Adsorption of phenylglycine and phenylalanine on TiO$_2$ rutile (110) and anatase (101) single crystal surfaces.

School of Physics and Astronomy, University of Manchester, Sackville Street Building, Manchester, M60 1QD

INTRODUCTION:
Titanium Dioxide is an important technological material with applications in pigments, biosensors, novel photovoltaic devices, photocatalysis to name but a few. In addition it is found at the surface of CP titanium and titanium alloys used in biomedical devices and is thought to contribute to the biocompatibility and high bonding strength to bone.

The surface structure and interactions of a number of low index faces of TiO$_2$ in the rutile form has been widely studied using high quality single crystals as model surfaces. However, there is still much that is unclear about surface geometrical structures, and the contribution of surface defects on the reactivity of the material. What is more many of the applications mentioned above use TiO$_2$ in the nanoparticulate anatase phase rather than the rutile form. Recent advances in growth of high quality single crystal anatase, in conjunction with thin film and epitaxial layer growth of anatase surfaces has allowed some of the complexities of this phase to be investigated [1,2]. In the work presented here we wish to understand the interaction between amino acids with TiO$_2$ surfaces in order to understand what may be happening in photocatalytic degradation of biological species, such as microbes in water purification. We also wish to investigate the stability of mode of adsorption of different amino acids, namely phenylalanine and phenylglycine, on these surfaces. It has been established that glycine adsorbs as a zwitterion and decomposes under low energy (ca 20-30 eV) photons [3], we wish to investigate the effect of the side group on the stability of the amino acids.


RESULTS & DISCUSSION: Phenylalanine adsorbed on anatase TiO$_2$(101) and rutile TiO$_2$ (110), appears to be more stable under illumination with VUV and soft x-ray synchrotron radiation between energies of 30 – 1000 eV, compared to glycine adsorbed on TiO$_2$ (110) [3] for exposure times of up to three hours. Loss of N was not observed in this time, which we believe is due to the different decomposition mechanisms between phenylalanine and glycine, resulting from the possible resonance structures which stabilise radical species formed during decomposition [4]. NEXAFS and core level photoemission indicate that phenylalanine adsorbs in an ordered fashion with hydrogen bonding between the amine groups and the carboxyl groups of first and subsequent layers of the molecules.

CONCLUSIONS: Phenylglycine undergoes decomposition when adsorbed on the (101) surface of anatase TiO$_2$. Phenylalanine adsorbed on the rutile (110) surface, on the other hand is stable and forms an ordered H-bonded multilayer.