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Interaction of Natural Organic Matter Molecules with TiO_2 Nanoparticles: An Experimental Adsorption and Aggregation study

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ABSTRACT

Mechanisms by which synthetic nanoparticles are released into natural environments and the potential impact of nanoparticles on living organisms have been discussed frequently over the past decade. Interactions of nanoparticles with dissolved ions and organic ligands such as natural organic matter (NOM) affect the surface potential, which in turn may lead to aggregation of the particles, thus affecting the colloidal stability. In this study, interaction of synthetic TiO_2 (anatase) nanoparticles with various organic ligands in aqueous suspension was investigated in terms of aggregation and adsorption. Aggregation was investigated by light scattering techniques to determine ζ-potential and z-average diameter, while batch adsorption experiments were used to quantify the amount of organic ligands adsorbed onto TiO_2 nanoparticles. Size, ζ-potential and adsorption mechanisms were affected by concentration and molecular structure of the organic ligand present. Infrared (IR) spectroscopy demonstrated that inner sphere and/or outer sphere complexes were formed depending on pH and type of organic ligands in solution. In conjunction with experiments, DLVO modelling supported enhanced colloidal stability with increasing concentrations of Suwannee river fulvic acid at pH 5 compared to at pH 2.8 A combined experimental and molecular dynamic (MD) investigation of 2,3-dihydroxybenzoic acid (2,3-DHBA) and SRFA complexation showed that the extent of NP aggregation depended on concentrations of the ligand as well as on added Zn^{2+} concentrations. MD calculations showed complexation between ligands and Zn^{2+} in solution, which together with experimental adsorption and aggregation data indicated possible co-adsorption and formation of ternary surface complexes at the TiO_2 surface.

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