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Discipline: Chemistry

Title: Bio/inorganic interfaces at the molecular level; The special case of amino acids and amorphous oxides

Abstract: Despite the intensive experimental work performed on peptide bond formation using silica, clays, alumina and other materials as catalysts, there is still no detailed molecular picture available for these processes. In recent years the theoretical approach became a very useful tool, because of significant improvement of computational power allowing to study complex systems with a high accuracy. Additionally, theoretical calculations can 'speed up' reactions that have a very slow rate in a real world, which is commonly the case in prebiotic chemistry.

A large number of different minerals can be found on the Earth's crust, however, most of them contains various forms of silicon oxide (aka silica, SiO_2), aluminum oxide (aka alumina, Al_2O_3) or titanium oxide (aka titania, TiO_2). Hence, these three species are the most abundant ones, accounting for about 70-80% of all mass of the Earth's upper lithosphere. Silica is a solid compound present in many different crystalline or amorphous forms. In nature, it is usually found as quartz, however, amorphous structures can be found as well. Likewise, alumina and titania also exist in many different allotropic forms, including crystalline and amorphous ones. Moreover, silica and alumina entities can bound to each other, creating a large family of aluminum silicates or aluminosilicates. They can also form amorphous structures like ASA – amorphous silica-alumina. Furthermore, silica and titania can form mixed materials, as well. While crystalline forms are easier to investigate experimentally, studies on amorphous forms are more complex due to the lack of regular lattice structure. Consequently, only several experimental techniques can give a detailed picture of those materials. Among them are IR, NMR, XPS and IRAS. Therefore, although amorphous materials have been studied experimentally since decades, progress in the site determination and surface interactions with adsorbed molecules has been slow and many features are still under debate. Very helpful can be computational approach which can provide complementary information, not accessible in experimental investigations.

Interactions of biomolecules with wet mineral surfaces and organic reactions at aqueous mineral interfaces are of crucial importance in prebiotic chemistry, biogeochemistry, astrochemistry and other fields like environmental chemistry. It was proposed that the biomolecules transformations involve reactions occurring on mineral surfaces. Hence, mineral surfaces can be viewed as a catalyst. Among different amino acids, glycine was very commonly used to study e.g. a peptide bond formation, because it is the simplest amino-acid. Reactions occurring in a homogeneous gas or liquid phases were found to be thermodynamically not favored. However, once surface of mineral is considered, transformations become more likely. Regarding ab initio studies in that field, most of them were performed in the absence of solvent, i.e., water. Solvent effects could play an important role here and this should be included in any realistic calculation. For example, it is still unclear whether solvent molecules participate in a proton transfer reaction facilitating peptide bond formation (or reverse reaction), or is it done exclusively by the surface hydroxyl groups.

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