Surface-enhanced Raman scattering and density functional theory studies of bis(4-aminophenyl)sulfone

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Raman and surface-enhanced Raman scattering (SERS) spectra of dapsone by using colloidal silver nanoparticles have been recorded. Density functional theory was used for the optimization of ground state geometries and simulation of the vibrational spectrum of this molecule. The SERS spectrum with a large silver cluster as a model metallic surface was simulated for the first time. Taking into account the experimental and calculated Raman as well as the SERS normal modes and the corresponding assignments, along with the modeling of the free dapsone and the one in the presence of the colloidal silver nanoparticles, the importance of the sulfone group on the SERS effect in dapsone was inferred.