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From the microscopic theory of the electrochemical atomic layer deposition (EC-ALD) to atomistic simulations

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The phenomenon of deposition of a monolayer amount of metal atoms onto a dissimilar, more noble metal electrode at a potential more anodic than expected from the Nernstian equilibrium potential was recognized about 70 years ago but it was not before 1974 that Kolb, Gerischer and Przasnyski explained theoretically this concept known as the underpotential deposition (UPD) ΔVupd. Using over 20 couples of metals these authors found that ΔV_{upd} followed the simple, linear equation $\Delta V_{upd}=½\Delta\phi$, where $\Delta\phi$ is the difference in work functions between the adsorbate and the substrate. For most of the metal couples investigated, the relation was verified. However, this seemingly oversimplified relation was soon after contradicted by Bewick and Thomas' experiments on the deposition of Tl and Pb on Ag single crystal electrodes. Henceforth, there has been tremendous works achieved by several authors to refine the microscopic understanding of the UPD process. These theoretical works were often accompanied by numerical simulation approaches at the atomistic level (Monte Carlo and kinetic Monte Carlo techniques) and quantum mechanical calculations. However, despite the increase of computer and softwares capabilities the models used in these studies cannot fully capture the whole complexity involved in the UPD process and simplified model systems had to be used. In this paper, the microscopic theory of UPD and the results obtained from computational, atomistic approaches will be reviewed, and the assets also the weaknesses and the foreseeable improvements in particular in the realm of the density-functional theory will be presented.

Biography

Pascal Boulet has completed his PhD in 2001 from both the University of Lyon (France) the University of Geneva (Switzerland). He then moved to University College London (England) as a Post-doctoral Fellow for two years. Since 2003, he is an Associate Professor at the Aix-Marseille University (France), where he works on materials for energy using computational chemistry tools. He has published over than 50 papers in reputed journals.

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