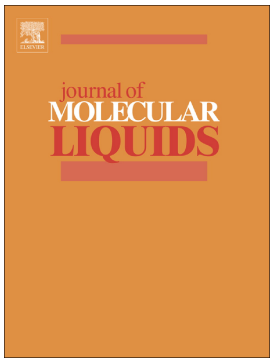

The simulation of the capturing of sodium ions in a monolayer consisting of polythiophene functionalised with crown ether side chains

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The simulation of the capturing of sodium ions in a monolayer consisting of polythiophene functionalised with crown ether side chains

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Abstract

When polythiophene is substituted in its '3' sites by 6-oxygen atom crown ether (CE) rings it forms a monolayer on a water surface. The migration of Na^+ ions from the aqueous layer to the CE is simulated by molecular dynamics and their complexation by the rings are studied. It is found that when electric fields (applied or local) overcome steric forces, the cations can access the CE rings and the formation of CE-Na^+ complexes is investigated. It is shown that the cations occupy sites near the rings but cannot migrate along their common axes. By conducting molecular dynamics over a range of temperatures two activated steps are found – the accession of the cations into the monolayer region and their subsequent release from the CE rings. Activation energies are found for each of these steps.

Keywords

Molecular dynamics; Polythiophene; Crown ether rings; Structure of Na^+ complexes; Electric fields; Activated complexation and decomplexation.

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