All-Atom Modelling of Charged Metal Oxide-Electrolyte Interfaces

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Exposed to an aqueous solution (electrolyte) at high pH, metal oxide surfaces acquire a negative charge due to release of protons. In this respect metal oxides remain ionic solids, whether they are insulators, semiconductors or even (narrow-band) electronic conductors. The negative surface charge is compensated by cations supplied by the electrolyte. The effective surface charge density of protonic double layers can be huge (several elementary charges per nm^2) as shown by colloid science. Modelling such highly charged interfaces in atomic detail remains a major challenge. An obvious problem is that the large dipoles of electric double layers are incompatible with the periodic boundary conditions used in all-atom modelling. In this talk we will outline how some of these complications can be overcome using finite electric field methods. While seemingly a technical issue for simulation, the problem of supercell modelling of electric double layers touches on fundamental questions concerning the microscopic definition of interface potentials and polarization and should therefore also be of interest to experimentalists.

After obtaining a PhD in physics from the University of Amsterdam followed by an extended period as postdoc Michiel Sprik joined the IBM Zurich research laboratory in 1990 as regular member of staff. In 1998 he left Zurich to take up a lectureship at the Department of Chemistry of the University of Cambridge and stayed there ever since. He was promoted to professor in 2004. His research interest have evolved over time from computational solution chemistry using density functional theory based molecular dynamics methods (“Car-Parrinello”) to the application of these methods to interfacial electrochemistry. The project which is the subject of this talk is in collaboration with Chao Zhang (Cambridge) and Jun Cheng (Xiamen).