SUPLEMENTARY INFORMATION

New details for assembling bioactive films from dispersions of amphiphilic molecules on titania surfaces

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FIGURE S 1 - HIGH RESOLUTION SPECTRA A) SI 2P AND B) P 2P FOR INVESTIGATED BULK ODPA ON A SILICON WAFER

For the investigated bulk DMOAP samples, the O 1s spectrum was fitted considering only one contribution, since there is only one oxygen neighbourhood based on DMOAP structure and inspection of the Si 2p region did not reveal signal contributions from the silicon wafer used as a substrate. The detected single peak centered at 532.6 eV is attributed to ester bonds ^{1,2}. The N 1s signal presented two peaks centered at 402.4 eV and 406.4 eV, attributed to quaternary ammonium cation and to species containing nitrogen-oxygen bonds, moreover, the DMOAP exposed to water did not show the N*-O contribution in the N 1s spectrum, but only the $-N^+$ contribution at 402.3 eV ^{3,4}. As compared to the stoichiometrically expected [O]/[N] concentration ratio of 3.0, for vacuum-dried DMOAP a value of 3.1 was found. The Si 2p signal presented only a centrosymmetric peak at 102.4 eV attributed to alkyltrialkoxysilyl moieties, with the expected binding energy ^{5,6}. The Cl 2p high resolution spectrum shows only the doublet and the binding energy is coherent with chloride present on DMOAP structure ⁷. In contrast, for the air-dried blot DMOAP a contribution of organic chlorine was detected and attributed to 3-chloropropyl)trimethoxysilane⁷ (see Figure S 2).



FIGURE S 2 - O1S, N1S, SI2P AND CL2P HIGH RESOLUTION SPECTRA FOR THE INVESTIGATED BULK DMOAP SAMPLES



Figure S 3 – C1s and O1s HIGH-RESOLUTION SPECTRA FOR OCTADECYLPHOSPHONIC ACID ADSORBED ON TITANIUM DIOXIDE



Figure S 4 - P 2p HIGH-RESOLUTION SPECTRA FOR OCTADECYLPHOSPHONIC ACID ADSORBED ON TITANIUM DIOXIDE



Figure S 5 - SI 2P HIGH-RESOLUTION SPECTRA FOR DMOAP ADSORBED ON TITANIA. WHERE "A" REPRESENT ADDITION OF AQUEOUS HCL ON THE SOLUTION AND "N" IS THE SOLUTION WITHOUT THE ADDITION OF HCl

References

- 1 G. Beamson and D. Briggs, 1992.
- F. C. Dos Santos, S. V. Harb, M. J. Menu, V. Turq, S. H. Pulcinelli, C. V. Santilli and P. Hammer, *RSC Adv.*, 2015, 5, 106754–106763.
- 3 A. Kepelová, J. Newberg, T. Huthwelker, H. Bluhm and M. Ammann, *Phys. Chem. Chem. Phys.*, 2010, **12**, 8870–8880.
- 4 W. He, Y. Zhang, J. Li, Y. Gao, F. Luo, H. Tan, K. Wang and Q. Fu, *Sci. Rep.*, 2016, 6, 1–9.
- 5 P. M. Dietrich, S. Glamsch, C. Ehlert, A. Lippitz, N. Kulak and W. E. S. Unger, *Appl. Surf. Sci.*, 2016, **363**, 406–411.
- 6 H. Zarrin, J. Fu, G. Jiang, S. Yoo, J. Lenos, M. Fowler and Z. Chen, *ACS Nano*, 2015, **9**, 2028–2037.
- 7 P. E. B. K. D. Moulder, J. F.; Stickle W. F.; Sobol, Handbook of X-ray Photoelectron Spectroscopy, 1993.