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Binding nature of fibrin molecules on to Au92 and Ag92 nanoparticles

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Density functional theory, and molecular dynamics simulations were used to study the nature of binding on Au- and Ag-nanoparticles and 1, 2, and 3-fibrin molecules. In the process, the negative adsorption energies acquired suggest that the fibrin molecules + Au-/Ag-nanoparticles reaction process is exothermic and energetically stable. Moreover, radial distribution functions and radius of gyration were utilised to explore the binding distance between the fibrin molecules functional groups atoms and Au-/Ag-nanoparticles surface atoms. To probe the mobility of the atoms in the fibrin-nanoparticle complexes, the mean square displacements graphs were plotted. Such plots together with the extracted diffusion constants suggest that H, C, N and O from the fibrin molecules functional groups, may diffuse easily into Au- and Ag-nanoparticles. Qualitatively, the H, C, N, and C atoms diffuse more readily in the Ag-nanoparticles compared to Au-nanoparticles.

Apply to be considered for a student ; award (Yes / No)?

YES

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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