Computational insights into ion-sorbent interactions for the design of functionalized PGME sorbents

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Abstract

Crosslinked macroporous copolymers based on glycidyl methacrylate (GMA) and ethylene glycol dimethacrylate (EGDMA), known as PGME, are characterized by a large specific surface area and the presence of reactive epoxide groups, making them highly attractive materials. Experimental adsorption studies in aqueous solutions have demonstrated their high efficiency toward a wide range of metal cations and oxyanions commonly found in wastewater (Cr(VI), Co(II), Ni(II), Cd(II), Pb(II)) [1,2]. In recent years, increasing attention has been devoted to developing model systems using molecular modeling approaches. Complementary quantum-chemical calculations enable the prediction of sorbent efficiency and selectivity under well-defined conditions, based on the interaction of a single ionic species in solution with an active site on the polymer surface (ligand) [3–6]. In this study, using vanadium sorption on a magnetic amino-functionalized macroporous PGME-deta copolymer as an example, a theoretical approach to modeling the single oxoanion–ligand interaction is presented. This approach is crucial for predicting sorption capacity and for the rational design of polymers tailored to specific applications.

References

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Figures

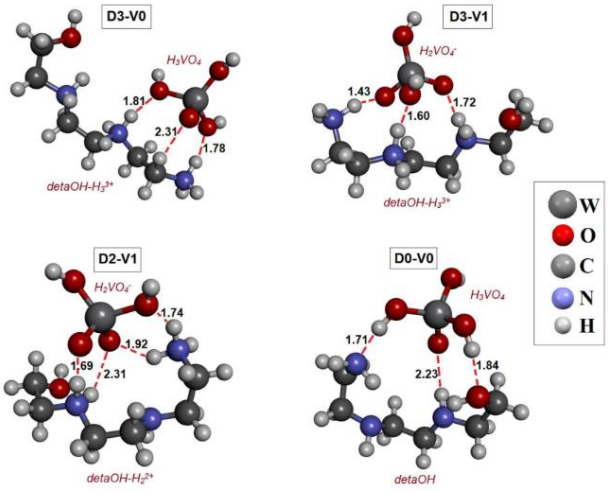

Figure 1: The optimized structures of dimers, used to estimate the interaction energies between vanadium (V) oxyanions and detaOH absorbent (D_3, D_2, D_0, V_0 and V_1 abbreviations in the labels of dimers refer to detaOH-H_3^{3+}, detaOH-H_2^{2+}, detaOH, H_3VO_4, and $H_2VO_4^-$, respectively) [6].