Prediction of the toxicity of Ag Nanoparticles using Molecular Dynamics

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Over the past two decades nanoparticles have gained lots of interest in industries such as cosmetics, medicine, biological sensing and more. However, in a biological environment, these nanoparticles tend to interact with the surrounding media, resulting to be toxic. It has been shown that the toxicity is brought about by the physicochemical characteristics (such as size, shape, surface functionalization and more) of these nanoparticles. However there is no or little research done on the systematic way of predicting the toxicity of these nanoparticles looking at their physicochemical properties. This research look at the physicochemical properties of the Ag nanoparticles to predict their toxicity using molecular dynamics. The physicochemical properties studied here are size, shape and surface functionalization by introducing polyethylene glycol (PEG) surfactants on the surface. The study uses the computational modelling (Monte Carlo) calculations, which is a powerful tool to understanding the fundamental properties of nanoscale systems.