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Study on the interactions of Ag nanoparticles with low molecular weight organic matter using first principles calculations

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ABSTRACT:

Experimental studies on environmental processes such as aggregation, disaggregation, dissolution, surface transformation, and adsorption of engineered nanoparticles(ENPs) in the aquatic systems are reported to be influenced by their interactions with natural organic matter (NOMs) and ENPs inherent physicochemical properties. Herein, density functional theory (DFT), classical lattice dynamics (CLD), and quantum mechanical calculations based on frontier molecular orbital (FMO) theory were applied to elucidate the interactions of ENPs and NOMs. Results were derived for the adsorption energies of formic acid (CH_2O_2), acetic acid ($C_2H_4O_2$), and ascorbic acid ($C_6H_8O_6$) on silver (Ag) ENPs (111) surface – and its shapes, namely: spherical, cylindrical, and different tetrahedron positions (faces, vertices and edges) using the DFT and CLD. Results showed that the adsorption energies increased as the molecular weight of the adsorbate increased; thus $C_6H_8O_6$ had the highest adsorption energies for surface, spherical- and cylindrical-shaped Ag ENPs. At different positions of tetrahedron Ag ENP (111) surface, results indicated faces exhibited higher adsorption energies compared to the edges; hence, likely to be the most preferred adsorption sites. Overall, results derived from both *in silico* techniques suggest that Ag ENPs are likely to be easily adsorbed by NOMs with larger molecular mass. In addition, calculations using FMO theory showed a direct relationship with each of the four parameters viz.: the dipole moment (μ), molecular surface area (MSA), absolute electronegativity (χ), and absolute hardness (η) to the molar mass of the adsorbate. Hence, from our theoretical results: μ, MSA, χ, and η properties, and the adsorption energies are likely quantum mechanical descriptors of ENMs adsorption to NOMs in the aquatic systems.