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Optimizing polyethylene glycol coating for stealth and biocompatible nanodiamonds

Nanodiamonds (NDs) have emerged as potential candidates for versatile platforms in nanomedicine, offering unique properties that enhance their utility in drug delivery, imaging, and therapeutic applications. To improve their biocompatibility and nanomedical applicability, NDs are coated with organic polymer chains, such as polyethylene glycol (PEG), which are well known to prolong their blood circulating lifetime by reducing the surface adsorption of serum proteins. Theoretical simulations are useful tools to define, at the atomic level, the optimal parameters that guide the presentation of the coating chains in the biological environment and the interaction of the coated NDs with proteins. In this work [1], we perform atomistic molecular dynamics (MD) simulations of several PEGylated spherical ND models, immersed in a realistic physiological medium. In particular, we evaluate the effect of the polymer chains terminal group, length, grafting density and of the ND core dimension on both the structural properties of the PEG coating and on the interaction of the nanoconjugates with the aqueous phase. Among all the parameters evaluated, we find that the PEG grafting density and the PEG chain length are key factors in determining the dynamic behavior of PEGylated nanosystems in solution, whereas the PEG terminal group and the ND dimension only play a marginal role. These factors can be strategically adjusted to identify the optimal conditions for enhanced clinical performance. Finally, we demonstrate the function of the PEG coating in preventing the aggregation of two ND particles. We believe that this computational study will provide valuable insights to the experimental community, supporting the rational design of polymer-coated inorganic NPs for more efficient nanomedical applications.

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