ANDREA PARIS ABSTRACT

Title: An XPS and DFT study of the interaction of a model polymer with silicon surfaces
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Understanding the interactions between polymers and surfaces is very important for the development of new, more effective materials such as glues and coating agents. The aim of this paper is to study the adsorption of polystyrene on model silicon surfaces and determine the extent to which the surface functionalisation influences the styrene adsorption. Different surface-modified silicon wafers were spin coated with layers of polystyrene. The functionalised surfaces studied included samples with terminating amine, methyl, thiol and hydroxyl groups with a hydrogen terminated silicon surface on which no hydrogen bonding could occur used as a control sample.

X-ray photoelectron spectroscopy (XPS) of the C1s shake-up satellites, which arise from π-π* transition of the aromatic ring of the polymer, was used to provide information on the nature of the interactions between the polymer and the functionalised silicon surfaces, with DFT modelling performed to establish a realistic model of the electronic structure of the adsorbed polystyrene's MO energies.