Gallium-Doped Zinc Oxide Semiconductor Nanoparticles for Plasmonic Applications: A Combined Experimental And Computational Study

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Gallium-doped zinc oxide (GZO) nanoparticles were synthesized using a sol–gel method followed by controlled thermal treatment, yielding nanocrystalline semiconductors with tuneable Ga concentrations for plasmonic applications. Structural and morphological characterizations via scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS) confirmed the successful substitution of Zn^{2+} by Ga^{3+}, while maintaining the wurtzite crystal structure. Optical properties were thoroughly investigated using UV–visible diffuse reflectance spectroscopy, where bandgap energies, derived through the Tauc method, demonstrated a progressive narrowing with increasing Ga doping. Notably, the real (ε_1) and imaginary (ε_2) components of the complex dielectric function revealed a distinct crossover of ε_1 from negative to positive values and a corresponding peak in ε_2 in the near-infrared region, indicative of plasmonic resonance. Furthermore, electron energy loss spectroscopy (EELS) exhibited a sharp loss peak at approximately 0 eV, confirming the presence of collective oscillations of free carriers (plasmons) in the doped system. To complement the experimental observations, first-principles density functional theory (DFT) calculations were performed, revealing an upward shift in the Fermi level and increased free carrier density due to Ga incorporation. This shift facilitates intraband transitions, enhancing the low-energy optical response and promoting a strong epsilon-near-zero (ENZ) effect. Collectively, these findings demonstrate the dual semiconducting and plasmonic nature of GZO nanoparticles, highlighting their potential in tuneable optoelectronic platforms, low-loss infrared plasmonics, and epsilon-near-zero photonic devices.

References

[1] A. Shabani, M. K. Nezhad, N. Rahmani, Y. K. Mishra, B. Sanyal, J. Adam, Adv. Photonics Res. 2, (2021), 2000086
[2] J. Kim, G. V. Naik, A. V. Gavrilenko, K. Dondapati, V. I. Gavrilenko, S. M. Prokes, O. J. Glembocki, V. M. Shalaev, and A. Boltasseva, Phys. Rev. X., 3, (2013), 041037

Figures

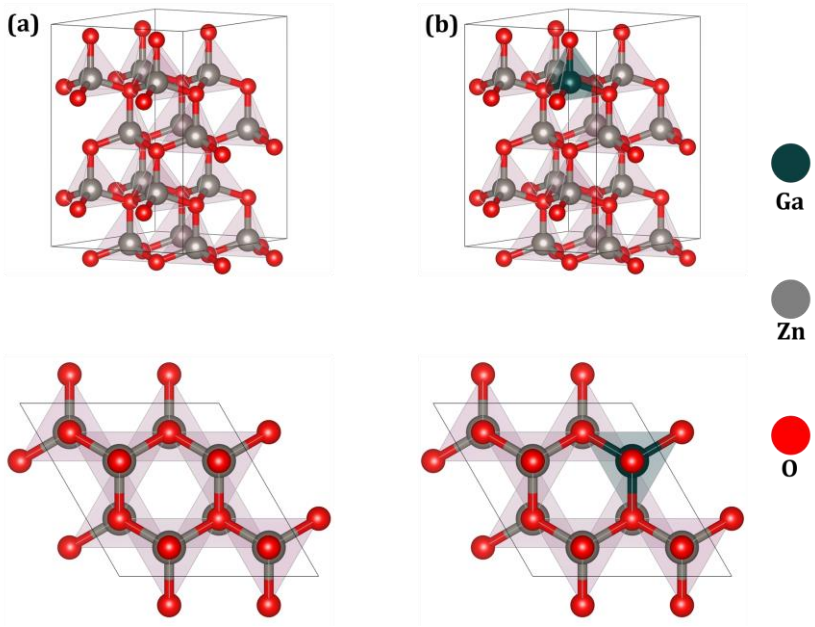

Figure 1: Wurtzite crystal structure of (a) pristine and (b) gallium-doped zinc oxide (GZO) for 2 × 2 × 2 supercell (6.25 at% Ga doped in ZnO), holding 16 Zn and 16 O atoms in a supercell.