Title: Molecular recognition of sulfonatocalixarene with organic cations at the self-assembled interface: a thermodynamic investigation

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Original article

Molecular recognition of sulfonatocalixarene with organic cations at the self-assembled interface: a thermodynamic investigation

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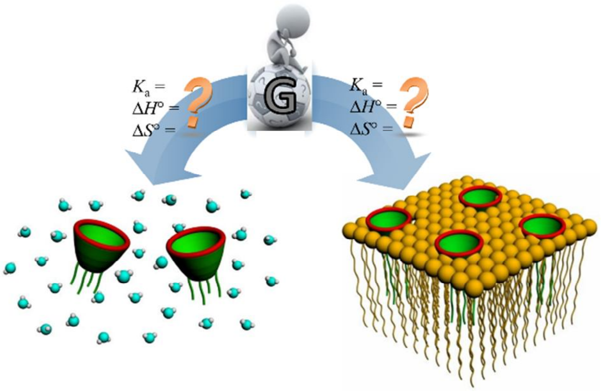
Graphical abstract



The molecular recognition of sulfonatocalixarene at self-assembled interface was investigated by means of microcalorimetry, which is definitely different from that in aqueous phase owing to the unique physicochemical characteristics of interfaces.

Abstract

A microcalorimetric study on molecular recognition of *p*-sulfonatocalix[4]arene derivatives at self-assembled interface in comparison with in bulk water was performed, inspired by the dramatic change in physicochemical characteristics from bulk water to interface. A total of six cationic molecules were screened as model guests, including ammonium (NH_4^+), guanidinium (Gdm^+), *N*,*N′*-dimethyl-1,4-diazabicyclo[2.2.2]octane ($DMDABCO^{2+}$), tropylium (Tpm^+), N-methyl pyridinium ($N\text{-}mPY^+$) and methyl viologen (MV^{2+}). The complexation with NH_4^+, Gdm^+ and $DMDABCO^{2+}$ is pronouncedly enhanced when the recognition process moved from bulk water to interface, whereas the complexation stabilities with Tpm^+, $N\text{-}mPY^+$ and MV^{2+} increase slightly or even decrease to some extent. A more interesting phenomenon arises from the NH_4^+/Gdm^+ pair that the thermodynamic origin at interface differs definitely from each other although with similar association constants. The results were discussed in terms of differential driving forces, electrostatic, hydrogen bond as well as π-stacking interactions, originating from the unique physicochemical features of interfaces, mainly the polarity and dielectric constant.

Keywords: Molecular recognition Calixarene Interface Thermodynamics Self-assembly