Computer simulation of surfaces and nanostructures I

Chair(s): Simon Crampin (University of Bath, UK)

Tuesday 14 December 2010

13.30 **Invited: He-Atom scattering from surfaces: calculating diffraction peak intensities from first principles**
R Martinez-Casado (Imperial College, London, UK)

14.00 **In search of the mechanism for tautomerization of naphthalocyanine: Density functional theory on a molecular switch**
F Hanke (University of Liverpool, UK)

14.30 **An ab initio description of the bulk and surface structures of UO2 using GGA+U and occupation matrix control**
A Devey (AWE, UK)

14.45 **A fast, stable method for density functional simulations of nanostructures**
P Hasnip (University of York, UK)

15.00 **Ab-initio multiscale method to address defects in metals**
G Schusteritsch (Harvard University, USA)

15.15 **An ab-initio method for complex unit cell materials with short-range ordering: the Non-Local Coherent Potential Approximation for multi-sublattices compound of arbitrary structure**
A Marmodoro (University of Warwick, UK)

15.30 **End of symposia**