

## ABSTRACT

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“Understanding and controlling dopant precursor chemistry at silicon surfaces in UHV”

Scanning tunnelling microscopy is an experimental technique that has provided unique insights into the nature of reactions at surfaces. In the case of small precursor molecules that deliver dopant atoms to host semiconductor surfaces, such insights are needed now more than ever.

Integrated circuit components are being shrunk to nanoscale dimensions and quantum computing schemes have been proposed that require accurate positioning of single dopant atoms. I will describe a long term project in which the interaction between a molecule and a surface (PH<sub>3</sub> and the (001) surface of silicon) has been characterised and ultimately controlled with an unprecedented level of detail. Processes of adsorption, dissociation, diffusion and incorporation are observed with STM and simulated with density functional theory (DFT) calculations. Sequences of STM images allow us to follow multi-step chemical reactions occurring on the surface and we determine the reaction pathways taken by a P atom during its transition from a component of a gas phase molecule to a dopant on the surface. In addition I will describe the use of a monolayer hydrogen resist mask, patterned using STM, to confine surface reactions to local areas of the Si(001) surface and ultimately incorporate P atoms in silicon at user defined positions, with atomic precision. I will end the talk with speculation about how the H-resist mask technique might be used to promote unconventional surface reactions by blocking off energetically favoured reaction pathways.