THEORETICAL STUDY AND ANALYSIS OF O-NITROPHENOL ADSORPTION USING LAYERED DOUBLE HYDROXIDES CONTAINING CA-AL, NI-AL AND ZN-AL

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Abstract

A theoretical assessment of the o-nitrophenol adsorption on layered double hydroxides containing different metallic species (Ca-Al, Ni-Al and Zn-Al) was performed. Experimental o-nitrophenol adsorption isotherms obtained at different adsorption temperatures with these layered double hydroxides were analyzed using a statistical physics monolayer model. Model calculations showed that the o-nitrophenol aggregation could occur with a high degree. It was estimated that the o-nitrophenol adsorption implied a non-flat orientation on all adsorbent surfaces and this process was multi-molecular. It was also demonstrated that there was no significant difference on the o-nitrophenol adsorption capacities of tested adsorbents, which varied from 77 to 135, 95 to 122 and 74 and 130 mg/g for Ca-Al, Ni-Al and Zn-Al layered double hydroxides, respectively. This finding suggested that the incorporation of Ca-Al, Ni-Al and Zn-Al in the layered double hydroxide structure played a similar role to adsorb o-nitrophenol molecules from aqueous solution. Calculated adsorption energies and thermodynamic functions confirmed an exothermic adsorption with the presence of physical-based interaction forces. This paper highlights the importance of reliable theoretical calculations based on statistical physics theory to contribute in the understanding of the adsorption mechanisms of a relevant water pollutant using layered double hydroxides as promising adsorbents for industrial applications.

Keywords

Layered double hydroxides; Modelling; Multi-molecular adsorption; O-nitrophenol