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Finite-Difference Time-Domain (FDTD) Modeling of Gold Core-Shell Structures with Different Shell Morphology for Surface-Enhanced Raman Spectroscopy (SERS)[1] ZOHRE GORUNMEZ, DEBRINA JANA, JIE HE, LAURA SAGLE, THOMAS BECK, University of Cincinnati — Core-shell (CS) nanostructures have received attention in recent years due to their usefulness in applications ranging from catalysis to cancer treatment. SERS has been shown to be one of the most sensitive techniques for molecular detection, achieving single molecule detection. It has been established that the electromagnetic mechanism (EM) provides the main contribution to SERS enhancement due to the normal Raman spectroscopy arising from coupling of both the incident and re-emitted fields. The FDTD technique has been developed to provide numerical solutions to Maxwells time-dependent curl equations in order to promise modeling capabilities for EM enhancement of SERS. Herein, we apply this method to the study of three morphologically different gold core-shell nanoparticles to investigate their contributions to SERS. In these structures, the dye/probe molecule resides in between the shell and the core and only the shell morphology is altered. The data shows that the surface plasmon resonances (PRs) influencing the SERS of the probe molecules, due to the coupling of the core and shell, are tunable by changing the shell morphologies and CS structures with sharp features on their surfaces highlight larger enhancements due to stronger localized surface PRs.

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