

Multi-level Modelling of Gold Nanoparticles in Various Environments

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Gold Nanoparticles (GNPs) have been demonstrated to be promising thanks to their tunable chemical, physical, and optical properties. The complexity of GNPs systems can be partly attributed to the dynamic interactions with surface ligands and solvent. Recently, computational approaches have been proven to be a powerful method to provide important atomistic insights. Therefore, our objective is to use multi-level computational approaches in an attempt to understand the interaction of GNPs with various environments.

The interfacial interaction of water on a series of increasing-size GNP has been systematically probed with classical molecular dynamics [1]. Many-body effects have been shown to play an essential role in these interactions. Therefore, the GAL forcefield, i.e. a recently developed forcefield for water-metal surfaces interactions, has been recently implemented in the Tinker software to allow the coupling with the polarizable AMOEBA force field. The parameters have been extracted from DFT reference data. The structural properties of the first solvation shell have been investigated, and the re-arrangement of the water network to form an extended 2D hydrogen bond network has been observed as the size of GNP increases.

Furthermore, the adsorption of organic molecules on GNP has been systematically investigated at the DFT level [2]. Recently, a series of substituted aromatic compounds adsorbed on Au₃₂ has been studied. Topological analyses have subsequently been performed to identify the formation of multiple non-covalent interactions with varied strengths. The energy decomposition analyses were computed to find that the electrostatic and dispersive interactions were the main contributors to these non-covalent interactions [3]. Vibrational analyses have been also performed to investigate how the adsorption on GNP affects the IR spectroscopy of the organic compounds.

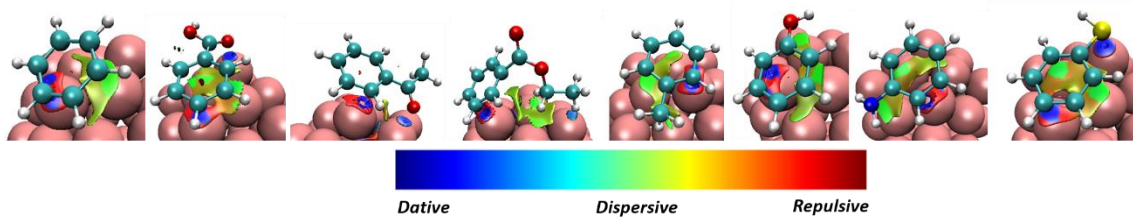


Figure – The Non-Covalent Interactions analysis on the complexes formed by Au₃₂ with benzene, benzoic acid, acetophenone, ethyl benzoate, toluene, phenol, aniline, and thiophenol [3].

[1] Rika Tandiana, Emilie Brun, Cécile Sicard-Roselli, Dominik Domin, Nguyen-Thi Van-Oanh, Carine Clavaguéra *J. Chem. Phys.* **154**:044706 (2021)

[2] Rika Tandiana, Nguyen-Thi Van-Oanh, Carine Clavaguéra *Theor. Chem. Acc.* **140**:118 (2021)

[3] Rika Tandiana, Cécile Sicard-Roselli, Nguyen-Thi Van-Oanh, Stephan Steinmann, Carine Clavaguéra *Phys. Chem. Chem. Phys.* **24**:25327 (2022)