Classical and DFT simulations of molecule adsorption and transport on mineral surfaces

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The type and the strength of the interaction of a molecular entity on a mineral surface depends on various fators, e.g. acid base properties, number of available sites, hydrophilicity, etc. To better understand the adsorption and transport of biomolecules in an aqueous solution, first-principle and classical methods are combined to firstly describe the surface sites at the atomic level and then evaluate the distribution coefficients, rates and geometries of adsorption of molecules. The influence of the temperature and partial pressures or concentration of species will be also considered using the chemical potential approach.

In this talk, I will illustrate some fundamental concepts in showing how small aminoacids and dioxins interact with oxides (such as alumina, silica, clays)[1-4]. Those studies aim to prevent pollution in soils, corrosion and they can be related to other area such as biocompatibility, pollutant removal, origins of life and catalysis.

References:

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