Minicolloque n° CPR8 **X Oral** **☐ Poster**

Charge transfer and work function modifications induced by molecules at gold nanoparticles surfaces

Olivier Pluchery [a*], Léo Bossard-Giannesini [a], Hervé Cruguel [a], Luis Lechaptois [a], Angeline Dileseigres [a]

a. *Institut des NanoSciences de Paris, Sorbonne Université, 4 place Jussieu, Paris, FRANCE*

* email : olivier.pluchery@insp.jussieu.fr

One key property of surfaces when dealing with electronic properties is work function. WF is clearly defined for a pure material with a planar and infinite interface. This is simply the energy needed for extracting an electron from the conduction band and placing it in vacuum in a rest position.

However, this notion becomes unclear when surfaces are rough, when they accommodate local charges or when they are functionalized with molecules [1]. Molecules will induce charge transfer and dipolar moments. The local surface radius related to surface roughness will also concentrate charges due to the lightning rod effect [2]. All these effects greatly influence the nanoscale chemistry and the surface reactivity. It will also influence the electric transport which is crucial when dealing with photovoltaics.

These various parameters will be discussed and studied with a special focus on the ideal case represented by gold nanoparticles. Gold nanoparticles allows easily adjusting their diameter and the surface chemical functionalization, without suffering from unwanted oxidation. The local work function is related to the so-called Contact Potential Difference (CPD) that is measured with a Kelvin Probe Force Microscope (KPFM). [3, 4]

Gold nanoparticles are also efficient nanoantenna for collecting electromagnetic excitations from light and transforming them into hot electrons. We will briefly mention some connections between this plasmon induced hot electrons and the electric properties of nanoparticles.

[1] Bossard-Giannesini, L. Measure and calculation of the work function of functionnalized gold nanoparticles. Sorbonne University, PhD thesis Paris, **2018**.
[2] Wood, D. M., Classical Size Dependence of the Work Function of Small Metallic Spheres. *Physical Review Letters* **1981,** *46* (11), 749-749.
[3] Zhang, Y.; Pluchery, O.; Caillard, L.; Lamic-Humblot, A.-F.; Casale, S.; Chabal, Y. J.; Salmeron, M., Sensing the Charge State of Single Gold Nanoparticles via Work Function Measurements. *Nano Letters* **2015,** *15* (1), 51-55.
[4] Zhang, Y.; Kang, J.; Pluchery, O.; Caillard, L.; Chabal, Y. J.; Wang, L.-W.; Sanz, J. F.; Salmeron, M., Nanoimaging of Organic Charge Retention Effects: Implications for Nonvolatile Memory, Neuromorphic Computing, and High Dielectric Breakdown Devices. *ACS Applied Nano Materials* **2019,** *2* (8), 4711-4716.