Abstract Submitted
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Acetophenone on Si(001) with STM and DFT[1] STEVEN SCHOFIELD, ADAM RAHNEJAT, London Centre for Nanotechnology and Department of Physics and Astronomy, UCL, London, UK, OLIVER WARSCHKOW, Centre for Quantum Computation and Communication Technology, University of Sydney, Australia, DANIEL BELCHER, MARIAN RADNY, PHILLIP SMITH, School of Mathematical and Physical Sciences, University of Newcastle, Australia — Organic molecules are likely to play an important role in future technologies, e.g., in novel devices where individual molecules are incorporated as active elements, and in extending the functionality of existing technologies. A detailed, atomic-scale understanding of the structural and electronic properties of molecules on surfaces is key to the development of these technologies. Here we present scanning tunnelling microscopy (STM) and density functional theory (DFT) data of the surface binding configurations of acetophenone adsorbed to Si(001). Topographic and spectroscopic tunnelling experiments were performed at 77 K and room temperature in the limit of very low coverage. We find in analogy to other similar molecules such as acetaldehyde [1], acetone [2,3] and acetic acid [4], acetophenone molecules covalently bond to the Si(001) surface in a variety of configurations that can be directly manipulated using the STM tip. In its most stable configuration, the adsorbate stands upright on the surface, attached via the C and O atoms of its acetyl group, producing a geometry that is robust and attractive for molecular electronics applications. [1] JCP 131, 104707 (2010), [2] PCCP 11, 2747 (2009), [3] JACS 129, 11402 (2007), [4] PRB 84, 153302 (2011).

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