯二胺合镍(Ⅱ)(PHDANI)的基态和离子态几何结构进行全优化, 模拟其双自由基特性. 运用势能面曲线法计算了PHDANI的空穴和电子重组能. 从晶体结构中选出所有可能最近的载流子传输路径, 计算相应的传输积分, 结合Marcus电荷转移理论探讨PHDANI的载流子传输性质. 计算结果表明, 在单重态双自由基特性下, 空穴和电子的迁移率分别达到0.253和0.135 $cm^2 \cdot V^{-1} \cdot s^{-1}$, 空穴和电子传输迁移率都很高且能达到平衡, 从理论层面上阐明了PHDANI可以作为很好的双极性传输材料.

关键词: 二邻苯二胺合镍(Ⅱ); 双自由基; 载流子传输; 密度泛函理论

Theory Study on Ambipolar Carrier Transport Properties of Bis(*o*-diiminobenzosemiquinonate) Nickel(Ⅱ) Complex

TANG Xiao-Dan[1], GAO Hong-Ze[2], Geng Yun[1], LIAO Yi[1,3*], SU Zhong-Min[1*]

1. Institute of Functional Material Chemistry, College of Chemistry, Northeast Normal University, Changchun 130024, China;
2. Fundamental Department, Chinese People's Armed Police Force Academy, Langfang 065000, China;
3. College of Chemistry, Capital Normal University, Beijing 100048, China

Abstract:

By means of the density functional theory level with UB3LYP function, the ground state and ionic structures of the complex bis(*o*-diiminobenzosemiquinonate) nickel(Ⅱ)(PHDANI) were optimized and the diradical character of PHDANI was successfully simulated. The hole and the electron reorganization energies were evaluated directly from the adiabatic potential-energy surface and the transfer integrals were calculated using direct method. Then, the charge carrier transport properties of PHDANI were investigated based on Marcus electron transfer theory. The results indicate that the hole and the electron mobilities of PHDANI, which are in the same order of magnitude, are 0.253 and 0.135 $cm^2 \cdot V^{-1} \cdot s^{-1}$, respectively. In theory, the transport properties of PHDANI are quite well as an ambipolar carrier transport material.

Keywords: Bis(o-diiminobenzosemiquinonate) nickel(Ⅱ); Diradical; Charge carrier transport; Density functional theory

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通讯作者: 廖奕, 女, 博士, 教授, 博士生导师, 主要从事量子化学研究. E-mail: liaoy271@nenu.edu.cn; 苏忠民, 男, 博士, 教授, 博士生导师, 主要从事量子化学研究. E-mail: zmsu@nenu.edu.cn

作者简介:

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