Adsorption of amino acids on passivated aluminium alloy surfaces: a DFT study

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The investigation of the adsorption of amino acids on the (0001) surface of α-alumina was initially undertaken to better understand the corrosive effects of proteins on aluminium alloy under a wet environment. The interaction of the different forms (neutral, anionic and cationic) of glycine (Gly)[1], lysine (Lys) and glutamic acid (Glu) with alumina surfaces have been studied using DFT (Density Functional Theory) methods. We found that the initially neutral amino acid molecule (without charges) becomes anionic or zwitterionic (ZW) with its adsorption on Al_2O_3. The forms of amino acids depend on their orientation, their coverage on the alumina surface and the hydroxylation state of the alumina surface. The alumina plays the role of a solvent by favouring the zwitterion form through hydrogen bonds with a parallel orientation of amino acids on the surface. In all cases, the carboxylic group interacts preferentially with the surface. An alumina amino acid complex is formed with the creation of a covalent bond Al-O(C), which induces the desorption of water molecules on the hydroxylated surface. An increase in the glycine coverage also has an effect on its crystallisation in 2D on the alumina surface. Finally, we found that the alumina stabilizes the peptide-bond formation with an epitaxial relationship allowing a bidentate adsorption of the dipeptide on the surface. It appears that the anhydrous alumina catalyses the peptide bond formation which is in fact important for a greater understanding of origin of life's reactions under prebiotic conditions.
A comparison with other materials reported in the literature has been examined in order to highlight some trends.

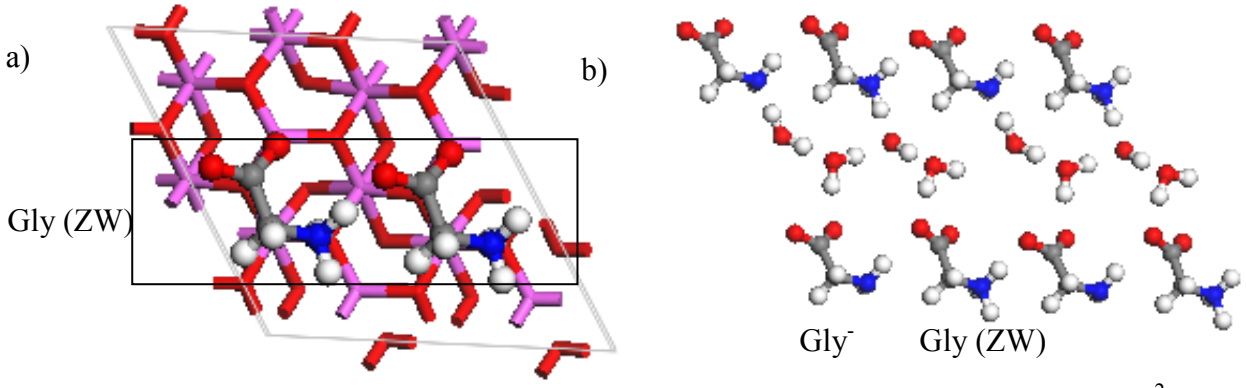

Fig: Top view of the more stable form of glycine at a coverage of 4.16 Gly μmol /m^2 on a) anhydrous and b) hydrated alumina, initially hydroxylated at 8.32 OH μmol /m^2

Keywords: surfaces, acid-base, bond formation, orientation.

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