ARTICLE

Structural-Morphological Insights into Optimization of Hydrothermally Synthesized $MoSe_2$ Nanoflowers for Improving Supercapacitor Application

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The $MoSe_2$ nanoflowers (MNF) have temperature-independent optical properties with direct energy band gap (E_g) of 1.76 eV.

Experimental

Characterization

UV-visible absorption spectroscopy was conducted on a Double Beam UV-Vis Spectrophotometer (Motra's UVPlus) in diffuse-reflectance mode to evaluate the optical absorption and band-gap of $MoSe_2$ nanostructures.

Results and discussion

Optical Properties

Fig. S1(a) elucidates the UV-Vis spectra of $MoSe_2$ nanoflowers obtained at three different synthesis temperatures via hydrothermal methodology. It is well accepted that an optical emission and/or absorption corresponds to the emission or absorption of photons by the defects. The three characteristics absorptions peaks of $MoSe_2$ are obtained for wavelength ranging 600-800 nm due to interband electronic excitation of the material indicating the formation of refined 2H phase $Mose_2$. The three excitons are obtained as; A (783 nm, 797 nm and 787 nm), B (687 nm, 699 nm and 697 nm), C (600 nm, 610 nm and 609 nm) for MNF_200, MNF_210 and MNF_220, respectively. Intriguingly, a red-shift is observed in exciton peak positions as we increase the synthesis temperature whereas a blue-shift is identified with further enhancement in temperature.

The optical energy band-gap (E_g) is evaluated from UV-Vis absorbance spectra using Tauc equation (1);

$$(\alpha h\nu)^n = A(h\nu - E_g) \quad ...(1)$$

Where, α is an absorption coefficient obtained using Beer-Lembert Law, ν is the incident photon frequency, h is Planck' constant, $h\nu$ is the energy of incident photons, n = 2 or ½ for direct or indirect band gap transitions and A is the characteristic of material with a constant value.

Fig. S1(b) displays the energy band-gap of $MoSe_2$ nanoflowers. The intercept on photon energy ($h\nu$) of the plot $(\alpha h\nu)^2$ versus $h\nu$ illustrates the optical energy band-gap values about 1.76 eV for all $MoSe_2$ nanoflowers synthesized at different temperature. It is obvious that there is a very weak effect of process temperature on the optical properties of $MoSe_2$ nanoflowers.

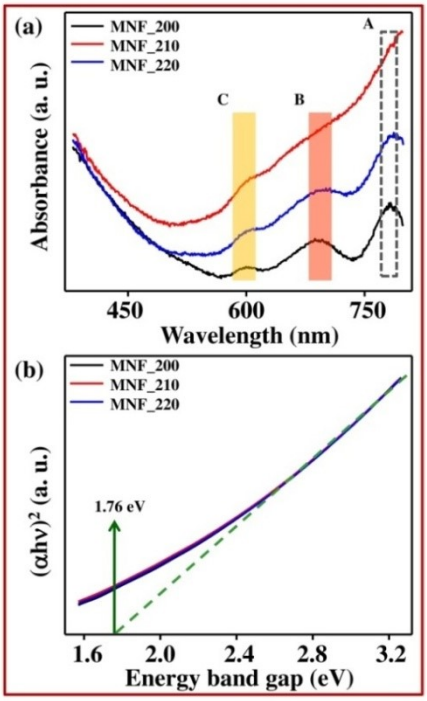

Fig. S1 (a) UV-Vis absorbance spectra; (b) Tauc plot depicting direct energy band gap of MNF_200, MNF_210, and MNF_220.

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