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Biosynthesis and computational analysis of amine-ended dual thiol ligand functionalized gold nanoparticles

The bio-synthesized DTAuNPs have an average size of 21 nm. The aggregation extent depends on the concentration of melamine, which was validated by UV-vis spectroscopy and hence a visual method for melamine detection was developed. The major observation in this method was the color change of DTAuNPs from red to purple due to the aggregation of ligand-capped gold nanoparticles initiated by melamine. The color change was due to the shift in hydrogen bonding between the nanoparticles and melamine. The ligand-capped gold nanoparticles was assessed for cytotoxicity against A549 cells which resulted in significant decreased cell viability. The DFT calculations were used to verify the characterization of the ligands. A frequency calculation was carried out to obtain the IR spectrum. Then the TDDFT[1] calculation was performed (both in the gas phase and in water) to obtain the HOMO and LUMO orbitals in the gas phase and transitions of electrons. The theoretical and experimental data compared favourably.

Figure 1. a) 3D structure of the APT molecule b) APT HOMO orbitals c) APT LUMO orbitals

References

1. Trani, F., Scalmani, G., Zheng, G.S., Carnimeo, L., Frisch, M.J., Barone, V. J. Chem. Theory Comput. 2011 7, 3304.

Presenter Biography

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