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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

[1].Oviedo, O.A., Leiva, E.P.M. Chapter 10: “Thermodynamic modeling of metallic nanoclusters” in the book Metal Clusters and Nanoalloys, Springer, New York, 2013, pag 305-350.