化学学报 2006 64 (16): 1659～1664 ISSN: 0567-7351 CN: 31-1320/06

研究论文

气液界面上阴离子表面活性剂单层膜的分子动力学模拟

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收稿日期 2005-11-2 修回日期 2006-3-1 网络版发布日期 2006-8-10 接受日期 2006-4-21

摘要 用分子动力学方法研究了阴离子表面活性剂十二烷基硫酸钠(SDS)在气液界面上的结构和动力学性质. 选择单分子占有面积分别为0.45和0.68 nm^{2}的两个模拟体系, 通过径向分布函数表征了单层膜的厚度, 并根据疏水链中碳原子与极性头中硫原子之间组成的矢量分布和取向函数, 对比了不同界面单层膜的有序排列情况. 结果表明在分子占有面积较小达到饱和吸附的情况下, 界面上的SDS具有较好的有序性. 通过计算气液界面附近水分子的扩散系数发现: 由于氢键和静电作用的影响, 界面区域内的水分子较本体溶液中的水分子有较弱的迁移能力.

关键词 分子动力学模拟 单层膜 气液界面

分类号

Molecular Dynamics on the Monolayer of Anionic Surfactant at Va-por/Liquid Interface

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Abstract The structures and dynamic properties of anionic surfactant sodium dodecyl sulfate (SDS) at the vapor/liquid interface were investigated using molecular dynamics method. Two systems in which the areas were 0.45 nm^2 and 0.68 nm^2 per molecule respectively were selected. The thickness of monolayer was calculated using radial distribution function (RDF), and the order of hydorcarbon chain at the interface for different systems were estimated through number density profiles and orientation correlation for the unit vector in different molecules. Using the diffusion coefficient calculated by mean square displacement (MSD) of water in the systems, it was found that the diffusion of water molecules in the interface was weaker than those in the bulky solution.

Key words molecular dynamics simulation monolayer vapor/liquid interface

DOI:

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