Integrated Materials Design Centre Seminar

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Silicon surfaces: fragmentation methods and thermal simulations

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Date: **Wednesday, 29th July 2015**
Time: **11:00 am – 12.00 pm**
Venue: Chemistry Building seminar room G05
Dalton Building (F12)

Abstract

Surface chemistry and the interactions between adsorbates and surfaces have a profound impact on modern life. The ability to accurately model and predict the outcomes of these processes can dramatically influence science and technology. Despite around 90% of industrial chemical production relying on heterogeneous catalysis, many aspects of gas-surface chemistry remain unexplained.

One method to calculate the properties of non-conducting crystals is systematic molecular fragmentation. This can equally be applied to crystal surfaces and adsorbate-surface interactions, yielding a linear scaling method that allows material surface reactivity to be modelled at any level of electronic structure theory. In this talk I shall describe fragmentation in general, its application to H + H-Si(111), and recent progress toward including surface temperature effects.

Biography

Dr Frankcombe is a Senior Lecturer at UNSW Canberra. He spent the period from 2004 to 2010 as a postdoctoral fellow, at universities in the Netherlands, Sweden and Australia. During this time Dr Frankcombe's projects ranged from solid state hydrogen storage to astrochemistry. From 2011 up to his appointment at UNSW Canberra he was employed as an ARC Future Fellow at the Australian National Univerity. Dr Frankcombe held the position of Associate Director of the National Youth Science Forum (a non-research position) from December 2010 to March 2011. His Research interests are diverse, broadly covering methodological and applied aspects of interactions in molecular and condensed phase systems, and how they impact on reactivity.