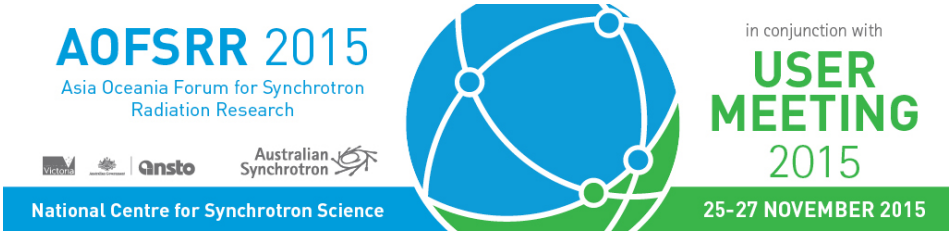

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Resolving conflicts in the understanding of molecular adsorption: benzonitrile on Si(001)

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Near-Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy is a powerful means of determining the orientation of molecular moieties with respect to a substrate. Still, interpretation is challenging in the case of small molecules on clean semiconductor surfaces. These surfaces are highly reactive and a typical molecule can adsorb in many ways. A classic example is benzonitrile on Si(001) where scanning tunneling microscopy (STM) studies [1] disagree with NEXAFS/photoemission studies [2] despite both being complemented by density functional theory calculations.

Here we show how this confusion arises as a function of molecular coverage. We use the Soft X-ray Spectroscopy beamline at the Australian Synchrotron to study the adsorption of benzonitrile at very low coverages (STM regime) using NEXAFS and photoemission. Using density functional theory to simulate NEXAFS spectra, it can be shown that the low coverage adsorption structure is the cross-row tripod structure found using STM, whereas at higher coverages the surface is increasingly populated by the 2+2 cycloaddition structure with a free-standing phenyl ring. Unlike our previous work with acetophenone [3], it is not possible to induce the free-standing structure with mild annealing. Instead, we observe rapid molecular dissociation confirmed with STM measurements at elevated temperatures.

[1] Belcher, et al, JACS 134, 15312 (2012)
[2] Rangan, et al, Phys Rev B 71, 165318 (2005)
[3] O'Donnell, et al, J Phys Condens Matter 27, 054002 (2015)

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