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The Raising Of A Molecular Flagpole: Acetophenone on the Silicon (001) Surface OLIVER WARSCHKOW, Centre for Quantum Computer Technology, School of Physics, The University of Sydney, STEVEN R. SCHOFIELD, London Centre for Nanotechnology, University College London, DANIEL R. BELCHER, MARIAN W. RADNY, PHILLIP V. SMITH, School of Mathematical and Physical Sciences, The University of Newcastle — The utility of scanning tunneling microscopy (STM) to image chemical processes on semiconductor surfaces is now widely appreciated. In addition to imaging, the STM may also be used as an invasive device to induce chemical reactions in a molecule under observation. This offers enticing prospects for directed single-molecule synthetic chemistry, provided the chemical processes observed are understood. This presentation reports a detailed density functional study to resolve the mechanism behind a series of STM-induced reactions in an acetophenone ($PhCOCH_3$) molecule on the Si(001) surface. Acetophenone follows the general reaction pattern resolved by us earlier for acetone [1] and acetaldehyde [2]; however, the presence of an aromatic ring introduces an important twist. [1] O. Warschkow, I. Gao, S.R. Schofield, D.R. Belcher, M.W. Radny, S.A. Saraireh, and P.V. Smith, Phys. Chem. Chem. Phys. 11 (2009) 2747. [2] D.R. Belcher, S.R. Schofield, O. Warschkow, M.W. Radny, P.V. Smith, J. Chem. Phys. 131 (2009) 104707.

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