Guest Articles

Chitosan-Stabilized Silver Nanoparticles: Molecular Dynamics Simulation on the Stability and *In-Vivo* Interactive Toxicity with Cadmium on an Aquatic Model *Moina macrocopa*

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The rapid rise of nanotechnology has resulted in minute particles, yet powerful such as silver nanoparticles (AgNPs) into countless products, from medical devices to household goods. These metallic specks, celebrated for their potent antimicrobial and catalytic traits, are driving innovation. Yet, as they move from the lab to market, a critical question remains: What happens when these engineered materials enter to environment, especially when they encounter other common pollutants. Recent studies suggest that AgNPs can undergo physicochemical transformations in the presence of other pollutants, such as heavy metals, altering their behavior and toxicity. Cadmium (Cd), a well-known toxic heavy metal, is frequently found in industrial effluents and can co-exist with AgNPs in aquatic habitats. The interaction between these two contaminants can result in synergistic or additive toxic effects, which remain poorly understood. Addressing this knowledge gap requires a multidisciplinary approach that combines material science, computational chemistry, and environmental toxicology.

A major hurdle for using nanoparticles is their inastability?? In water, unprotected AgNPs tend to clump together, which can drastically change their properties and environmental behavior. Our research sought a sustainable solution to address this issue. Chitosan, a natural, renewable polymer derived from crustacean shells. AgNPs were successfully synthesized via a simple, heated reaction. During AgNP synthesis, chitosan plays a dual role: it acts as a green chemical reductant, converting silver ions (Ag^{+}) into metallic silver (Ag^{0}), and, most importantly, as a stabilizing cap to synthesized AgNPs. Chitosan polymer, rich in amine and hydroxyl groups, wraps tightly around the silver, creating a robust shield that prevents the particles from collapsing.

Analytical tests confirmed the formation of the metallic core and secured the presence of the chitosan coating, revealing uniformly dispersed, stable nanospheres. In order to truly validate the effectiveness of the chitosan shield, we moved beyond the physical laboratory into the realm of computational chemistry. This is where Molecular Dynamics (MD) simulations provided atomic-level insights into the system's stability.

To model this accurately the CHARMM force field (Chemistry at Harvard Macromolecular Mechanics) was used with the GROMACS software. A force field is essentially the mathematical blueprint used to calculate the energy and forces acting on every atom in the simulation, allowing us to predict their movement over time. In the CHARMM model, the total energy of the system is the sum of bonded interactions (like the spring-like forces holding the chitosan molecule together) and non-bonded interactions (like the attractions and repulsions between different molecules). The non-bonded terms, which include van der Waals forces and electrostatic forces (based on atomic charges), are critical for modeling the securing interaction between the chitosan and the silver surface.

The MD simulations, powered by this precise force field, confirmed that the CS-AgNPs remained structurally sound and highly stable over the entire simulation period. This demonstrated that the non-covalent, hydrogen-bonding forces exerted by the chitosan are highly effective in maintaining the nanoparticle's integrity in an aqueous setting, reinforcing the synthesis success computationally.

The final, and most crucial, step was to test the environmental impact of AgNPs when released to water bodies. *Moina macrocopa*, a common freshwater crustacean was chosen as the model organism for *in-vivo* toxicity assessment. The individual effects of CS-AgNPs and heavy metal toxin Cadmium (Cd), and their combined presence on *Moina macrocopa* were assessed.

As anticipated, CS-AgNPs exhibited only mild toxicity to *Moina macrocopa*, suggesting the protective polymer coating was effective. Cadmium, a well-known pollutant, caused significant harm even at low concentrations. However, the results from the combined exposure were alarming: the toxicity was synergistic. The organisms suffered a far steeper decline in survival, growth, and reproduction when exposed to both contaminants than would be expected from simply adding their individual effects. This synergistic effect suggests that the chitosan, while stabilizing the silver core, might also be complexing with the cadmium ions. This new interaction could potentially enhance the uptake of the highly toxic metal species by the *Moina macrocopa*, highlighting a hidden hazard in complex aquatic systems.

This research stands as a powerful demonstration of the need to merge experimental chemistry with advanced computational prediction. We have successfully proven that chitosan is an excellent green stabilizer for silver nanoparticles. However, the discovery of enhanced toxicity in the presence of cadmium serves as a vital environmental warning.

Moving forward, the development of nanotechnology must be guided by this holistic approach. We must evaluate nanomaterials not in isolated, pristine laboratory conditions, but under environmentally realistic scenario where interactions with co-existing pollutants like heavy metals are the norm. This work provides a robust framework, accelerating the rational design of future materials that balance high performance with necessary environmental safety.

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