CHAPTER III

Abstract

SERS of N-(1-(2-chlorophenyl)-2-(4-nitrophenyl)ethyl)-4-methylbenzenesulfonamide (CNPSA) by Ag NPs was investigated using Raman spectroscopy. Ag NPs were synthesized by solution combustion method using citric acid as fuels. The prepared Ag NPs were characterized by XRD, UV, HR-TEM, FESEM and SERS studies. The prepared Ag NPs exhibit cubic crystalline structure with grain size 46nm. The surface plasmon resonance peak was found at 380nm. The spherical shape of Ag NPs was confirmed by FESEM and HR-TEM. The orientation of CNPSA molecule on Ag NPs has been inferred from nRs and SERS spectral feature. The molecule is adsorbed on the Ag NPs with the benzene ring in a tilted orientation. The presence of amino and sulfate group vibrations in the SERS spectrum reveal the interaction between amino and sulfate.

CHAPTER IV

Abstract

Ag NPs were synthesized using a solution combustion method with glycine as fuel. Ag NPs were characterized by XRD, UV, HR-TEM and FESEM. The prepared Ag NPs exhibit cubic crystalline structure with grain size of 59nm. The spherical shape of Ag NPs was confirmed by HR-TEM and SEM. HR-TEM images show that the Ag NPs have five-fold symmetry formed by twinning in the crystal structure. SERS spectra of N-(1-(4-fluorophenyl)-2-(4-nitropheny) ethyl)-4-metylbenzenesulfonamide (CFSA) adsorbed on Ag NPs were studied. The C-H in-plane bending mode and in-plane mode in C-F were high intensity and they were broadening in SERS spectrum with respect to nRs was observered. The spectral analysis reveals that the CFSA adsorbed ‘stand-on’ orientation on the Ag NPs.

CHAPTER IV

Abstract

SERS technique has been employed to investigate the orientation of 2-bromo-3-methylamino-1,4-naphthoquinone (BMANQ) molecule on Ag NPs. Ag NPs have been prepared by solution combustion method with citric acid as fuel. The observed intense C=O stretching, C–Br stretching, in-plane of C-H mode and NH2 vibration suggests that the BMANQ molecule may be adsorbed in a ‘stand-on’ orientation to

the Ag NPs. The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy show that charge transfer occurs within the molecule.

CHAPTER VI

Abstract

Ag NPs have been prepared by solution combustion method with glycine as fuel. Ag NPs were characterized by The orientation of 1,4-dibromonaphthlaene (1,4-DBrN) on Ag NPs has been inferred from nRs and SERS spectral features. The absence of a C–H stretching vibrations, observed high intense C–H in-plane bending modes and high intense C–Br stretching vibration suggest that the 1,4-DBrN molecule may be adsorbed in a ‘stand-on’ orientation to the Ag NPs. The HOMO-LUMO analyses explain the charge transfer taking place within the molecule.

CHAPTER VII

Abstract

SERS has been employed to investigate the orientation of 1,4-dimethoxy-2-nitro-3-methylanthrance-9,10-dione(DMNMAD) molecule on Ag NPs. The Ag NPs were synthesized using a solution combustion method with citric acid as fuel. The nRs and SERS spectrum of DMNMAD molecule and DMNMAD molecule on Ag NPs have been simulated using DFT calculation at B3PW91 level of theory. The very good correlation found between experimental and theoretical data is a clear evidence for a reliable assignment of the vibrational bands. The large enhancement of C=O stretching and C-H in-plane modes in the SERS spectrum indicates that the molecules adsorbed on the Ag NPs may be adsorbed in a ‘stand-on’ orientation. The calculated HOMO and LUMO energy shows that charge transfer occurs within the molecule.

CHAPTER VIII

Abstract

Ag NPs were prepared by solution combustion method with glycine as fuel. SERS of 1,4-dimethoxy-3-bromomethylanthracene -9,10 dione (DMBMAD) adsorbed on Ag NPs has been investigated. The orientation of DMBMAD on Ag NPs has been inferred from nRs and SERS spectral features. The observed spectral feature corroborated that DMBMAD would adsorb on Ag NPs by ‘stand-on’ orientation

through the high intensity of C-H in-plane bending mode, C-Br stretching, ring stretching and C=O. In present case, the DMBMAD molecule and Ag NPs as component molecules for energy gap analysis, where as DMBMAD serve as donor and Ag NPs as acceptor. The calculated HOMO and LUMO energy gap shows that charge transfer occur within molecule and Ag NPs.