Morphological Effects on the Plexitonic Interaction in Au@$MoSe_2$ Nanodisk Dimer

UT San Antonio[1], Univ. Paul Sabatier[2], CEMES Toulouse, FR[3]

Emil Penafiel[1,*], Ines Abid[2,3], Adnen Mlayah[2,3], Nicolas Large[1]

E-mail: ecpenafiel@live.com; nicolas.large@utsa.edu

Here, we report on the surface-enhanced resonant Raman scattering (SERRS) in hybrid $MoSe_2$@Au plasmonic-excitonic nanostructures and focus on the situation where the localized surface plasmon resonance (LSPR) of Au nanodisks is finely tuned to the exciton absorption of monolayer $MoSe_2$. Using a combination of experimental and computational techniques, we estimate the relative contributions from the localized surface plasmons and the confined excitons to the Raman scattering enhancement. By exploring the optical properties of the hybrid $MoSe_2$@Au nanostructure we investigate the SERRS efficiency dependence on the nanodisk surface morphology. We investigate the effects of rough interfaces in a gold-molybdenum diselenide (Au@$MoSe_2$) nano-disk dimer system by numerically solving Maxwell's equations using the finite-difference -time-domain (FDTD) method. We simulated a system consisting of a gold dimer with a diameter of 140 nm and a height of 16 nm. The 2 nm $MoSe_2$ layer is added on top of the dimer to complete the system. The gap between the dimer is varied with three different gap lengths: 20 nm, 45 nm, 100 nm to capture the varying resonance wavelengths for each system. For each configuration, three varying degrees of surface roughness ranging from smooth, rough, to super rough interfaces are simulated. We show that morphological defects have negligible effects on the resonance wavelengths and far-field properties of the system and that other parameters such as dimer gap width and dimer diameter have a more significant impact in determining the resonance wavelength. However, we show that such surface defects strongly impact near-field properties. As the surface roughness increases, local electric fields are redistributed around the nanodisks and within the $MoSe_2$, thus leading to a modification of the plasmon-exciton coupling [1]. We demonstrate that the surface roughness of the metallic nanostructures is the main limiting factor of the SERRS efficiency.

Keywords: Hybrid Au-$MoSe_2$, Plexcitons, Raman Scattering Enhancement, Interface Morphology

References:

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