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MTDTPY.TCNQ及MTDTPY.CHL电荷转移复合物晶体的电子能带结构 及其与导电性能 关系的研究

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摘要 用紧束缚近似的EHMO方法对αMTDTPY.TCNQ(1)、β-MTDTPY.TCNQ(2)及MTDTPY.CHL(3)三种电荷转移复合物晶体的电子能带进行了计算。在1中,电子施体(D)分子MTDTPY及受体(A)分子TCNQ形成交替重叠的一维分子柱(M),柱间无净电荷转移。能隙E~G=0.15eV,载流子的产生主要来自热激发。在2及3中,电子施体(D)MTDTPY及受体(A)TCNQ及CHL分子分别相对独立的D及A一维分子柱,载流子的产生主要来自柱间的电荷转移。由电子能带结构及关于载流子迁移的Frohlich-Sewell公式,得出上述三种晶体的室温电导率之比为σ1:σ2:σ3=3.75×10^-^1^0:1:1.15,与实验事实基本一致。关于各分子柱对σ的贡献,2中D柱:A柱～10^3:1;3中D柱:A柱～2:1。根据计算结果,本文还对载流子的迁移机理进行了讨论。

关键词 导电性能 电子能带结构 晶体 电荷转移复合物 EHMO方法 紧束缚近似 电荷转移 载流子 电导率 迁移机理

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Electronic energy band structure of charge transfer complex crystals MTDTPY.TCNQ and MTDTPY.CHL and the relations between the band structure and the electrical conductivity

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Abstract The electronic energy bands of charge transfer complexes α-MTDTPY. TCNQ(1), β-MTDTPY.TCNQ(2) and MTDTPY.CHL(3) were calculated by tight binding EHMO. In 1, the electron donor, molecule MTDTPY, and the electron acceptor, molecule TCNQ, form a quasi one-dimensional mixed molecular column with alternative packing, and there is no net intercolumn charge transfer. The energy gap E=0.15eV. The charge carriers are created by thermo-exciting from band E~H~O to E~L~U. As for 2 and 3, the electron donor, molecule MTDTPY and electron acceptor, molecules TCNQ and CHL appear in relatively separated quasi one-dimensional molecular columns respectively. Charge carriers mainly come from inter-column charge transfer. Based on the calculated structure of energy bands and according to the equation of the migration of charge carriers of Frohlich-Sewell, the proportion of the room temperature electrical conductivities for these crystals is σ1:σ2:σ3=3.75×10^-^1^0:1:1.15, and it is fundamentaly coincide with the relevant experimental results. In 2, the ratio of contributions of molecular column MTDTPY (D) and TCNQ (A) to electrical conductivity is σD:σA=10^3:1, and for 3, the corresponding ratio of MTDTPY (D) and CHL (A) is σD:σA=2:1. Besides, the migration mechanisms of charge carriers of these crystals have been discussed.

Key words CRYSTALS CHARGE TRANSFER COMPLEX CHARGE TRANSFER CHARGE EARRIER (CARRIER) ELECTRICAL CONDUCTIVITY MIGRATION MECHANISM

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