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碘和氧修饰银**(110)**表面对甲醇吸附的影响**:** 密度 泛函理论的计算研究

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摘要 用密度泛函理论(DFT)的B3-LYP方法和原子簇模型研究了碘和修饰银(110)表面对甲醇吸附的影响。结果表明，甲醇分子在干净的银表面吸附很弱甚至不吸附，但在氧或碘修饰过的银表面上，由于预吸附导致吸附能的增加而变得容易吸附。并进一步采用目前较新的映像电荷模型计算验证了在甲醇部分氧化制甲醛反应中氧或碘对银催化剂表面修饰的本质是电荷修饰这一推论，为实验中如何筛选修饰提供了良好的判据。

关键词 碘 氧 银 甲醇 吸附 密度泛函理论

分类号 064

Effects of iodine and oxygen modification on the adsorption of methanol on the Ag(110) surface : A density-functional theory approach

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Abstract The effects of iodine and oxygen modification on the adsorption of methanol on the Ag(110) surface were studied by density-functional theory (DFT) method using cluster model approximation. It is found that methanol was weakly adsorbed in the form of physisorption on a clean silver surface. However, after the surface was modified by oxygen or iodine, methanol can undergo a stable form of molecular chemisorption because the pre-adsorption of iodine and oxygen increases the adsorption energy of methanol. And image charge model was used to verify our deduction that charge modification is the essence of modification of iodine and oxygen on the surface of silver catalyst in partial oxidation reaction of methanol to formaldehyde. This may help with the selection of promoter for this kind of reaction.

Key words IODINE OXYGEN SILVER METHANOL ADSORPTION

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