Surface modifications for improving properties of materials.

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The structure and chemical activity of the surfaces of numerous solid materials are important for various processes taking place in nature or in industrial activities. For example, adsorption and accumulation of environmental pollutants on soil components is responsible for buffer function of soils. Another example is preparation of new materials by surface modifications (e.g., chemically) such as new catalysts for industry or adsorption materials with increasing efficiency in removing of pollutants from the environment (e.g., water sources) by remediation processes.

By chemical modification of surfaces, we can fine-tune their properties in a desired way to enhance their functions – e.g., optimize their hydrophobicity/hydrophilicity, increase their specific selectivity for adsorption, or increase catalytic activity. There is an intensive effort in material science to prepare such materials. An important aspect of these activities is application of molecular modeling methods for better understanding of surface properties on a molecular scale, which could help in the effective design and planning of experimental work. In this talk, we will give several examples in this regard. Specifically, we present three studies, in which molecular modeling methods accompanied experiments and were applied to explain mechanisms of a) modification of alumina surfaces by fluorination, b) silanization of silica by organofunctional alkoxysilane moieties to tune surface wettability, and c) modification of zero-valent iron nanoparticles by nitriding and sulfidation for improving dechlorination of chlorinated hydrocarbons.