

# Applied Surface Science

## Adsorption and coadsorption of single and multiple natural organic matter on Ag (111) surface: A DFT-D study

Nyangiwe, Nangamso N  
Council for Scientific and Industrial Research  
Pretoria, 0001, South Africa  
Email:

### Abstract

The nature of the interaction of low molecular weight natural organic matter (NOM) with the Ag (1 1 1) surface is of crucial importance in the environment. The low molecular weight organics used in this study are formic acid (FA), acetic acid (AA1) and ascorbic acid (AA2). In this study, we think of a realistic environment where single, multiple or even a mixture of NOM's can attach on one Ag (1 1 1) surface. Such critical information is relevant in order to understand the behaviour of engineered nanoparticles (ENPs) when they get into the environment. To bridge this gap, we investigate the adsorption and co-adsorption properties of NOM's on Ag (1 1 1) surface using dispersion-corrected density functional theory (DFT-D) in the gas phase and water as a solvent. Throughout this paper, the number behind the letter represents the number of molecules i.e. nFA, nAA1, nAA2 (n = 1, 2, 3, 4). The results of the calculated adsorption energy suggest that the interaction of 4FA, 2AA1 and 2AA2 molecules with Ag (1 1 1) surface is the strongest with the most negative values (-6.54 and -3.84 eV) in both gas phase and COSMO respectively which reveals that is the most stable system. The global reactivity descriptors in the gas phase and water as a solvent were calculated.