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Discrete dipole approximation to determine the optical properties of ZnO polymer nanocomposite

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Optical properties have been simulated by DDA for ZnO NPs and ZnO-PVP composite for different particle size with complex dielectric function as input. The absorption efficiency factor for ZnO NPs of size 26 nm and that for ZnO-PVP of size 28 nm in simulation matches well with the experimentally obtained absorbance data. When ZnO is simulated for the particle size of 26 nm, the electric near-field intensities on the edges show fewer intensities compared with the center. The simulation of ZnO-PVP composites of 28 nm results in a spherical electric near-field with a larger diameter. Since ZnO is a hexagonal structure, the near-field appears to be most intense at the center followed by the edges of the NP. The increase of near electric field due to the presence of local dielectric medium may be the possible reason to behave a particle within the dielectric medium as the particle with higher effective radius. So, in ZnO-PVP composite, ZnO NPs act as a particle with higher effective radius. As a result, in presence of dielectric medium, the absorbance peak of same NPs shifts towards higher wavelength. The dielectric medium perturbs electron-phonon interaction as well as the optoelectronic properties. Moreover, the luminescence properties of the materials are affected due to composite formation. In case of NP-polymer composite, NPs are capped and there is negligible further adsorption and desorption of O_2 molecules occurred on the surface. This increases the photocurrent as well as photosensitivity, which makes the ZnO-PVP composite as a suitable candidate for visible-blind UV detector.

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