Theoretical study of phosphate adsorption from wastewater using Al-(hydr)oxide

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ABSTRACT

The overabundance of phosphorus in water causes eutrophication of aquatic environments. As a consequence, developing an adsorbent and understanding the adsorption process to remove phosphate is vital for the prevention of eutrophication in lakes. In this study, quantum chemical calculations were used to simulate the adsorption of phosphate on variably charged Al-(hydr)oxide, taking into account both explicit and implicit solvation. The corresponding adsorption reactions were modeled via ligand exchange between phosphate species and surface functional groups ($-H_2O/-OH^-$). Gibbs free energies of phosphate adsorption, for inner and outer sphere complexes, using three different simulated pH conditions (acidic, intermediate, and basic) were estimated. The theoretical results indicate that the thermodynamic favorability of phosphate adsorption on Al-(hydr)oxide is directly related to pH. At intermediate pH condition, H-bonded and MM_1 complexes present the most thermodynamically favorable mode of adsorption with –126.2 kJ/mol and –107.8 kJ/mol, respectively. At high pH, simulated IR spectra show that the values of P–O and P–OH stretching modes shifted to higher frequencies with respect to those at low pH.

Keywords: Al-(hydr)oxide; Adsorption; Phosphate; DFT; pH; Gibbs free energy; Wastewater, IR

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