Journal of Material Science and Mechanical Engineering (JMSME)
p-ISSN: 2393-9095; e-ISSN: 2393-9109; Volume 4, Issue 1; January-March, 2017 pp. 14-16

http://www.krishisanskriti.org/Publication.html

Understanding The Adsorption of Zein on the Surface of Gold Nanoparticles using Molecular Dynamics Simulation

Lovika Moudgil[1], Baljinder Singh[2] and Aman Kaura, Gurinder Singh[3]

[1,2]Department of Physics, Centre of Advanced Study in Physics, Panjab University, Chandigarh
[3]Department of UIET, Panjab University SSG Regional Centre Hoshiarpur, Panjab
E-mail: [1]lovikamoudgil@gmail.com, [2]baljinder.vehniwal@gmail.com

Abstract—*Protein amongst the most abundant organic molecules in living systemhaving diverse structure and various functions than the other classes of macromolecules. We have done Molecular Dynamics (MD) simulation of zein protein , one of the best understood protein in the presence of gold naoparticles (AuNPs). MD results helps us to recognize the amino acids that play chief role to make the interaction possible between protein and Au surface. We discussed about the nature and the surface adsorption of zein in the presence of AuNPs. Reults are further analyzed to understand the protein interaction up to molecular level.*

1. INTRODUCTION

A single cell can contain thousand of protein each with a unique function. Proteins that originate from plant or animal can be produced or processed on an industrial scale for applications in food. Technologies that are involved in separation and sources to these proteins need to give specific attention or alternative sources to develop the research of new proteins and methods to isolate proteins. Proteins have many functions in food applications like techno-functional properties [1] and bio-functional properties. Chemical character of a protein decides the functionality of protein which can also be changed by modification methods. This further gives us new and innovative applications of proteins to increase their applicability. The most important thing to understand is the chemical character and functional behavior of a protein. These factors will additionally help us to understand the possible applications of protein in a particular field. Research in these days is helping us to study these proteins and to apply them on industrial and academic level. In food industry Corn is the largest and most important agricultural commodity and zein one of the component of corn, has long been investigated for use other than food and feed. Zein is a unique and complex material and it is one of the few cereal proteins extracted in a relatively pure from. Zein is an industrial protein well-known for its vast application in food and pharmaceutical industries [2-3] with highly hydrophobic nature and robust structure [4]. Here we investigate the theoretical aspect of zein in the presence of AuNPs to analyze its behavior and to understand its adsorption on AuNPs surface which have very important aspect in biotechnology [5] and biomaterial [6] synthesis. MD simulation helps us to understand this on microscopic level.

2. COMPUTIONAL DETAILS

MD simulation is performed using the GROMACS (GROningen Machine for Chemical Simulation) program (version 4.6.5) and the OPLS-AA (Optimized Potentials for Liquid Simulations) force field was used to describe the system in periodic boundary conditions. For the interactions of protein with gold, we choose a limited number of amino acid residues for zein to explain the interaction. As a linear chain of amino acid residues called polypeptide. For most of the complex proteins it is preferred to consider the polypeptide or peptide chain rather than the whole protein. So we have chosen a peptide cahin (MET-ALA-ALA-LYS-ILE-PHE-LYS-LEU-ILE-MET-LEU-LEU-GLU) for zein. A conventional molecular dynamic simulation of 5.0ns at temperature 310K was employed for zein and gold slab. Before MD simulation the system was solvated in explicit SPC water (simple point charge). Periodic image separation in the system was about 1.2nm so that there is no interaction via van der waals potentials. A tolerance of 1000KJ/mol was achieved by system through step by step steepest descent interaction via van der waals potential. A tolerance of 1000KJ/mol is achieved by system through step by step steepest descent energy minimization. An NVT (constant number of atoms, volume and temperature) simulation is performed to bring the system to the target temperature, followed by an NPT (constant number of atoms, pressure and temperature) simulation to allow the system to find the correct density. For temperature coupling Nose-Hoover thermostat is used to have correct ensemble of kinetic energies than other methods. The electrostatic interactions are calculated by using the particle-Mesh-Ewald(PME) algorithm. A time step of 1 fs

is used to study the interaction of protein and gold surface. LINCS (Linear Constraint Soiver) algorithm is used to constrain the length of bonds.

3. RESULTS AND DISCUSSION

MD study is appropriate to pinpoint certain amino acid residues which extract the results to understand the nature of complex and the interaction between zein-gold surface (Fig. 1). The total energy versus time graph at 310K for Zein-Gold surface indicates the overall stability of system (Fig. 2).

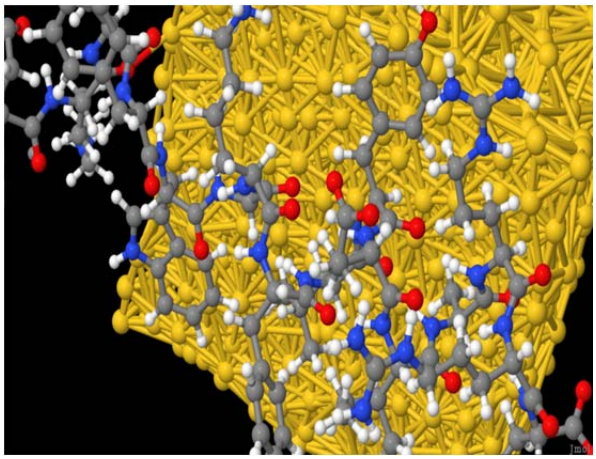

Fig. 1: Zein protein in the presence of Au slab.

Zein mainly interacts through –OH and –NH_2 groups of SER and GLN amino acids through hydrogen bond. These residues have polar uncharged side chains respectively. Other residues MET and LEU having hydrophobic side chain and lie next to SER. These hydrophobic domains of zein derive the non polar interactions between zein surface.

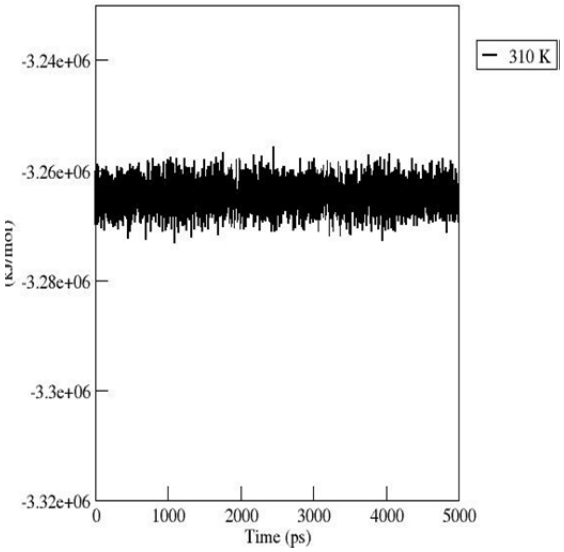

Fig. 2: The total energy versus time graph at 310K for zein-gold surface system.

Hence zein is dominated by hydrophobic nature. Fig. 3 represent hydrophilic and hydrophobic surface of protein. As electrostatic interactions play very important role to understand interactions, (Fig. 4) represent the electrostatic potential map around zein.

Blue region have positive, red region have negative and white region have neutral charges on the surface of protein. As SER is included in the part of one of three polar surfaces on the helical wheel of zein. SER have nonpolar side chain which makes it to have high empathy for hydrogen bonding which dominates and helps the zein to interact with gold suface. Such ruling nature of zein i.e. nonpolar, is bringing out by SER residue giving it significant surface adsorption.

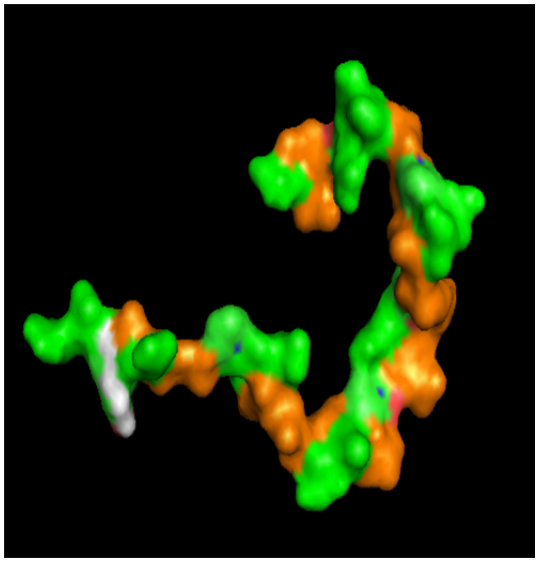

Fig. 3: Zein protein showing hydrophilic (green) and hydrophobic (orange) regions.

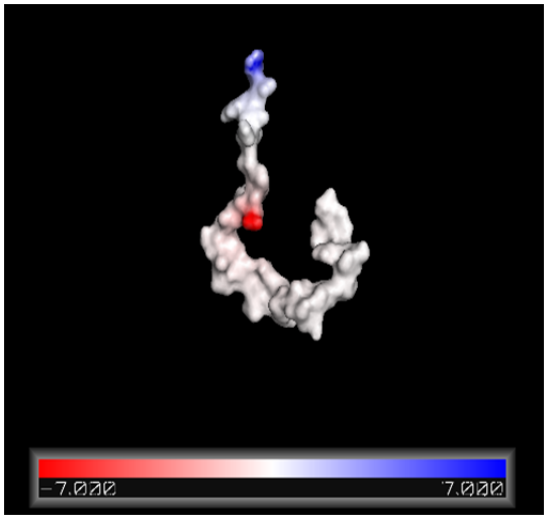

FIG. 4: The electrostatic surface potential on the solvent accessible surface of zein.

4. CONCLUSION

Results from the molecular dynamic simulation of the interaction of protein with gold slab shows that the interaction between them is triggered by the residues like GLN and SER through hydrogen bonding. As in zein we have polar uncharged side chains so non polar interactions play a predominant role. Such nonpolar nature of zein driven by SER residue allows its significant adsorption on the Au surface.

REFERENCES

[1] Schmitt, C., Sanchez, C.,Desobry-Banon, S.,Hardy, J, "Suctural and technofunctional properties of protein-polysaccharide complex: A review", *Food Science and Nutrition*,38 (8), 1998, pp. 689-753.

[2] Alkan, D., Aydemir, L. Y., Arcan, I., Yavuzdurmaz, H., Atabay, H. I., Celyan, C., Yemenicioglu, A., "Development of flexible antimicrobal packaging materials against campylobacter jejuni by incorporation of gallic acid into zein-based films", *J.Agri.Food Chem.*, 59,2011, pp. 11003-11010.

[3] Bakshi, M. S., Kaur, H., Khullar, P., Banipal T. S., Kaur, G., "Protein films of bovine serum albumen conjugated gold nanoparticles: A synthetic route from bioconjugated nanoparticles to biodegradable protein films", *J. Phys. Chem. C.*, 115, 2011, pp. 2982-2992.

[4] Mahal, A., Khullar, P., Kumar, H., Kaur, G., Singh, N., Jelokhani-Niaraki, M., Bakshi, M. S "Green chemistry of zein protein toward the synthesis of bioconjugated nanoparticles:understanding unfolding, fusogenic behaviour and hemolysis", *ACS Sustainable Chem. Eng.*, 1, 2013, pp. 627-639.

[5] Zhdanov, V. P.; Kasemo, B., "Bistability in catalyic reactions on nm scale", *Surf. Sci.*,496, 2002, pp. 251-263.

[6] Ratner, B. D.; Bryant, S. J., "Where we have been and where we are going", *Annu. Rev. Biomed. Eng*, 6, 2004, pp. 41-75

[7] Goshisht, M. K., Moudgil, L., Rani, M., Khullar, P., Singh, G., Kumar, H., Singh, N., Kaur, G., and Bakshi, M. S., "Lysozyme Complexes for the Synthesis of Functionalized Biomaterials To Understand Protein–Protein Interactions and Their Biological Applications", *J Phys. Chem. C*, 118, 48, November 2014, pp. 28207-28219.