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环状聚茚并茚及其取代衍生物电子结构和磁性研究

黄俭根

井冈山师范学院化学系

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摘要 采用半经验的AM1法，对环状聚茚并茚及其取代物的电子结构进行了计算研究 ，探讨了其磁性和取代基效应. 计算得到，环状聚茚并茚及其取代物皆表现半导体性质且发现其中一种异构体可能具有磁性. 取代基效应表明，吸电子基团的取代使 聚合物的电子亲合势增大，而给电子基团的取代则导致电离势减少，但取代基效应 不能改变聚合物的半导体性质. 此外，无论吸电子基团还是给电子基团的取代都不 能改变聚合物的磁性特征.

关键词 环状化合物 聚合物 茚 P 电子结构 半导体 磁性 取代基效应

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Theortical Studies on Cyclic-polyindenoindenes and Their Derivatives

Huang Jiangen

Department of Chemistry, Jinggangshan Normal University

Abstract The electronic structures of cyclic-polyindenoindenes (PInIn) and their derivatives have been studied by restricted Harlxee-Fock at AMI level. The substituent effect is discussed also. The calculated results show that these polymers are semiconductors, and although the band gap decreases for most of the substituted derivatives of polyindenoindenes, the polymers can not be conductors in intrinsic state by the substitution. Electron affinity of the substituted PMns chain is raised due to the substitution of electron-withdrawing substituents, while the ionization potential is decreased by electron- donating substituents. Therefore, the substitution of electron-donating group is favorable to p-type doping, while the substitution of electron-withdrawing group to n-type doping. In addition, one of cyclic-polyindenoindenes is a high-spin polymer and might become a magnetic material. Neither the electron-donating group nor the electron-withdrawing group can alter the magnetism of cyclic- polyindenoindene.

Key words CYCLIC COMPOUNDS POLYMER INDENE P ELECTRONIC STRUCTURE SEMICONDUCTOR MAGNETISM SUBSTITUENT EFFECT

DOI:

通讯作者