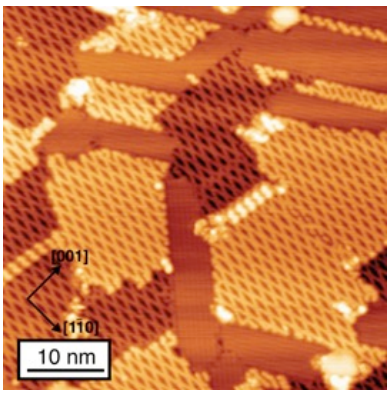
PhD in Multiscale Modelling of Corrosion Scales

Supervisor: Nicholas M Harrison



We are all familiar with corrosion and its significant economic and environmental consequences. The cost to industry in 2012 was estimated to be over $2 trillion *per annum* [1]. Current theories of corrosion are in large part based on the phenomenology of average behaviour and predict more of less successfully average corrosion rates for widely used metallurgies [2,3]. This is often insufficient to allow us to generate new strategies for detecting, controlling and ultimately preventing corrosion especially in extreme environments. Recent advances in multi-scale modelling and in the *in situ* measurement of atomic scale processes in corrosion layers [4] suggests that it is now possible to develop a multi-scale predictive model of corrosion that addresses behaviour at macroscopic length and time scales but is rigorously based on a new understanding of atomic scale processes.

Applications are invited for a fully funded 4-year studentship in the combined quantum, atomistic and continuum modelling of the nucleation, growth and degradation of corrosion scales in the Computational Materials Science Group at Imperial College London (http://www.imperial.ac.uk/computational-materials-science).

The project involves the development of a meso-scale model that will use the *local corrosion approximation* to model the growth and degradation of typical iron carbonate scales that form on steel surfaces in various environments. The solution chemistry, mass transport, reaction kinetics, diffusion and charge transport processes underpinning the model will be obtained from a combination of detailed experimental characterisation to be performed by collaborating groups and from large scale quantum mechanical calculations.

This work will be conducted as part of a wider collaboration involving the Universities of Leeds, Edinburgh, Manchester and Cambridge within which state of the art *in situ* measurements of microscopy and spectroscopy will be used to elucidate the composition and structure of growing and degrading scales. The long term aim is to develop strategies for the prevention, mitigation and detection of corrosion.

This PhD studentship will be part of the BP International Centre for Advanced Materials (BP-ICAM: http://www.icam-online.org) community. BP-ICAM was set up by BP in autumn 2012 with a $100 million investment over 10 years; it has recently been extended for a further 5 years. It brings together the strengths of world-leading universities and BP's expertise in oil and gas to create an international centre of excellence in advanced materials research. The partnership between The University of Manchester (Dr Robert Lindsay), the University of Cambridge (Dr Stuart Clark), Imperial College London (Prof Mary Ryan), the University of Sheffield (Dr Kyra Campbell), the University of Leeds (Dr Rick Barker) and BP's corrosion engineers brings game-changing capabilities in structural materials, corrosion, separations, surfaces, deposits, imaging, modelling and self-healing materials.

Application process

Applicants should submit a CV, a brief statement of research interests, and the names of two referees by e-mail to Prof. Nicholas Harrison (nicholas.harrison@imperial.ac.uk).

1. Hays G. F. *Now is the Time*, World Corrosion Organisation (2012)
2. *Atkinson A, Rev. Mod. Phys., 57, 437 (1985)*
3. *Cabrera N, Mott N, Theory of the Oxidation of Metals, Rep. Prog. Phys. 12 163 (1949)*
4. M Tautschnig, NM Harrison, MW Finnis, *Acta Mater.,* **132,** 503 (2017) [https://doi.org/10.1016/j.actamat.2017.04.059]