Supramolecular Binding of Small Molecules on Self-Assembled Monolayer Protected Gold Nanoparticles

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Abstract:
Various strategies have been developed for construction of molecular aggregates with rationally designed properties, geometries, and dimensions that promise to provide solutions to both theoretical and practical problems in areas such as drug delivery, medical diagnostics, and biosensors, to name but a few. Several studies have reported an enhanced antimicrobial activity of the antiseptic photosensitizer crystal violet (CV) in the presence of gold nanoparticles covered with self-assembled monolayers. While the effectiveness of CV against gram-negative and gram-positive bacteria was demonstrated on multiple occasions, the detailed molecular mechanism of the synergistic interaction pathway between gold nanoparticles and CV remains poorly understood. We conducted a systematic investigation on the binding principles for CV attachment to the nanoparticle shell through a combined computational and experimental approach.
In particular, 2 nm gold core nanoparticles coated with undecanesulfonicacid (MUS)-containing ligands were considered.
The evidences obtained so far show a significant influence of the environmental conditions on CV interaction properties. Moreover, based on computational models resembling experimental conditions, the molecular binding principles were elucidated, showing a preferential binding mode of the CV to the monolayer.

Keywords: gold nanoparticles, self-assembled monolayer, molecular simulation, supramolecular binding, biomedical applications.

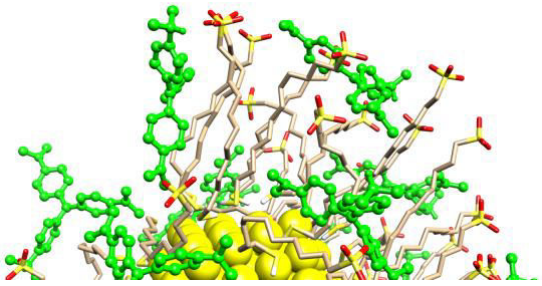

Figure 1: Molecular view of the interaction mode of CV and MUS-coated gold nanoparticle in solution.

References:

Macdonald, T. J. et al. (2016) Thiol-Capped Gold Nanoparticles Swell-Encapsulated into Polyuretane as Powerful Antibacterial Surfaces Under Dark and Light Conditions, *Sci. Rep*. **6**, 39272

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