Impact of organic molecules on the colloidal stability of silica nanoparticles – simulations and experiments

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The use of engineered metal (-oxide) nanoparticles in a variety of applications and products is rapidly increasing. Among engineered nanoparticles, silica nanoparticles (often referred to as colloidal silica) is by far the most common industrial product, with extensive use in drug production, paper making, paints and sealants etc. Silica nanoparticles are generally considered to be non-toxic, but details of their interaction with environmental organic material are scarce, especially considering the multitude of available surface modifications. Interaction between nanoparticles released into the environment and natural organic material will change the physical and biological characteristics of the nanoparticles and affect their fate. However, the structure and dynamics of the particle-ligand interface are not well understood.

We will present the experimental data on the effect of organic molecules on the adsorbed amount and colloidal stability of silica nanoparticles. The molecular level description of the interfacial interactions will be provided by molecular dynamics simulations yielding adsorbed amount, binding patterns and role of molecular geometry and functional groups. As model molecules, dihydroxybenzoic acid (2,3-DHBA and 3,4-DHBA) and benzenetricarboxylic acid (1,2,4-BTCA) will be used.

Both experimental and simulation results will be presented for a range of pH values. The interactions appear to be relatively weak, especially for dihydroxybenzoic acid, but they do have a measurable effect on the stability of the silica suspension.

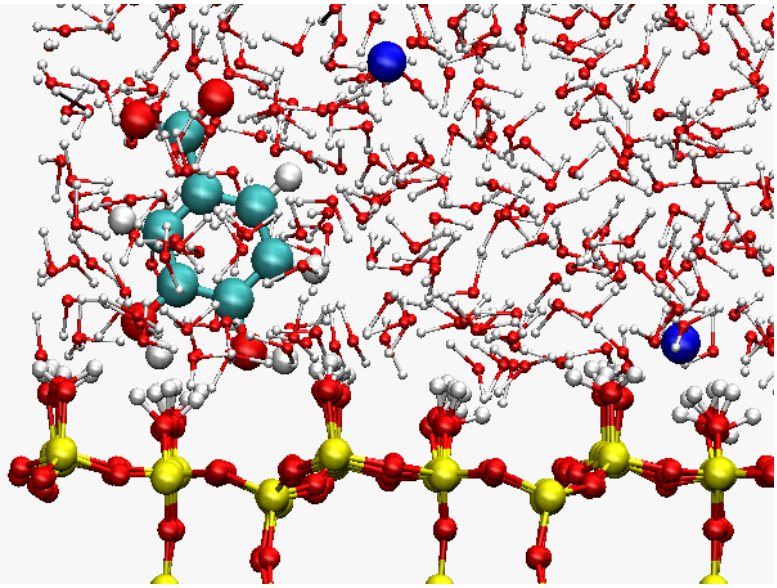

Figure 1: Snapshot of one adsorption pattern of 3,4-DHBA on neutral quartz (101) surface.