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[CuCo(CO)4]n的能谱和能带研究

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摘要 应用EHMO方法计算了[CuCo(CO)4]n低聚物的能谱和无穷链能带.简单分析和具体计算表明,Cu-Co之间以双电子双中心键结合,Cu-Cu之间则成键较弱.对单体的电子结构研究表明,AuCo(CO)4是不稳定的,因Au尚有余价,能与Lewis碱配位体结合或自身多聚.由四聚体[CuCo(CO)4]4的能谱可以得到[CuCo(CO)4]的近似能带,从而可以在统一基础上解释低聚体的能谱与无穷链的能带,
为利用低聚物的理论计算和实验结果预言高聚物的物理及化学性质提供近似依据.

关键词 羰基络合物 铜络合物 能带结构 钴络合物 能带理论 休克尔分子轨道

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A study on energy spectrum and energy band of [CuCo(CO)4]n

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Abstract EHMO calcns. were carried out for the homologous series [CuCo(CO4)]n with n either finite or infinite. Bi-center bonding is essentially existed between Cu-Co couple but almost neglected with respect to a Cu-Cu pair. The monomer species is active because of a low lying empty frontier orbitals with large populations around Cu (or Au) atom which favors combination with a donor or self-polymd. The relation between the infinite chain and oligomers is well indicated by the likeness of band and approx. band derived from energy spectrum of the tetramer. This perhaps provides a possibility to predict and rationalize the polymer behaviors in terms of those known events of the oligomers.

Key words CARBONYL COMPLEX COPPER COMPLEX BAND STRUCTURES COBALT COMPLEX BAND THEORY HUCKEL MOLECULAR ORBITAL

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