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Molecular insight to biocompatibility of carbon-based nanomaterials

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Biomaterials are widely used for manufacturing implants. One of the most common reasons for implant failure is its immune rejection. Changes in the conformation of blood proteins (e.g., fibrinogen) due to their binding to nonbiological surfaces are the initial step in a chain of immunological reactions to foreign bodies. Despite the large number of experimental studies that have been performed on fibrinogen adsorption to nonbiological surfaces, a clear picture describing this complex process has eluded researchers to date. Here we focus on modeling the interaction between carbon-based nanomaterials and fibrinogen at the microscopic level by taking into account the physico-chemical properties of the surfaces with the use of empirical force field potential within molecular dynamic (MD) simulations. Carbon-based materials are chosen as a model system for this study due to an increasing interest in their bio-medical applications and the possibility of functionalization (e.g., graphene oxide). The accuracy of the force field was verified by comparing the adsorption energies of individual amino acids on graphene surface with *ab initio* calculations. All-atom MD simulations of the adsorption of a fibrinogen fragment onto a graphene surface reveal significant conformational changes on immune-reactive sites. In contrast, the interaction with polyethylene glycol (PEG) does not induce structural rearrangements in fibrinogen, which is consistent with the bio-inert nature of PEG

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