Polymer-Coated TiO_2 Nanoparticles: Mechanistic Insights into Antimicrobial Activity via Particle–Membrane Interactions

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Surface modification is a widely employed strategy to enhance the antimicrobial performance of photocatalytic nanoparticles (NPs); however, the underlying particle–membrane interactions remain insufficiently understood. In this work, we investigate how coating TiO_2 nanoparticles with the cationic polymer PDMAEMA (poly((2-dimethylamino)ethyl methacrylate) methyl chloride quaternary salt) influences their interactions with bacterial membranes.

Compared to bare TiO_2, PDMAEMA-coated nanoparticles exhibit significantly enhanced adsorption to negatively charged bacterial cells and model membranes. Upon UV illumination, this increased association leads to enhanced membrane permeabilization driven by reactive oxygen species (ROS) generation. Importantly, the polymer coating does not hinder ROS production and remains stable under UV exposure over timescales relevant for membrane binding and disruption.

The observed membrane damage is highly localized near nanoparticle binding sites. Notably, coated nanoparticles show preferential accumulation at poles and division sites of *Escherichia coli* . We hypothesize that this localization is driven by interactions with anionic lipid domains, particularly cardiolipin. This hypothesis is supported by experiments on giant unilamellar vesicles, where nanoparticles preferentially bind to cardiolipin-rich regions, whether uniformly distributed or phase-separated.

These findings demonstrate that antimicrobial activity of photocatalytic nanoparticles is governed not only by bulk ROS generation but also by localized nanoparticle–membrane interactions. Our results highlight the importance of spatial heterogeneity in bacterial membranes and provide new insights for the rational design of nanoparticle-based antimicrobial systems.

Keywords:
Antimicrobial nanoparticles, cationic modification, lipid membrane, reactive oxygen species, membrane permeation, mechanism

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