



Characterisation of the cell surface of three bacterial strains and the interactions at the cell-mineral interface by combining potentiometric titrations, XPS and ATR-FTIR.

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Cell surface properties of *Pseudomonas putida* (Gram-negative bacterium) and two *Rhodococcus sp.* strains (Gram-positive bacteria) were examined by potentiometric titrations, modelling, XPS and ATR-FTIR spectroscopy. By combining ATR-FTIR data at different pH values and potentiometric titration data with thermodynamic model optimisation, the presence, concentration and changes of organic functional groups on the cell surface (e.g. carboxyl, phosphoryl, amine groups) were inferred. The pH of zero proton charge, pHzpc, found from titrations at different electrolyte concentrations and resulting from equilibrium speciation calculations suggests that the net surface charge is negative at neutral pH values in the absence of other charge determining ions. In situ flow-cell ATR-FTIR using a Hematite coated germanium crystal was used to describe and monitor chemical interactions between the bacteria and Hematite in real time. ATR-FTIR spectra of bacteria growing on Hematite showed differences in the polysaccharide and phosphoryl regions when compared to the samples obtained from the planktonic culture. A shift in the carboxylate signal was also observed. XPS analysis was performed to quantify the elemental surface composition, to assess the local chemical environment of carbon and oxygen at the cell wall and to calculate the overall concentrations of polysaccharides, peptides and hydrocarbon compounds of the cell surface. Thermodynamic parameters for proton adsorption are

compared with parameters for other Gram-negative and Gram-positive bacteria. This work shows how the combination of potentiometric titrations, modelling, XPS and ATR-FTIR allows a more comprehensive characterisation of bacterial cell surfaces and cell wall reactivity as the initial step to understand the fundamental mechanisms involved in bacterial adhesion to solid surfaces and transport in aqueous systems.