# Orientation change and structure according to the various pH conditions of 4-amino-4'-cyanobiphenyl on silver surfaces: SERS and DFT study

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Surface-enhanced Raman Scattering (SERS) spectra of 4-amino-4'-cyanobiphenyl (44ACBP) adsorbed on Ag colloidal nanoparticles were measured in various pH conditions. In neutral and alkaline solutions, the molecule should be adsorbed flat on the surface whereas in acidic solution, the molecule should vertically be adsorbed through the CN-metal bonding due to protonation in the amine group. The peaks observed in the spectra were assigned in comparison to those in the normal Raman spectra taking advantage of quantum chemical density functional theory (DFT) calculations. The adsorption behavior could be identified from spectral analyses of relative enhancement of the in-plane against the out-of-plane vibrational modes observed in the SERS spectra. The orientation of 44ACBP adsorbed on the Ag surface could be reversibly controlled to flat or vertical orientation by changing pH in solution.