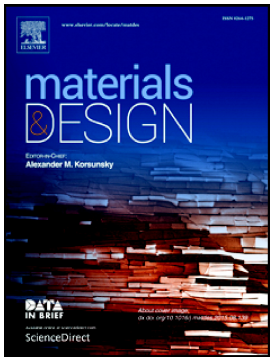

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Amino Acid Functionalized Zinc oxide Nanostructures for Cytotoxicity Effect and Hemolytic Behavior: Theoretical and Experimental Studies

Satvinder Singh[$,a], Baljinder Singh [$,a], Prateek Sharma[b], Anu Mittal[c], Sanjeev Kumar[b], G.S.S. Saini[a], S.K. Tripathi[a], Gurinder Singh[d] and Aman Kaura[d,*]

[a]*Department of Physics, Centre of Advanced Study in Physics, Panjab University, Chandigarh, 160014, India*
[b]*Centre for Biosciences, Central University of Punjab, Bathinda, 151001, India*
[c]*Department of Chemistry, Guru Nanak Dev University College, Chungh, Distt. Tarntaran*
[d]*Department of UIET, Panjab University SSG Regional Centre Hoshiarpur, Panjab, 146001, India*
** Corresponding author, Tel.: +91-9501911977, Fax: +91-1882-282221*
***Electronic mail:** amankaura1979@gmail.com; aman_kaura@yahoo.co.in
[$] First two authors have equal contribution

Abstract

Blending of theoretical and experimental approach, provide an important strategy in designing the nanostructure at a microscopic level and helps in predicting the response of synthesized material towards inhibition of the growth of breast cancer cell. In this work, ab initio calculations using super cell approach are performed for three different amino acids (AAs)- Histidine (His), Arginine (Arg) and Aspartic acid (Asp) coated Zinc oxide (ZnO) nanostructures to explain the growth mechanism of nanoparticles (NPs) of different shapes. Based on the first principles calculations, we reveal that ZnO-AA (Arg and Asp) NPs results in rod like and ZnO-His NPs lead to tablet like configuration. Similar morphologies are fabricated using AAs through synthetic route. The effect of concentration ratio of reactants and pH has been studied. As synthesized samples, are characterized by using Transmission Electron Microscopy (TEM), X-ray diffraction (XRD), Fourier Transform Infrared (FTIR) and UV-Vis spectroscopy techniques. Based on the results, a plausible mechanism of formation of nanostructures has been proposed. The nanostructures with rod like morphology are found to be biocompatible with normal red blood cells and show cytotoxic effect as evaluated from hemolysis and cytotoxicity assays on breast (MCF-7, T47D, MDA-MB-231) & prostate cancer (PC-3) cell lines.

Keywords: Zinc Oxide nanoparticles; Binding energy; Cytotoxicity; Hemolysis; Partial Density of States