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Molecular Dynamics Study of Uranium Extraction from TBP/Dodecane Solutions Using Amidoxime-Grafted Silica

The production of energy from nuclear sources generates a variety of radioactive wastes, and in particular Radioactive Liquid Organic Waste (RLOW). RLOW contains a wide range of organic molecules and radioactive species along with halogens, heavy metals, nitrates, carbonates, sulfates and other components. To be compatible with existing waste management systems, RLOW must undergo pre-treatment. Current treatment methods of RLOW consists in incineration-vitrification and hydrothermal oxidation, and complementary methods are being researched in order to selectively remove the radioactive species from the liquids.

Recent studies have demonstrated that functionalized silica materials exhibit strong potential for uranium extraction from acidic sulfate solutions via liquid-solid extraction [1,2]. Molecular dynamics simulations have contributed to giving insights on phenomena surrounding the speciation of uranium by ligands grafted onto mesoporous silica at the aqueous phase/solid interface [3].

Extending our study to organic-phase systems, we simulate a TBP/dodecane solution of uranyl nitrate in contact with amidoxime-grafted silica. The objective is to examine the speciation behavior of uranyl cations at the organic-phase/solid interface and to assess the influence of water and acid in the solvent phase. A key challenge lies in developing a simplified yet realistic surface model while incorporating polarization effects in classical molecular dynamics simulations. With our results we intend to offer insight into uranium coordination and extraction mechanisms in organic medium relevant to RLOW treatment.

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