

Application for Class A usage of ICHEC facilities on the successor of Stoney/Stokes II

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Project title: Highly-parallel *ab initio* molecular simulation and dynamics studies of metal oxide-water interfaces  
Duration: 24 months requested, with proposed start date of 1 Jan 2014 (ideally). As late as 1 May 2014 is also quite acceptable, however.  
Core-hours: 3.5 million  
Funding: SFI-funded three-year Research Frontiers project, 10/RFP/MTR/2868 (the theoretical aspects of which hinge on DFT simulation of metal oxides with a view towards applications in photovoltaics, and more specifically hydrogen production from water-splitting).

In addition, there is a pending funding application under review by SFI for their Investigators programme (with final decision expected around Jan./Feb. 2014), entitled ‘Innovative, low-cost advanced electrode Materials for enhancing water Electrolysis Systems and distributed Hydrogen production (I-MESH)’ – here, the application of DFT towards water-splitting for hydrogen production is a key feature.

Abstract

Highly-parallelised molecular simulation and *ab initio* dynamics (AIMD) will be performed of interfaces between metal oxides and liquid water, to capture the rich tapestry of chemical and physical adsorption interactions in all of their physico-chemical complexity, employing state-of-the-art treatments of dispersion. Partial and full coverage of chemically and physically adsorbed water molecules will be investigated, as well as full condensed phases of liquid water in contact with metal oxide surfaces. A particular focus will be on the dynamical properties of hydrogen bonds between protons in water molecules and the bridging oxygen atoms at the surface, as well as the variation in bond-stretch and bond-angle bending modes in the water molecules. The dipolar orientation of the water molecules vis-à-vis the surface-normal will also be studied, as well as water-dissociation kinetics and thermodynamics on these surfaces. The importance of kinks and surface irregularities will also be studied very closely. It is to be expected that this will contribute to our somewhat lacking understanding of water interactions with metal oxide surfaces, to enhance efforts in the optimal design of nano-material surfaces for photo-catalytic water-splitting.