Au- and Ag-Nanoparticles Interaction with Fibrin Protein Molecules

Malesela Walter Makgoba, Thuto Mosuang, Abram Mahladisa, Malili Matshaba, Lucky Sikhwivhilu and Teboho Mokhena

EasyChair preprints are intended for rapid dissemination of research results and are integrated with the rest of EasyChair.

August 21, 2023
Au- AND Ag-NANOPARTICLES INTERACTION WITH FIBRIN PROTEIN MOLECULES

MW Makgoba1*, TE Mosuанг1, MA Mahladisa1, M Matshaba1, LM Sikhwivhilu2, T Mokhena2

1*Department of Physics, University of Limpopo, South Africa, makgoba.walter@gmail.com
2DSI/Mintek Nanotechnology Innovation Centre, Advanced Materials Division, Mintek, South Africa.

ABSTRACT

The interaction of Au- and Ag-nanoparticles with fibrin molecules have been investigated using Monte Carlo, density functional theory and molecular dynamic simulations. The negative adsorption energies are recorded whenever fibrin molecules get adsorbed onto either Au- or Ag-nanoparticles. The binding distance between the terminal functional group atoms and either Au or Ag nanoparticles were estimated using the radial distribution functions. The mean square displacement and diffusion constants were also used to probe the possibility of O, H, N, and C atoms diffusion into the Au- and Ag-nanoparticles matrices.

*Corresponding author

INTRODUCTION

When some nanoparticles infiltrate physiological fluids, certain proteins get adsorbed onto the nanoparticles surfaces leading to the formation of the nanoparticle-protein coronas [1, 2]. In the process, the free energy of the entire nanoparticle-protein corona is reduced [3]. Thermodynamically, this is expressed as \( \Delta_{\text{ads}} G < 0 \) where \( \Delta_{\text{ads}} G \) is the net change of the Gibbs free energy by binding; the change is negative indicating that the adsorption process occurs spontaneously [3]. In this article; 19, 38, 55, 79 atoms aggregates of Au- and Ag-nanoparticles interaction with 1, 2, 3, and 4-fibrin protein molecules respectively were modelled according to the methods explained in the following section.

METHODS

- Monte Carlo (MC) approach was utilised for the adsorption of fibrin molecules onto Au and Ag nanoparticles using the Universal Force Field (UFF) along with fine convergence tolerance test.
- DFT procedure which uses the generalised gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) exchange correlation energy functional was applied for geometry optimisations.
- MD simulations were also performed to achieve total energies of the nanoparticle-protein corona systems. The NVT ensemble at room temperature (298 K) with a time step of 1.0 fs and a total dynamic time of 100 ps was maintained.

RESULTS

The total energy of the nanoparticle-protein corona system decreases with the increasing number of the fibrin helix chains. The negative adsorption energies suggest possible and stable nanoparticle-protein corona formation. The RDFs suggest Au-H and Ag-H interactions having shortest binding distances. Such can be interpreted on the hydrogen bonds as the most favourable binding with the Au- and Ag-nanoparticles. The mean square displacement graphs suggests that upon adsorption, all the atoms of the fibrin molecules may diffuse easily into the Au- and Ag-nanoparticles. Diffusion suggest possible disintegration of the corona upon reaching required destination.

CONCLUSION

REFERENCES