سمینارهفتگی ماده چگال نرم

عنوان سمینار

Interactions of Azurin with Nanosheets for Medical Applications

ارائه دهنده

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چکیده

Azurin as an electron transfer protein plays an important role in the biological process such as killing the cancerous cells. In the present study, the molecular dynamics techniques are exploited to investigate the interaction and immobilization of Azurin on the surface of nanosheets such as graphene monoxide, silicon carbide and boron nitride at 310 K. To analyse the simulation results, structural parameters such as root mean square fluctuation (RMSF), root mean square deviation (RMSD), radius of gyration (R_g), the distance between the centre of the mass of immobilized protein and the surface of the considered nanosheets and surface accessible solvent area (SASA) were measured. Additionally, the interaction energy of the protein on the surface of the nanosheets by considering structural and energetic parameters of the protein and nanosheets such as residue polarity, charge density, hydrophilicity and hydrophobicity were investigated. The simulation results demonstrate that Azurin adsorbed and immobilized on the targeted surfaces with the kept of its native state. As well as our results exhibit that the stabilization of the azurin with native structure represents its protection against stomach acids and, therefore, it reveals a promising potential to be used in smart delivery and release application in medicine and cancer therapy.

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