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Size-dependent and intra-band photoluminescence of NiS2 nano-alloys synthesized by microwave assisted hydrothermal technique

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Abstract

Synthesis of nickel disulfide (NiS2) nano-alloys capped and uncapped with hexadecylamine (HDA) was carried out. A cubic phase NiS2 formation was confirmed by X-ray diffraction (XRD) analysis. An average crystallite size of 35 nm was obtained for the uncapped nanostructures and 9 nmwas obtained for the capped nanostructures estimated using the Scherrer equation. Unexpected ultra-violet (UV) emission as well as near infrared (IR) emissions were attributed to intra-band energy state transitions that occur as a result of the porous structure of the material. Enhanced UV and near IR PL emissions due to the smaller crystallite size of the capped NiS2 nanostructures was also observed. Band energy and local density of states calculation for NiS2 were used to support the experimentally observed luminescence results. The luminescence features at wavelengths of 400 nm (3.10 eV), 428 nm (2.90 eV), 447 nm (2.77 eV) and 464 nm (2.67 eV) can be attributed to some of those electrons de-exciting from S (3p) levels down to the Ni (3d) (blue to UV emission) whereas those features at wavelengths of 710 nm (1.75 eV), 751 nm (1.65 eV), 754 nm (1.64 eV), [NiS2/HDA-capped NiS2] and 784 nm (1.58 eV) respectively seem to result from de-excitations between either Ni(3d) or S (3s, 3p) levels and Ni–S hybridization levels (red to near IR emission).