

Title: General linear model-predicted and observed toxicity of three organo-coated silver nanoparticles: Impacts of particle size, surface charge and dose

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ABSTRACT: Intrinsic to the myriad of nano-enabled products are atomic-size multifunctional engineered nanomaterials, which upon release contaminate the environments, raising considerable health and safety concerns. Despite global research efforts, mechanism underlying nanotoxicity has remained elusive. Here we consider three types of organo-coated silver nanoparticles (AgNPs): citrate-coated AgNP (Citrate-AgNP), polyvinylpyrrolidone-coated AgNP (PVP-AgNP), and branched polyethyleneimine-coated AgNP (BPEI-AgNP), with different surface charge scenarios and core particle sizes, and systematically evaluate the potential role of particle size, surface charge, and concentration on the toxicity of the three types of AgNPs against two model organisms, *Escherichia coli* and *Daphnia magna*. We found particle size, surface charge, and concentration dependent toxicity of all the three types of AgNPs against both the test organisms. Notably, Ag⁺ (as added AgNO₃) toxicity was greater than each type of AgNPs tested and the toxicity followed the trend: AgNO₃ > BPEI-AgNP > Citrate-AgNP > PVP-AgNP. Modeling AgNP physicochemical properties using the General linear model (GLM), a significant interaction effect of primary particle size and surface charge emerged that explained empirically-derived acute toxicity with great precision. The model explained 99.9 % variation of toxicity in *E. coli* and 99.8% variation of toxicity in *D. magna*, revealing satisfactory predictability of the models to predict nanotoxicity of the three organo-coated AgNPs. We anticipate that the use of GLM to satisfactorily predict nanotoxicity based on NP physicochemical characteristics could contribute to our understanding of nanotoxicology, and suggest considering interaction effects among nanoparticle properties when explaining nanotoxicity.