Journal of Nanomaterials

Special Issue on

Multiscale Modeling in Design of Nanoparticles for Targeted Drug Delivery

CALL FOR PAPERS

Freely administrated drug molecules cannot be efficiently delivered to diseased cells to treat physiological disorders due to sequestration in the reticuloendothelial system, cellular uptake by immune cells, and degradation by protein adsorption. The accumulation of these freely administered drug molecules in tumors is usually at levels ≤0.1% of the injected dose per gram tissue (% ID/g). However, when these molecules are encapsulated into liposomes, the peak drug accumulation can be increased by one to two orders of magnitude. To date, several classes of nanoparticles (NPs) (e.g., polymeric and metal nanoparticles, liposomes, micelles, quantum dots, and dendrimers) have demonstrated promising properties as therapeutic carriers. By loading the drug molecules into these NPs, their pharmacokinetics, toxicity, and biodistribution can be significantly improved, compared with their freely administered counterparts. They have been shown to efficiently deliver drug molecules into diseased cells to treat numerous physiological disorders. In the design of efficient therapeutic carriers for targeted drug delivery, the size, shape, stiffness (material composition), and surface properties of NPs have been identified as the most important design factors. However, simultaneously optimizing these factors in design of efficient NP-based drug carriers is a forbidden challenge for experiments, as it is very time consuming and cost-inefficient. To overcome this challenge, multiscale modeling is a promising way to accelerate the design process. Through the multiscale and multiphysics computational modeling, the detailed physical mechanisms behind the NP-mediated drug delivery process will be well-understood. In the meantime, by elucidating the different roles played by the size, shape, stiffness (material composition), and surface properties of NPs, design paradigms will be immediately available.

This journal is a peer-reviewed, open access journal that aims to bring science and applications together on nanoscale and nanostructured materials with emphasis on synthesis, processing, characterization, and applications of materials containing true nanosize dimensions or nanostructures that enable novel/enhanced properties or functions. It is directed at both academic researchers and practicing engineers. It will highlight the continued growth and new challenges in nanomaterials science, engineering, and nanotechnology, both for application development and for basic research. We invite researchers to submit their original research papers and review articles to this special issue on multiscale and multiphysics modeling of nanoparticle-mediated drug delivery. Both theoretical and computational studies on the roles of nanomaterials in drug delivery and their effects on biostability and cytotoxicity are within the scope of this special issue.

Potential topics include, but are not limited to:

- Self-assembly of nanoparticles under different environments (e.g., pH, light, and solvent quality)
- Interaction between the nanoparticles and drug molecules (e.g., doxorubicin hydrochloride (DOX), and ibuprofen)
- Microcirculation of nanoparticles within blood flow, interacting with red blood cell, white blood cell, and platelets
- Diffusion of nanoparticles within tumor tissue
- Endocytosis of nanoparticles by diseased cells and related uptake mechanisms
- Physics and chemistry of biological membranes
- Toxicity of different nanomaterials (e.g., polymeric and metal nanoparticles, liposomes, micelles, quantum dots, and dendrimers)

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