

Title Interaction of Organic Molecules with Metal Passivated Silicon Surfaces Studied via STM

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Abstract Organic molecules offer a wide range of optical, electronic or chemical properties. Coupling them to silicon could pave way to novel applications and devices, however, a controlled molecular functionalization of silicon remains challenging due to the presence of highly reactive dangling bonds on its surfaces. We attempt to decrease the reactivity of low index silicon surfaces with an ultra-thin layer of a metal adsorbates and study their interaction with organic molecules via scanning tunnelling microscopy. In the first part we investigate the interaction of ethylene, a small unsaturated molecule, with tin and indium 1D chains grown on Si(001) – 2×1 . The chains consist of dimers structurally analogous to the dimers of the underlying Si(001) – 2×1 surface. Aided by photoelectron spectroscopy we find that the Sn chains are less reactive than the Si(001) surface and that the absence of a π dimer bond renders indium chains inert. In the second part we study the interaction of copper phthalocyanine, a small macrocyclic heteroaromatic compound, with the Si(111)/Sn – $\sqrt{3} \times \sqrt{3}$ substrate. We find that despite the presence of dangling bonds on the tin atoms, the reactivity of the Sn layer is significantly decreased with respect to a bare Si(111) – 7×7 . Substitutional defects, however, significantly increase the reactivity locally and strongly bind CuPc. Other Sn and In reconstructed Si(111) surfaces exhibit a similar trend, albeit the strength of the interaction at defect sites is noticeably weaker as CuPc can hop between defects.

Keywords adsorption, phthalocyanine, CuPc, ethylene, ethene, silicon, Si(111), Si(001), Si(100), surface, tin, indium, defects, STM, STS, PES, XPS