

**SUPPORTING INFORMATION**

Characterisation of the cell surface and cell wall  
chemistry of drinking water bacteria by combining  
XPS and FTIR spectroscopy, modelling and  
potentiometric titrations

*Jesús J. Ojeda<sup>1</sup>, María E. Romero-González<sup>\*1</sup>, Robert T. Bachmann<sup>2</sup>, Robert G. J. Edyvean<sup>2</sup> and  
Steven A. Banwart<sup>1</sup>.*

(1) Cell-Mineral Interface Research Programme, Kroto Research Institute, The University of  
Sheffield, Broad Lane, Sheffield, S3 7HQ, UK.

(2) Department of Chemical and Process Engineering, Sir Frederick Mappin Building, The  
University of Sheffield, Mappin Street, Sheffield, S1 3JD, UK.

\* e-mail: [m.e.romero-gonzalez@shef.ac.uk](mailto:m.e.romero-gonzalez@shef.ac.uk)

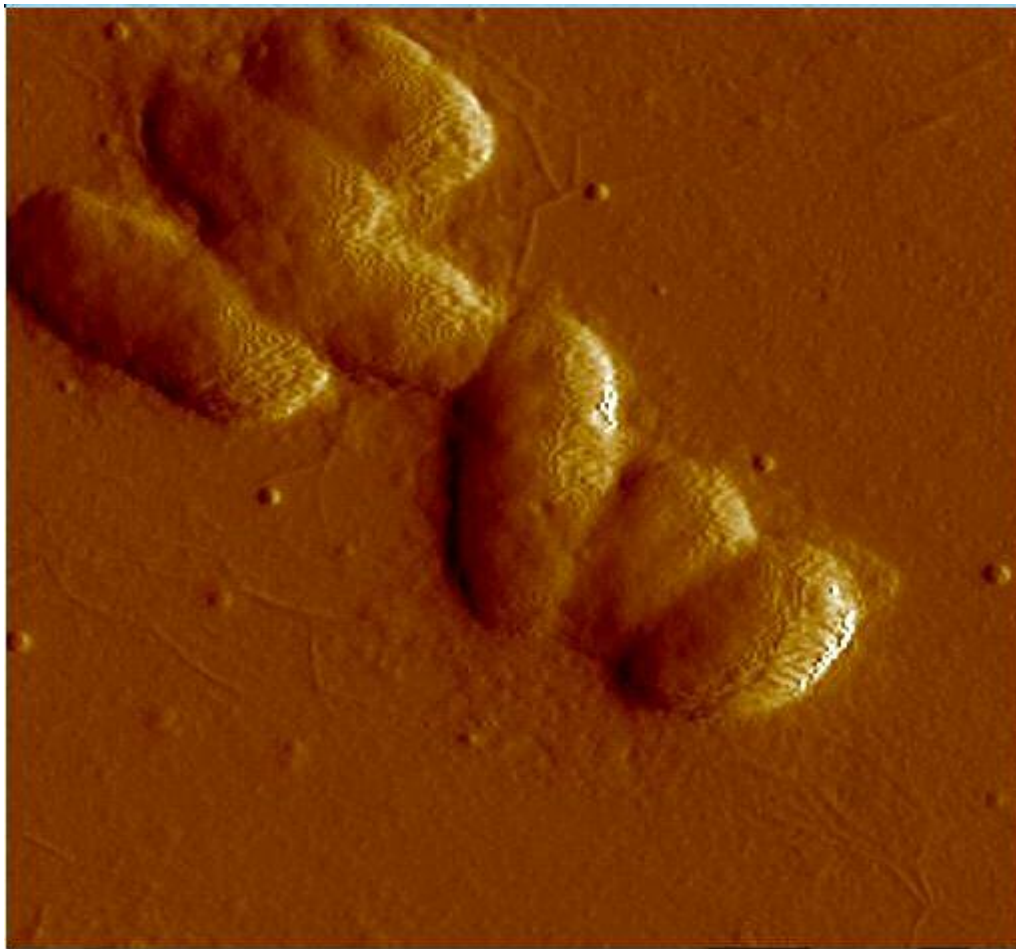
### **Atomic Force Spectroscopy images to calculate bacterial dimensions**

Atomic Force Microscopy (AFM) images of *A. commune* were made using a Dimension 3100 (Digital Instrument) in tapping mode and using a silicon tip. The images were processed using the Dimension 3100 software “Nanoscope”.

Bacterial surface area was calculated according to Fein et al. [1], since traditional solid surface area techniques cannot be used for microbial species, as untreated bacterial cells will not remain intact when placed under vacuum conditions. Therefore, the specific surface area was estimated using a geometric approach by measuring the external bacterium dimensions using atomic force microscopy (AFM). Figure S 1 shows that *A. commune* is rod shaped and the average long axis is  $2.92\mu\text{m}$  and the short axis is  $1.21\mu\text{m}$ . Based on these observations, the optical density measurements and the cell number per unit dry weight, a surface area of  $80\text{m}^2/\text{g}$  was calculated.

### **Titration of biomass at different ionic strength:**

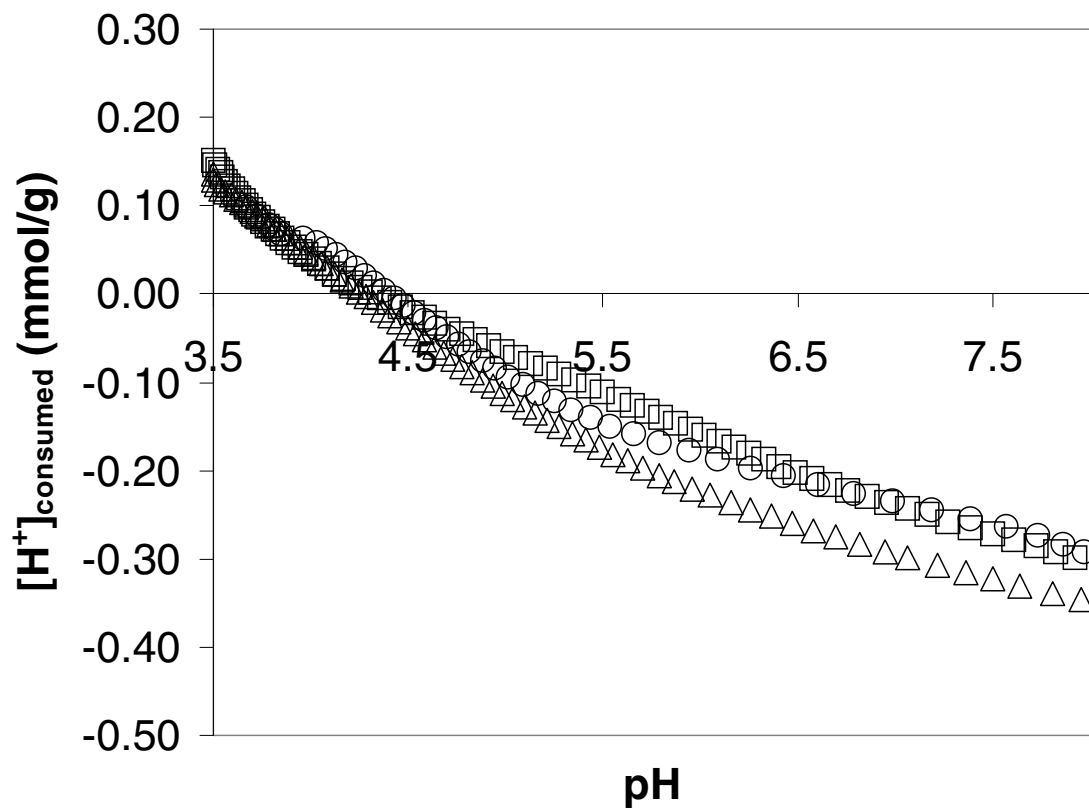
Figure S 2 compares the results from titrations with different ionic strength conditions. Although a possible ionic strength effect can be observed over the range studied, these effects are weak compared to the relatively large experimental uncertainties associated with biomass titrations [1,2,3,4,5,6]. The data shows an intersection point around pH 3.6-3.7, where there is no effect of the salt concentration. This value is similar to the pH of zero proton charge ( $\text{pH}_{\text{zpc}}$ ) calculated by PROTOFIT using the surface complexation model.



0

4.11  $\mu\text{m}$

1  
2 Figure S 1: AFM image of *Aquabacterium commune*.



1  
 2 Figure S 2: Potentiometric titration data for suspensions of 4.0g/L (dry weight) of *Aquabacterium*  
 3 *commune* in 0.01 (squares), 0.1 (circles) and 1.0 (triangles) M  $\text{NaClO}_4$ .

## 1 Literature Cited

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- [1] Fein, J.B.; Daughney, C.J.; Yee, N.; Davis, T.A. A chemical equilibrium model for metal adsorption onto bacterial surfaces. *Geochim. Cosmochim. Acta.* **1997**, *61*, 3319-3328.
- [2] Fein J.B.; Boily, J.; Yee, N.; Gorman-Lewis, D.; Turner, B.F. Potentiometric titrations of *Bacillus subtilis* cells to low pH and a comparison of modeling approaches. *Geochim. Cosmochim. Acta.* **2005**, *69*, 1123-1132.
- [3] Yee N.; Fein, J. Cd adsorption onto bacterial surfaces: A universal adsorption edge? *Geochim. Cosmochim. Acta.* **2001**, *65*, 2037-2042.
- [4] Martinez, R.E.; Smith, D.S.; Kulczycki, E.; Ferris, F.G. Determination of intrinsic bacterial surface acidity constants using a Donnan shell model and a continuous pK<sub>a</sub> distribution method. *J. Colloid Interface Sci.* **2002**, *253*, 130-139.
- [5] Daughney, C.J.; Fein, J.B. The Effect of Ionic Strength on the adsorption of H<sup>+</sup>, Cd<sup>2+</sup>, Pb<sup>2+</sup>, and Cu<sup>2+</sup> by *Bacillus subtilis* and *Bacillus licheniformis*: A surface complexation model. *J. Colloid Interface Sci.* **1998**, *198*, 53-77.
- [6] Cox, J.S.; Smith, D.S.; Warren, L.A.; Ferris, F.G. Characterizing heterogeneous bacterial surface functional groups using discrete affinity spectra for proton binding. *Environ. Sci. Technol.* **1999**, *33*, 4514-4521.