具有**Cn**对称性的大分子的能带结构研究 **1:** 计算方法

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摘要
利用环间和环内Bloch函数建立了一组新的原子轨道基函数。首次设计了适用于一维具有旋转对称性的大环分子的能带程序。计算了酞菁、
四氮卟吩、四苯并卟啉,四苯基卟啉的能带结构,
较好地解释了卟啉类化合物导电性能不如酞菁类的事实。还计算了酞菁铜和酞菁锰的能带结构,
讨论了酞菁与酞菁简化模型的能带结构以及晶体轨道的差异。
关键词   能带结构   导电性   晶体轨道   卟啉   酞菁   四氮卟吩
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Study on the energy band for macromolecular crystal with Cn symmetry 1: Calculating method

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Abstract In this paper a new basis set of atomic orbitals with Bloch functions of inter-ring and intra-ring is built. The new energy band program for One-D macrocyclic molecular crystal with Cn symmetry was designed by use for the first time. the energy band structures of phthalocyanine (Pc), tetrazaporphin (TAP), tetrabenzoporphyrin (TBP) and tetraphenylporphyrin (TPP) compounds are calculated. The fact that the properties of conductance for porphin compound is not as good as that for phthalocyanine is explained well. The energy bands of PcCu and PcMn are calculated. The difference of the energy band and the crystal orbitals between Pc and Pc' (the simplest model) are discussed.

Key words BAND STRUCTURES   ELECTRICAL CONDUCTIVITY   CRYSTAL ORBIT   PORPHYRIN   PHTHALOCYANIN (=PHTHALOCYANINE)   TETRAZAPORPHIN (=PORPHRAZINE)

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