Raising a Molecular Flagpole on the Silicon Surface.

The utility of scanning tunnelling 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 with applications in molecular electronics and atomic-scale device fabrication. A key requirement is that the chemical processes observed and induced are understood, which heavily relies on theoretical modelling. This presentation reports a detailed density functional theory study to resolve the mechanism behind a series of STM-induced reactions in an acetophenone (PhCOCH3) molecule on the silicon (001) surface. We find that acetophenone follows the general reaction pattern of the smaller analogues acetone and acetaldehyde; however, the presence of an aromatic ring introduces an important twist.

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