

DIPOLE-INDUCED ORIENTATION OF FLUOROPHENOLS ON SI(111)

Fan Zheng, J. L. McChesney, Xiaosong Liu, Franz Himpsel

Department of Physics, University of Wisconsin Madison, Madison, Wisconsin 53706

Our group has developed a memory system where each bit is represented by the presence or absence of a single silicon atom [1]. Because Si atoms are difficult to move at room temperature it is desirable to replace them by molecules that can be switched electronically, for example by a change in shape conformation, orbital configuration, oxidation state, optical properties, or dipole moment. We select polar molecules with a rotatable dipole with the intent to flip the axis of the polarization electrostatically with a biased STM tip. In order to carry out such a program one has to first characterize the adsorption and orientation of these molecules on silicon.

The adsorption of phenol and two of its fluorinated versions (4-fluorophenol and 2,3,4-trifluorophenol) on Si(111)7×7 is studied by the near edge x-ray absorption fine structure (NEXAFS) spectroscopy. The polarization dependence of the π^* transitions indicates a preferred orientation for the fluorinated phenols which is absent for phenol itself (Figure 1). The orientation is attributed to dipole-dipole interactions between the aromatic groups that are polarized by fluorine ligands. Two models are developed for the quantitative analysis of NEXAFS data from a molecular layer with two angular degrees of freedom, i.e., the tilt of the supporting chain and the rotation of the end group about its bond to the chain. More generally, this work addresses the NEXAFS analysis of molecular layers with customized end groups [2] that are used in molecular electronics and for making inorganic surfaces bio-compatible.

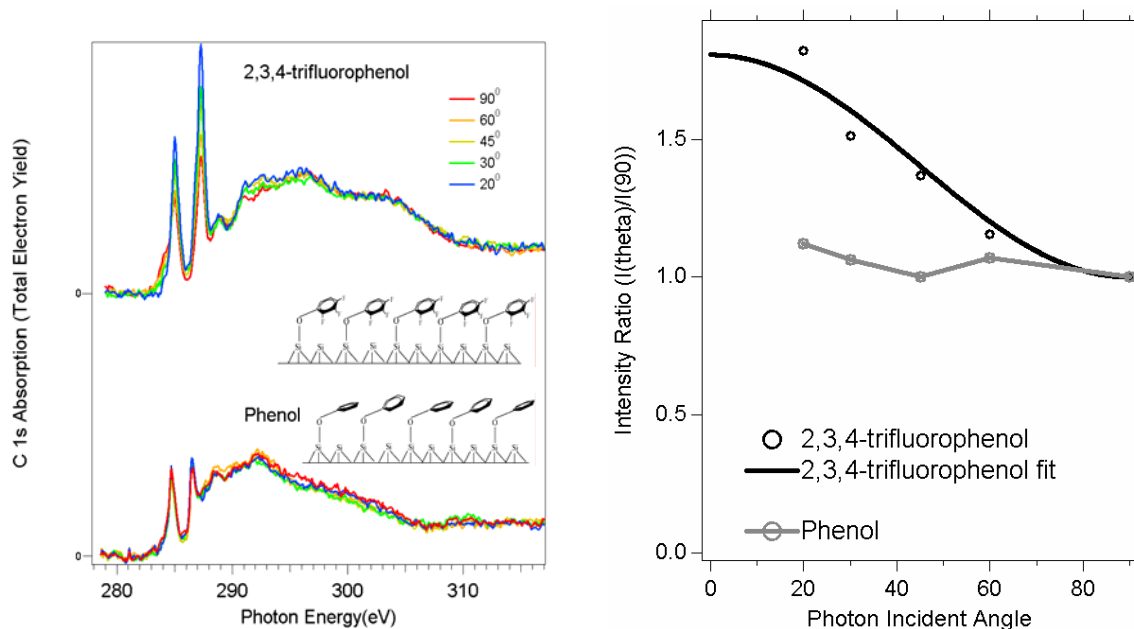


Figure.1. Polarization-dependent NEXAFS spectra at the C1s edge for 2,3,4-trifluorophenol (top) and phenol (bottom). In contrast to phenol, the fluorinated phenol shows a strong polarization dependence which indicates a well-defined orientation (right).

[1] R. Bennowitz et al., *Nanotechnology*, **13**, 499 (2002).

[2] Y.-Y. Luk et al., *Chem. Phys.* **120**, 10792 (2004).