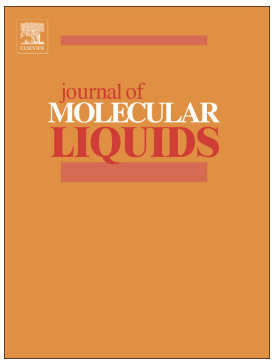


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# Screening of commercial sorbents for the removal of phosphates from water and modeling by molecular simulation

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## Abstract

Eight commercial sorbents of different origin and nature were studied in the present work for the removal of phosphate from water using synthetic solutions and a wastewater from an anodizing company. The materials included activated carbons, bone char, catalytic carbon, natural silica, natural zeolite, a manganese(II) oxide composite and iron(III) hydroxide. These materials were characterized with different analytical techniques such as nitrogen adsorption isotherms at -196 °C, FT-IR spectroscopy, SEM/EDX analysis and X-ray diffraction. The adsorption studies were performed in batch systems. Iron(III) hydroxide was found the best sorbent, showing a maximum adsorption capacity of 193.75 mg/g at pH 7 in contrast with natural zeolite and silica, which registered very low adsorption values (2.92 and 4.17 mg/g, respectively). According to molecular simulation studies, the adsorption of phosphates from water on iron(III) hydroxide allowed the formation of the complex $\equiv FePO_4H_2$, with a Gibbs free energy of -21.38 kcal/mol, showing that it is possible to recover

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