Monolayer protected gold nanoparticles, on the move: Toward nanoreceptors with intelligent recognition abilities

Marco De Vivo

Molecular Modeling and Drug Discovery Lab, Istituto Italiano di tecnologia, Genova, Italy

The self-assembly of a monolayer of ligands on the surface of noble metal nanoparticles allows the realization of ordered and complex molecular structures, with applications that span from materials science and electronics, to bioimaging, nanomedicine and even catalysis. Here, we will show how molecular dynamics (MD) simulations of realistic 3D models built using our recently released NanoModeler webserver (www.nanomodeler.it), can help in characterizing, with unprecedented detail, the fundamental molecular mechanisms of binding pockets formed into the monolayer of monolayer-protected gold nanoparticles (AuNPs). Notably, NanoModeler is the first webserver designed to automatically generate and parameterize model systems of AuNPs and gold nanoclusters. Our extended simulations, integrated with experiments, explain the selectivity and sensitivity observed for different organic analytes in NMR chemosensing experiments. Thus, our findings advocate for the rational design of tailored coating groups to form specific recognition binding sites on monolayer-protected AuNPs. These may find applications for detecting small molecules such as drugs, metabolites, illegal drugs, and small molecular markers for cancer.