

论文

铁原子簇的交换劈裂和磁性研究

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摘要: 用MS-X $\alpha$ 方法研究了Fe<sub>8</sub>原子簇(具有D<sub>6h</sub>对称)和Fe<sub>15</sub>原子簇(具有O<sub>h</sub>对称)的电子结构. 结果表明: (1) 两种原子簇中的Fe原子磁矩及其d能带中的交换劈裂性质互不相同; (2) 两类原子簇中的电荷分布不是均匀的, 电荷倾向于从外围原子向内部原子上转移, 并且被转移电子的自旋方向(正自旋或负自旋)与原子簇的对称性质密切相关.

关键词: 铁原子簇 电子结构 对称性 交换劈裂

STUDY ON THE EXCHANGE SPLITTING AND MAGNETISM OF IRON CLUSTERS

LI Hua, DONG Jianmin, MEI Lianmpo, HU Jifan, GAO Ruwei, DING Xuehou (Shandong University, Jinan 250100) (Manuscript received 1996-08-26, in revised form 1996- 12-26)

Abstract: The electronic structures of cluster Fe<sub>8</sub> with D<sub>6h</sub> symmetry and Fe<sub>15</sub> with O<sub>h</sub> symmetry have been studied by MS-X $\alpha$  method. The results show that (1) The exchange splittings of the d-band and the magnetic moments of the Fe-atoms are different in the two clusters; (2) The charge distribution in both clusters is not uniform, showing that the electrons are transferred from peripheral atoms to inner atoms, and the spin-direction (up or down) of the electrons transferred is in accordance with the symmetric characteristics of the clusters.

Keywords: iron atom cluster electronic structure symmetry exchange splitting

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