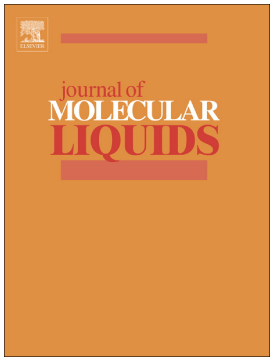

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Molecular Arrangement between Electrolytes and Alcohol at the Air/Water Interface

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Abstract

While it is conventionally believed that interaction between electrolytes and surfactants at the air/water interface can have profound impact on surface tension, a quantitative description remains elusive. In this study, the surface arrangement of MIBC at 1M and 2M NaCl solution was investigated by molecular dynamics. The main aim of simulation was to explore the molecular arrangement and explain the synergistic effect, which was evidenced by existing experimental data. The simulation was able to confirm experimental results as well as the underlying molecular arrangement. Specifically, it was found that Na^+ and Cl^- has an opposite effects on surface tension. The net effect of Na^+/Cl^- on surface tension is determined by the relative ratio between the two ions near the interface. This relative ratio, in turn, depends on MIBC concentration. As a result, NaCl decrease tension at low MIBC and increase tension at high MIBC. The mechanism should be the same governing principle for other surfactant/electrolyte mixture. The findings lay an important foundation for mixed surfactant/electrolyte systems.

Keywords: surface tension; air/water interface; molecular simulations

Introduction

The adsorption of solutes into air/water interface is a fundamental topic in surface science. Due to experimental difficulties, the adsorption is often obtained via theoretical modelling and surface tension. In an early study, the adsorption was modelled from the molecular arrangement between the solutes and surface water [1]. Such model was limited to certain molecules and cannot be extended to