**Towards a Realistic Modelling of Electrified Interfaces the Nanoscale**

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In this talk I will introduce some issues connected with the simulation of electrified

interfaces at the nanoscale focusing on simulating the effect of an applied potential to an electrochemical (EC) cell, using realistic models for the charged electrode electrolyte interface. I will present some recent progress in the simulation of the double layer of the fundamental Pt-water interface and its response to changes of potential applied to the cell [1]; this is obtained applying a general ab initio electrode-charging approach I have developed. If time allows, I will illustrate how combining knowledge from molecular electronics and DFT based methodologies to simulate atomic dynamics could lead to a more sophisticated description of EC phenomena.

[1] R. Khatib, A. Kumar, S. Sanvito, M. Sulpizi and C. S. Cucinotta\*, The nanoscale structure of the Pt-water double layer under applied potential revealed, 2021, 391, 138875

