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Pt-Ru合金系的特征原子序列和催化性能

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摘 要： 依据特征晶体理论(CC)确定Pt-Ru合金系中的特征原子序列和特征晶体序列的电子结构、势能、原子体积、晶格常数和结合能等，研究合金催化剂的稳定性、催化性能及成分配比；计算Pt-Ru有序合金中Pt和Ru配比分别为31:1、1:和3:1的合金的势能和晶格常数，并分析组元Pt的组态变化；计算Pt-Ru无序合金的平均性质和组元Pt的电子结构。研究结果表明：随着Ru含量的增加，势能降低，合金稳定性增强，晶格常数随之减小，组元Pt的d空穴增加，提高了催化活性；合金中Pt与Ru的最佳原子个数之比约为11:。

关键字： Pt-Ru合金；电子结构；催化性能

Catalytic performance and characteristic atom sequences of Pt-Ru alloy system

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Abstract: Using the characteristic crystal theory(CC), the electronic structures, potential energies, atomic volumes, lattice constants and cohesive energies of characteristic atom sequences and characteristic crystal sequences of Pt-Ru alloy were determined. The stability， catalytic performance and ratio of composition of alloy catalyst were discussed. The potential energies and lattice constants of Pt-Ru ordered alloys in which the atomic ratios of Pt to Ru are 31:1 ,1: and 3:1, respectively, were calculated. The configuration of component Pt was analyzed. The average properties of Pt-Ru disordered alloys and electronic structures of Pt-component were calculated. The results show that when the content of Ru increases, the potential energy decreases, the stability increases, the lattice constant decreases and the d-orbital vacancy is enlarged, which is advantageous to reaction. The most proper atomic ratio of composition of alloy as catalyst is 11:.

Key words: Pt-Ru alloy; electronic structure; catalytic performance

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