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Comparative Study of W(VI) and Cr(VI) Oxyanions Binding Ability with Magnetic Polymer Nanocomposite

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Extended Abstract

Magnetite particles are widely used as sorbents for removal of heavy metal ions, organic dyes, drug delivery, cell labelling, magnetic resonance imaging, sensing, etc. [1,2]. Also, the functionalization of polymer by specific ligands enables customizing these composites for specific applications.

Magnetic crosslinked macroporous copolymer of glycidyl methacrylate, GMA, and ethylene glycol dimethacrylate, EGDMA, mPGME was synthesized by suspension copolymerisation of GMA and EGDMA, in the presence of inert component (mixture of cyclohexanol and aliphatic alcohol) [3] and magnetite nanoparticles coated with (3-aminopropyl)trimethoxysilane (APTMS) as silanization agent. The sample was additionally functionalized with diethylene triamine mPGME-deta. Magnetic amino-functionalized copolymer was fully characterized in terms of its structural and magnetic properties using: FTIR analysis, SEM/EDX, XRD and SQUID magnetometry.

Synthesized magnetic macroporous copolymer mPGME-deta was tested as sorbent of W(VI) and Cr(VI) oxyanions from diluted aqueous solutions (C_i=25 ppm) in a batch system, under uncompetitive conditions, at room temperature (T=25 °C). The oxyanions concentrations in solution after 60 min of sorption, were determined by inductively coupled plasma atomic emission spectroscopy (ICP-AES).

The maximal experimental values of oxyanions sorption capacities (Q_{max} μmol/g) were compared with theoretically values determined by theoretical modeling, using quantum-chemical methods: Density Functional Theory (DFT), statistic analysis of the crystal structure extracted from the Cambridge Structural Database (CSD) and by implicit solvation model (SMD).

It was found that the process is spontaneous and exothermic, and that the active sites of magnetic copolymer sorbent are amino groups (of diethylenetriamine and APTMS) which forms electrostatic interactions with oxianions W(VI) and Cr(VI).

References

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