COMPUTER DESIGN OF NANOMATERIALS

Centre for Natural Sciences and Technologies

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RESEARCH/TECHNOLOGY INTRODUCTION

Within the given research topic we deal with computer modeling of complex molecular systems. In particular, we focus on:
- **computer modeling of potential drug carriers at the molecular level**, especially for gene therapies. In particular, we focus in polymeric hyperbranched molecules called dendrimers. In cooperation with domestic and international workplaces, dealing with the synthesis and experimental research of dendrimers for medical purposes, we participate in research into the use of these molecules also for other medical applications (antiviral drugs, bactericides). In addition to modeling the dendrimers or dendrons themselves, we typically simulate (with respect to a given application) various molecular complexes (usually in an aqueous environment) containing, in addition to dendrimer molecules, e.g. oligonucleotides or other molecules transported into cells, proteins or lipid bilayers or liposomes. These complexes are then analyzed in terms of their spatial arrangement, possibly in terms of their stability or dynamics of interaction processes.
- **molecular modeling of chemically modified polymer surfaces in the context of development of antimicrobial filter media** based on polymer nanofiber textile, modified with an antimicrobial substance. Based on model calculations, it is possible, for example, to determine the interaction energy between a polymeric nanofiber and an antimicrobial additive, or to determine (at a given concentration) the distribution of antimicrobial ligands on the nanofiber surface in air, water or other environments. This information can be used to find the optimal polymer / additive combination for a given application.

Of course, we are able to model and analyze other molecular systems as well at this level and possibly provide other available characteristics (e.g. transport characteristics).

POTENTIAL USERS

We welcome cooperation with any company or research organization from the pharmaceutical industry or research, or from the production and development of surface-modified nanofiber materials, but also from other areas of nanomaterial design.

ADVANCEMENT OF TECHNOLOGY AND MARKET APPLICATION

Molecular simulations **enable the study of molecular systems at the atomistic level** and thus provide detailed information about the behavior and properties of the studied systems under given conditions. This approach thus suitably complements or it even partially replaces experimental techniques. The great advantage of this approach, where the real experiments are replaced by the realistic computer experiments, are also low economic and time requirements, which here also significantly increases the potential for streamlining development and research not only in the areas specified above.

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ADDITIONAL INFORMATION

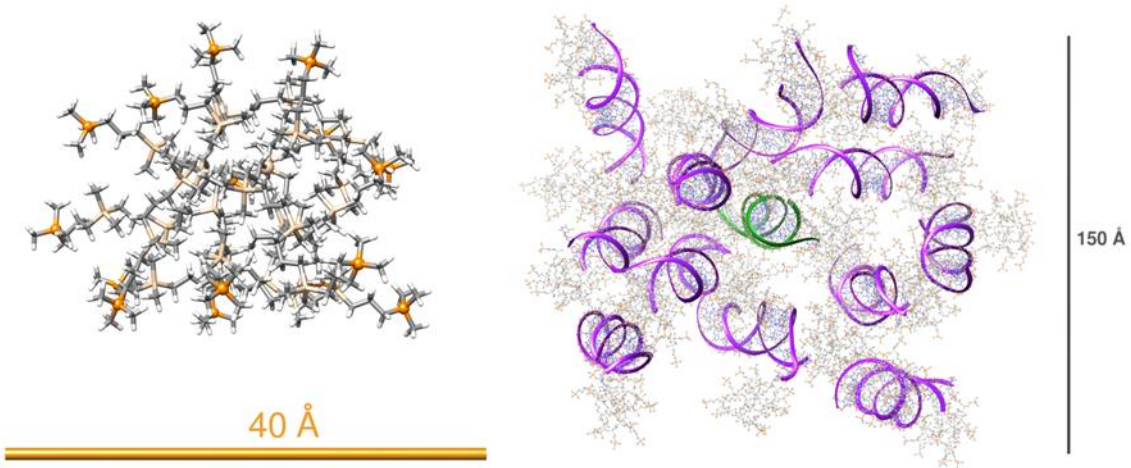

Figure 1: Computer model of the cationic carbosilane dendrimer (3rd generation) with phosphonium (PMe3) end groups (left) and a simulated dendriplex consisting of 36 of these dendrimers and 13 siRNA molecules (right). In both cases, the simulations were done in aqueous environment.

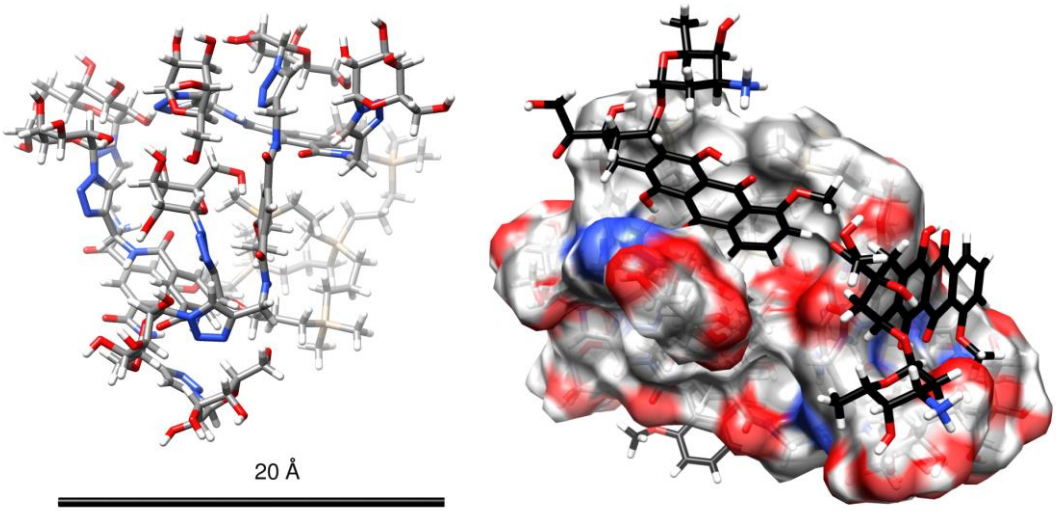

Figure 2: Computer model of a carbosilane dendrimer (1st generation) with galctose end groups (left) and the simulated complex of this dendrimer and 3 molecules of doxorubicin (right). In both cases, simulations were done in an aqueous environment.

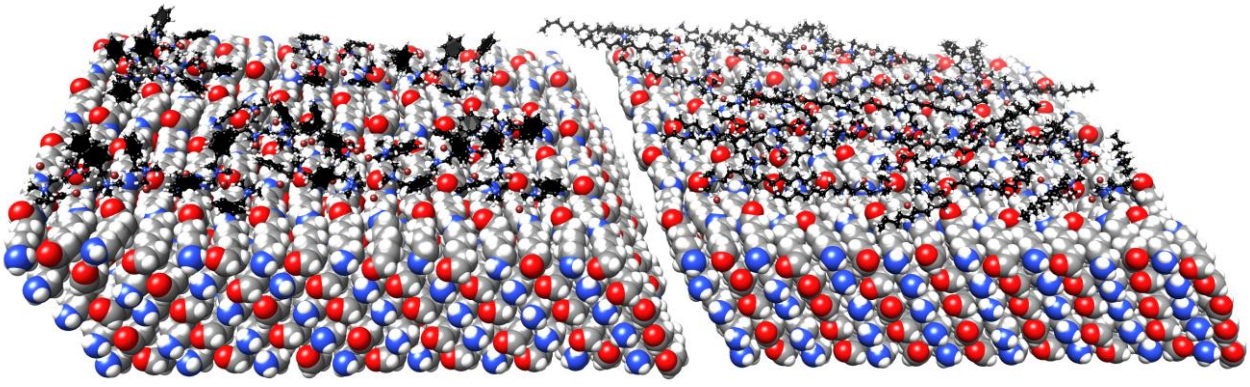

Figure 3: Modeled surface of nylon nanofiber with antibacterial surface modification (benzyltrimethylammonium bromide - left, 1-dodecyltrimethylammonium bromide - right).