

Orientation Studies of Si-phthalocyanine Sulfonic Acids Cast on SiO_x Substrates

G. Appel, H. Ade (North Carolina State U.), and S. Stadler (NRL)

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Phthalocyanine (pc) sulfonic acids are an interesting class of materials for molecular electronics. If used as dopants of conjugated polymers, they strongly influence the morphology [1] and the electronic structure [2] of these materials. The newly synthesized dihydroxy silicon phthalocyanine tetrasulfonic acid (Fig. 1a) and especially its oligomer [3] (Fig. 1.b) are expected to have an even stronger impact due to their high accumulation of anionic groups. We prepared layers of these substances by solution casting and investigated their orientation relative to the substrate by NEXAFS spectroscopy. The results of the NEXAFS studies were compared with atomic force microscope images.

The monomeric and the oligomeric pc were dissolved in methanol and parts of the solution were membrane filtered. These solutions were either spin cast or drop cast onto silicon substrates. Sample current NEXAFS spectra were taken at different angles of incidence.

Fig. 2a shows the NEXAFS spectra of a monomer sample, which was spin cast from a unfiltered solution. The dependence of the π^* -intensities at 285.4 and 287.7eV on the angle of incidence indicates that the molecular plane and the substrate plane are preferably parallel to each other or form an acute angle. This is consistent with the large flat crystals, which can be seen in the AFM image (Fig. 2b). The spectra of an oligomeric sample, drop cast from a filtered solution, also show a significant dichroism (Fig. 2c) but this time they indicate a rather perpendicular orientation. The AFM image again shows large flat areas of (probably) crystalline material (Fig. 2d).

We believe that these differences in the orientation behavior are governed by interactions of the pcs with the SiO_x-substrate and by possible impurities.

References:

- [1] B.R. Saunders, K.S. Murray, R. J. Fleming, R. Cervini, N.S. Allen, "Handbook of organic conductive molecules and polymers", edited by H.S. Nalwa, John Wiley and Sons, Vol. 3, p. 633, New York 1997.
 [2] G. Appel, O. Böhme, R. Mikalo, D. Schmeißer, *Chemical Physics Letters*, **313** (3-4), 411-415, 1999.
 [3] A.G. Guerek, G. Appel, R.P. Mikalo, D. Schmeisser, *Journal of Porphyrins and Phthalocyanines*, **5** (10), 751-757, 2001.

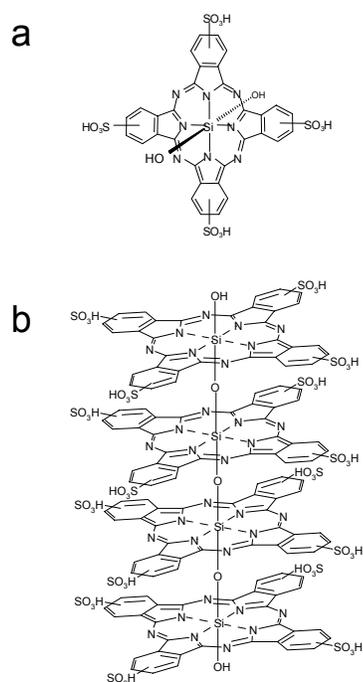


Figure 1: Structures of Dihydroxy silicon phthalocyanine tetrasulfonic acid (a) and its oligomer (b).

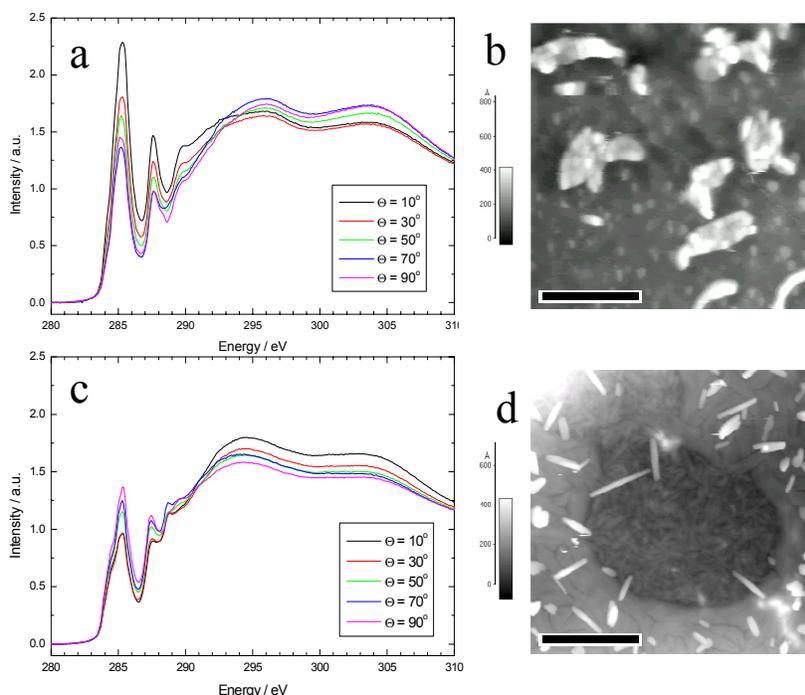


Figure 2: C-K edge NEXAFS spectra (a, c) at different angles of incidence Θ (angle of the electric field vector and the sample normal) and AFM topography images (b, d) of #2 (monomer, spin cast, unfiltered): a, b and #7 (oligomer, drop cast, filtered): c, d. The black bars indicate 1 μ m.