Recent advances in the theory and simulation of Underpotential Deposition

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The electrochemical formation of non-bulk surface (sub)monolayers at potentials more positive than the reversible Nernst potential for the bulk deposition of the adsorbate, popularly denominated underpotential deposition (upd), has been observed with a great variety of substrate/adsorbate combinations, including nanoparticles (NPs). The latter have awaked great interest in both the scientific and technological communities, and the size-dependence of their thermodynamic properties has been a hot topic of research in recent years[1].

In the present talk we will address three different aspects of upd:
1- We will consider upd on surfaces with different curvatures, and we will show that in the case of surfaces with positive curvatures (NPs) the upd phenomenon should vanish in the nanoscale.
2- We will show how to deal with upd modeling in the presence of anions, and show that in some systems the presence of anions may be essential for the existence of upd.
3- We will analyze how to calculate the entropic contribution to the stability of upd deposits.

References