Biological solid waste mediated synthesis of silver nanoparticles for removal of anthropogenic pollutant: Optimization modelling by response surface methodology (RSM), artificial neural network (ANN) and DFT studies

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Green synthesis has gained worldwide attention among researchers as a sustainable, affordable and eco-friendly process for fabrication of various materials and nanomaterials. The traditional methods of nanoparticle synthesis are costly, toxic, and harmful to the environment. The green approach of synthesis facilitates the overcome of the destructive effects of these methods (Khan and Al-Thabaiti, 2019). Utilization of waste fruit peel has been done in this study for the successful synthesis of silver nanoparticles (AgNPs) via a low-cost and single-step process. *Citrus limetta* peels extract was used as a reducing, capping, and stabilizing agent. The biobased AgNPs possessed high stability in an aqueous colloidal solution. Central composite design (CCD) of response surface methodology (RSM) was applied to optimize the process conditions of AgNPs synthesis. It helps to reduce the number of experiments. Three empirical factors of synthesis, including temperature, the concentration of $AgNO_3$ solution and time of reaction, were used as independent variables of the model at five different levels (−α, −1, 0, +1, and +α) and the dependent variable is the peak intensity of localized surface plasmon resonance (LSPR). The UV-Visible spectroscopy showed characteristic for synthesized AgNPs show absorption maxima in the wavelength ranging from 430nm to 470nm (Fig. 1). The response variable was found to be significant for the process parameters analyzed from response surface methodology. The quadratic model was significant with a p-value < 0.05 and R^2 value 0.9365. Furthermore, the mathematical modeling of optimization was done using an artificial neural network (ANN) to determine the capabilities of prediction of the response for greater accuracy (Rao and Paria, 2015). The physico-chemical characterization of the prepared AgNPs was conducted by Fourier transform infrared spectroscopy (FTIR), powder x-ray diffraction (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive x-ray spectroscopy (EDX), dynamic light scattering (DLS), and zeta potential. The FTIR analysis showed that AgNPs were capped by various biological molecules. Phytochemical screening was also performed to confirm the presence of flavonoids, alkaloids, terpenoids, proteins, and reducing sugars. SEM and TEM images of the formed AgNPs confirm the spherical shape of the nanoparticles. XRD pattern reveals significant diffraction peak at 38.01°, 44.22°, 64.45°, 77.42° and 81.51° attributing to (111) (200) (220) (311) and (222) planes of FCC crystal structure of polycrystalline silver. The size of nanoparticles was found to be approx. 60 nm diameter. The AgNPs obtained from the optimization process were analyzed for its ability of degradation of para-nitrophenol. DFT studies revealed that the compounds gallic acid, limonene, ferulic acid, *p*-coumaric acid and linalool present in the *C. limetta* peels extract demonstrated great reducing and stabilizing properties for the fabrication of AgNPs.

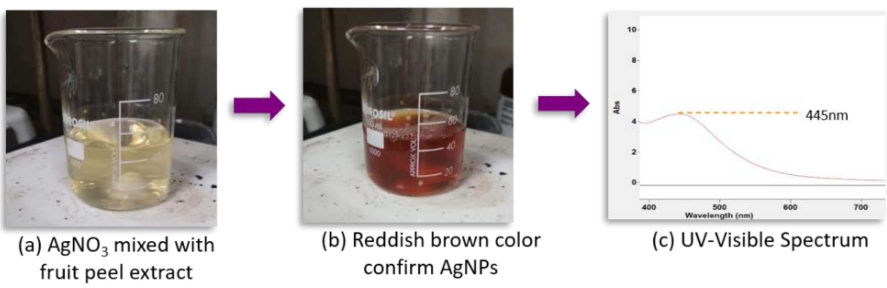

Fig. 1: Green synthesis of AgNPs mediated by fruit peel extract. (a) orange peel extract is mixed with $AgNO_3$ salt solution to obtain the biobased silver nanoparticles. b) The change in color of the solution to reddish brown confirms the synthesis of silver nanoparticles c) also confirmed by UV spectroscopy).

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