化学学报 2005 63 (8): 769-773 ISSN: 0567-7351 CN: 31-1320/06

研究简报

银纳米粒子表面油酸盐吸附的分子模拟

杨春杰[1]，陈晓*[1]，赵继宽[1]，刘成卜[2]

([1]山东大学胶体与界面化学教育部重点实验室 [2]理论化学研究所 济南 250100)

收稿日期 2004-7-5 修回日期 2004-12-26 网络版发布日期 接受日期

摘要 采用分子力学方法模拟了油酸盐分子在银纳米粒子(111)表面的两种主要吸附形态: 双键吸附和羧基吸附, 计算了不同溶剂环境中油酸盐分子的吸附能和振动频率. 结果表明:
作为银纳米粒子保护剂的油酸盐能够稳定地存在于极性和非极性溶剂环境中,
与银表面的作用方式随溶剂极性的改变而改变, 水相中以双键吸附为主, 而在有机相中主要是羧基吸附.
这与红外光谱实验的推论基本吻合. 从而在分子水平上为实验结果提供了有价值的理论支持和微观信息.

关键词 分子模拟 油酸盐 分子力学 吸附

分类号

Molecular Modeling of Oleate Adsorption on Silver Nanoparticle Surface

YANG Chun-Jie[1], CHEN Xiao*[1], ZHAO Ji-Kuan[1], LIU Cheng-Bu[2]

([1] *Key Laboratory of Colloid and Interface Chemistry, Ministry of Education,*
[2] *Institute of Theoretical Chemistry, Shandong University, Jinan 250100*)

Abstract Molecular mechanics calculations were carried out to model the oleate molecule (OLM) adsorption on silver nanoparticle surface. Eight OLM solutions in different solvents on the given Ag(111) surface were chosen to present the adsorption system. The energy minimizations of all systems were performed with full atomic representation model. A series of relative adsorption energies for two different adsorbing modes of OLM, via double bond or carboxylate group, were calculated and compared in the presence of water or isooctane. Results show that the OLM is stable on the Ag surface as a stabilizer either in polar or nonpolar solvents. The favorable adsorption mode of OLM was transformed with changing solvent polarity from the double bond anchoring in the water to the carboxylate group anchoring in the isooctane solvent. Furthermore, the computed vibrational frequencies of these two stable systems and isolated pure Na oleate and Ag oleate components were basically agreed with the experimental values of IR spectroscopy, providing a better understanding of molecular adsorption nature on metal surface.

Key words molecular modeling oleate molecular mechanics adsorption

DOI:

通讯作者 陈晓 xchen@sdu.edu.cn