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Simulating the sensing properties of silver nanoparticles for identifying molecular structures using modified discrete dipole approximation method

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Abstract

By making a modification to the usual discrete dipole approximation (DDA) method, the effect of different molecules on the plasmonic properties of silver nanoparticles was investigated. Several calculations were performed for molecules with different structures, sizes and concentrations. The obtained results indicated that considering that the modified DDA method is very sensitive to the geometrical details and the type of atoms of the guest molecule, the smallest change in the dimensions and also the type of atoms of the guest molecule leads to a change in the peak wavelength of the absorption spectrum of silver nanoparticle. These changes are unique for different molecules with good accuracy.

Keywords: discrete dipole approximation, molecular polarizability, sensing properties of silver nanoparticles

For full article, refer to the Persian section