Chapter 6

Concluding remarks and future directions

6. Concluding remarks and future directions

6.1Conclusions

Significant findings of the thesis can be summarized as follows.

a) A novel approach of solid state reactions to synthesize MoS_2 NPs, WS_2 NPs and NPs of bimetallic ternary compound of Mo, W and S namely MoW-disulfide1(having molar ratio of Mo:W equal to 1:1) and MoW-disulfide2(having molar ratio of Mo:W equal to 10:1) was successfully achieved. The formation of desired materials having a nanoscale dimension was determined by analyses using XRD, SEM, TEM, EDX and Raman spectra. All the materials exhibit Hexagonal structure which was confirmed by XRD and TEM analyses. The combining effect of the sulfides of W and Mo gives rise to different optical properties. UV-vis absorption spectra analysis determined the multiple BG nature of the nano materials. This outcome promises that the materials can give good photocatalytic activity. There is an enhancement of PL emission near 463nm blue wavelength in the ternary compound MoW-disulfide1 as compared to the other as-synthesized materials.

b) MBG values of the as-synthesized nanomaterials enhance their photocatalytic activity by providing absorption of a wide range of radiation at multiple wavelengths. A large value of BG in MoW-disulfide1 (2.84eV, 2.41eV) facilitates the materials to absorb the intense part of visible solar spectra. As the energy of the band gap lies in the atmospheric window of the solar spectra, which has larger photon density, generation of more number of exciton pairs takes place under the influence of this visible light exposure. A comparative study shows that as-prepared ternary compound MoW-disulfide1 has come out to be better photocatalyst than MoS_2 and WS_2 NPs. BET and BHJ analysis showed that MoW-disulfide1 NPs has maximum surface area and larger pores which leads to better photocatalytic activity. About 99% degradation in just 90 minutes of irradiation is observed in case of the compound MoW-disulfide1 NPs catalyst. The photodegradation mechanism is found to follow Langmuir-Hinselwood (L-H) pseudo first-order kinetics under experimental conditions. The reusability of the compound MoW-disulfide1 catalyst makes the catalytic process a reliable and cost-effective technique.

c) A computational investigation of the effect of W on the MoS_2 system using density functional theory (DFT) revealed that insertion of W in the MoS_2 system makes the ternary compound system more stable. Among the three clone models in our DFT simulation study, the system $Mo_8W_8S_{16}$ comes out to be the most stable system. DFT study concluded that W insertion in MoS_2 system makes the compound system a direct BG semiconductor when W and Mo are equal in content which agrees with the experimental results. The direct BG nature as determine in DFT simulation also gives good support to the experimental results of enhancement in PL and photocatalytic activity of the ternary compound MoW-disulfide1 NPs.

6.2 Future directions

The work done in this thesis can be extended in many ways. We shall highlight some of the points where these work may lead to,

a) The as-synthesized ternary compound NP catalyst is found to be efficient in degrading our chosen model dyes. The study could be extended for several other organic and inorganic dyes. It has potential applications in the field of wastewater treatment and dye pollution controlling process.
b) Since the as-synthesized ternary material has a suitable high value of BG (2.84eV) covering the water-splitting potential, it has probable application in the generation of hydrogen and oxygen by water splitting via the photocatalytic mechanism.
c) The enhanced blue PL emission indicates the material's good applicability in luminescent devices.
d) Study of the bimetallic ternary compound with combinations of elements other than M and W is a potential area for future research.