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TH-P-1

Korelacija eksperimentalnih podataka sa teorijskim predviđanjem sorpcije jona teških metala na makroporoznom amino-funkcionalizovanom sorbentu

Ljiljana Suručić, Aleksandra Nastasović[*], Aleksandra Rakić[**], Bojana Marković[*],

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Decenijama se različiti sorbenti primenjuju za tretman otpadnih voda kontaminiranih jonima teških metala, koji ozbiljno ugrožavaju živi svet. Makroporozni funkcionalni polimeri pokazuju visok afinitet za jone teških metala, pri čemu efikasnost sorpcije i selektivnost direktno zavise od prirode funkcionalnih grupa sorbenta i jona metala. U radu je predstavljena korelacija teorijskih predviđanja i eksperimentalnih podataka dobijenih ispitivanjem sorpcije katjona Cu^{2+}, Co^{2+}, Ni^{2+} i Cd^{2+} u konkurentnim i nekonkurentnim uslovima u vodenom rastvoru na makroporoznom amino-funkcionalizovanom sorbentu poli(glicidil-metakrilat-*co*-etilen glikol dimetakrilat), PGME-deta. Kvantno-hemijskim proračunima procenjene su energije vezivanja metalnih jona za aktivna mesta sorbenta na model sistemima pojedinačnih fragmenata, metal-ligand, dobijenih statističkom analizom podataka baze kristalnih struktura. Ovakav teorijski pristup pokazao je visok stepen korelacije sa eksperimentalnim podacima u jednokomponentnim sistemima.

Correlation of experimental data and theoretical predictions of heavy metal sorption by macroporous amino-functionalized sorbent

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Over the decades, various sorbents have been used in the treatment of wastewater contaminated with heavy metal ions, which seriously endanger the living world. Macroporous functional polymers show a high affinity for sorption of these ions, where sorption efficiency and selectivity directly depend on the nature of the functional groups of sorbent and metal ions. In this study, we performed a correlation of theoretical predictions and experimental data obtained by investigation of Cu^{2+}, Co^{2+}, Ni^{2+} and Cd^{2+} cations sorption under competitive and uncompetitive conditions from aqueous solutions on macroporous amino-functionalized sorbent poly(glycidyl methacrylate-*co*-ethylene glycol dimethacrylate), PGME-deta. Quantum-chemical calculations estimated the binding energies of metal ions to the active sites of the sorbent, on the model systems of individual fragments, composed of metal ions and ligands, based on statistical analysis of data obtained from crystal structures. By this theoretical approach, the high degree of correlation with experimental data was observed for mono-component system.

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