2° Simposio sobre Adsorción Adsorbentes y sus Aplicaciones

MOLECULAR SIMULATION STUDY OF PROTONATED DYE ADSORPTION

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ABSTRACT

Hydrotalcite like compounds are anionic clays of scientific and technological interest due to its use as ion-exchange materials[(1)], catalysts[(2)], antacids[(3)] and modified electrodes[(4)]. For those applications a study of the material surface properties is required. Although conventional analytical methods have provided considerable insight of the behavior of layered clays in solution, an atomic level evaluation of the dynamic of its ionic interaction is lacking. Molecular computer simulations have become extremely helpful in providing this perspective. Thus, the goal of this study is to evaluate, using molecular simulation techniques, the adsorption of 5-benzoyl-4-hydroxy-2-methoxybenzenesulfonic acid (MBSA), an anionic dye reference model, concerning its surface positioning and protonation. For this purpose, Monte Carlo simulation in the canonical ensemble were performed with $MBSA^{1-}$ and hydrotalcite model using a clay forcefield[(5)], in order to simulate the ionic interaction with the surface and also the charge stabilization of the system. With our molecular model was possible to reproduce atomic force microscopy experimental data[(6)]. Protonation influences on the adsorption process are also presented.

Keywords: *Adsorption, Hydrotalcite, MBSA, Dye.*

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