



Iranian Journal of Physics Research, Vol. 23, No. 2, 2023  
DOI: 10.47176/ijpr.23.2.51683

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

Araz Siabi-Garjan

Department of Engineering Sciences, Faculty of Advanced Technologies, University of Mohaghegh Ardabili, Namin, Iran

E-mail: a\_siabi@uma.ac.ir

(Received 10 May 2023 ; in final form 25 May 2023)

---

### 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