

Organization and plasticity of the nanoparticle-coating monolayer control its conformation, solubility and molecular recognition ability

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ABSTRACT

The self-assembly of a monolayer of ligands on the surface of noble metal nanoparticles allow the realization of ordered and complex molecular structures, with applications that span from materials science and electronics, to bioimaging, nanomedicine and even catalysis.[1] We present a combined computational–experimental study that demonstrates how functionalized coating thiols can self-organize to form transient pockets in monolayer-protected gold nanoparticles (AuNPs). These transient cavities explain the selectivity and sensitivity observed for different organic analytes in NMR chemosensing experiments.[2] Thus, our findings advocate for the rational design of tailored coating groups to form specific recognition binding sites on monolayer-protected AuNPs.

[1] A. Quarta, A. Curcio, H. Kakwere, T. Pellegrino, Polymer coated inorganic nanoparticles: tailoring the nanocrystal surface for designing nanoprobcs with biological implications, *Nanoscale*. 4 (2012) 3319.

[2] M.-V. Salvia, G. Salassa, F. Rastrelli, F. Mancin, Turning supramolecular receptors into chemosensors by nanoparticle-assisted “NMR chemosensing,” *J. Am. Chem. Soc.* 137 (2015) 11399–11406.