Molecular Dynamic Simulations of the Effect of Interfacial Water on the Interaction between Silica Nanoparticles

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Adhesion forces between nanoparticles depend on the amount of condensed water adsorbed from ambient atmosphere. Liquid water forms bridges in the cavities separating the particles, giving rise to the so called capillary forces which, in most cases dominate the van der Waals and long range electrostatic interactions. Capillary forces influence agglomeration of particles to large clusters and the flow of powders in processes. Molecular Dynamic (MD) simulation was used to calculate the structure of the liquid bridge between two silica wafer or nanoparticles. The PMF (potential of mean force) method [1] was used to calculate interparticular forces from the molecular structure of the interfacial water. ClayFF was used as force field for the silica interactions including the silanol groups which are responsible for the hydrophilicity of the surface. MD simulations were performed for silica nanoparticles with different numbers of adsorbed water layers. Results for the particle-particle interactions are discussed and compared to AFM and small angle X-ray scattering results.

[1] S. Leroch, J. Fischer, M. Wendland. Mean Force Simulation of the Adsorption of Aqueous Dilute Solutions. Soft Materials 2012, in print.