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George R. Brown Convention Center

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### 784-2 Molecular Mechanisms of Glutamic and Aspartic Acid Sorption to Oxyhydroxide Minerals.

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Knowledge of amino acid sorption to mineral surfaces is important for understanding bacterial adhesion, biomolecule transport, mineral dissolution, elemental cycling, and the origin of life. The amino acids, glutamic and aspartic acid, contain carboxyl and amine groups whose dissociation over a pH range results in changes of molecular charge and reactivity. This research uses attenuated total reflectance (ATR) Fourier transform infrared (FTIR) spectroscopy and quantum chemical calculations to elucidate the influence of solution chemistry (pH, electrolyte composition) on the binding mechanisms of glutamic and aspartic acid to rutile (TiO<sub>2</sub>). Data for glutamic acid (100 mM NaCl, pH 3 and 7) reveals increased sorption with decreasing pH, with binding occurring primarily through carboxyl groups. At pH 3, a decrease of IR bands corresponding to protonated carboxyl groups is observed upon reaction with TiO<sub>2</sub> and indicates involvement of carboxyl groups during sorption. Changes in IR bands corresponding to amide moieties are also observed during reaction, perhaps an indirect result of bidentate-binuclear species forming with TiO<sub>2</sub>.

This surface species requires both carboxyl groups to bind with surface Ti<sup>4+</sup>, forming a ring-link structure. In this conformation, the amide group is brought towards the surface and may weakly interact with TiO<sub>2</sub>. Additional FTIR experiments will be carried out using D<sub>2</sub>O, to eliminate overlapping OH bands from H<sub>2</sub>O, permitting enhanced analysis of IR bands corresponding to amide and carboxyl groups. Quantum chemical calculations are ongoing to further investigate the binding mechanisms of these amino acids to TiO<sub>2</sub>. This research builds on our fundamental knowledge of sorption mechanisms and surface coordination of carboxylated amino acids on oxyhydroxide minerals. A basic understanding of this initial binding is needed to evaluate subsequent geochemical processes, ranging from organic contaminant fate and transport to understanding the formation of organic templates in early earth environments.

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