ФИЗИКА КОНДЕНСИРОВАННЫХ СРЕД

STRUCTURAL, OPTICAL AND PHOTOCATALYTIC PROPERTIES OF CUBIC AND HEXAGONAL CdS:Fe NANOCRYSTALS

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Present work successfully demonstrates controlled doping of transition metal Fe (0.5%, 1% and 1.5%) into cubic and hexagonal lattice structure of CdS nanocrystals. The paper includes detailed studies on the structural, optical and photocatalytic properties of CdS:Fe nanocrystals. The estimated average crystallite sizes of CdS:Fe in cubic and hexagonal phases are 5 nm and 3 nm, respectively as revealed by the XRD analyses. Smaller crystallite sizes ofh-CdS:Fe nanocrystals result in larger band gap compared to its cubic counterpart. The variations in the band gaps of CdS:Fe nanocrystals in cubic and hexagonal phases with different doping percentages of Fe do not follow any trend. Photoluminescence (PL) spectra reveal that the crystal structure of h-CdS:Fe nanocrystals contain more crystal defects compared to c-CdS:Fe nanocrystals. In addition, the prepared nanocrystals are tested as photocatalyts by observing photodegradation of Methylene blue (MB) solution with the the prepared materials immersed in it. Hexagonal phase of CdS:Fe nanocrystals have shown better photocatalytic behaviour compared to the cubic phase owing to the presence of more defects in their crystal structures than their cubic counterparts. Doping with transition element Fe into the crystal structure of cubic and hexagonal CdS nanocrystals significantly affects their photocatalytic performances.

Keywords: semiconductor, doping, transition metal, photocatalytic property.

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1. Introduction. CdS is one of the most talked group II–IV chalcogenide semiconductors due to its unique size dependent chemical and physical properties [1]. It crystallizes in three crystal structures-cubic zinc blend, hexagonal wurtzite and rock-salt structures [2]. The thermodynamically stable structure for CdS at room temperature is the hexagonal wurtzite structure, while cubic zinc blend structure has appeared for smaller particle sizes and rock salt structure has been observed only at high pressure (61 GPa) [3, 4]. Since CdS is chemically more stable than other II–IV chalcogenides, it has found extensive applications in the field of optoelectronics as light emitting diodes, solar cells and optical devices [5–8].

One of the most widely used strategies to modify various properties of CdS such as optical, magnetic, electrical and structural is to dope it with transition metal ions such as Ni^{2+}, Mn^{2+}, Fe^{2+}, Cu^{2+} and Co^{2+} [3, 9–11]. It has been reported that doping with Mn and Cu lower the band gap of CdS [12, 13], while Zn doped CdS exhibit larger band gap compared to undoped CdS thereby increasing the photostability and conductivity of CdS [14]. As per literature survey, CdS acquires paramagnetic behaviour upon doping with Fe and Co [15–17]. Doping with Zn enables CdS to be used as window layers in solar cells [18]. Raju et al. have shown that doping with Ni^{2+} ions in $Cd_{0.9}Zn_{0.1}S$ nanostructures decreases the crystallite size from 6.9 to 4.3 nm and also micro-strain is introduced in the system [19]. Very recently, Ranjan et al. has explored that the nanoparticle size of Co doped CdS declines when Co^{2+} ion has substituted Cd^{2+} ion in the Cd-S lattice due to the smaller ionic radius of Co [20]. Especially, doping with Fe^{2+} into CdS nanocrystals has attracted wide attention of the researchers [21–24]. Thambidurai et al. has studied the structural properties and optical absorption properties of Fe doped CdS quantum dots [21]. Shkir and Alshahrani have tuned the physical properties of CdS thin films through doping with Fe dopant for photodetector application [22]. Work of Saikia et al. have shown that CdS nanoparticles acquire ferromagnetic behavior when doped with lower concentrations of Fe, they become anti-ferromagnetic if the doping concentration of Fe is raised [23]. Moslem et al. have shown the effect of Fe doping on the structural, optical and magnetic properties of CdS quantum dots [24]. Due to its direct band gap of 2.42 eV and suitable band position, CdS can be a good photocatalyst for visible-light driven photocatalysis [25–28]. But, CdS does not exhibit overwhelming photocatalytic property [29]...

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