CHAPTER VII

Conclusion and future directions

The salient features of this thesis are

- ✓ A novel core-shell nanocomposite Ag_2S-HgS is synthesized through a simple laboratory procedure. The synthesized core-shell structure which is TYPE 1 for a 0.1 M Hg^{2+} concentration is transited to TYPE 2 while changing the shell precursor concentration to 0.2 M Hg^{2+}. Earlier this type of phenomenon is observed in case of inverted core-shell structures. The TYPE 2 core-shell Ag_2S-HgS (0.2 M Hg^{2+}) is tested for photocatalytic performance and it has been able to successfully degrade Methylene Blue dye under daylight illumination. The degradation efficiency of the core-shell structure is found to be improved than its core counterpart.

- ✓ TiO_2 nanoparticles are synthesized via a standard sol-gel procedure. The core TiO_2 nanoparticles were coated with an insulating material MgO (bulk band gap 7.8 eV). The properties of the core material were studied by annealing at different temperatures and a phase transition from anatase to rutile was observed at 650 ºC and almost completely transformed to rutile at 850 ºC. Again to see the effect of insultaing coating layer on the core particle, MgO nanoparticles were prepared and their optical properties were also extensively studied through UV-vis and photoluminescence (PL) spectroscopy. A detailed report on PL properties of MgO nanoparticles has been provided in the thesis which as per our knowledge has not done so far. The absorption spectra of MgO contain oxygen defect related absorption peaks spanning the entire energy spectrum from ultraviolet to visible region. The corresponding emission spectra are obtained at three different excitations 206 nm, 270 nm and 330 nm. Each excitation results in an intense emission associated with F^+, F_2^{2+} and F-type defect centers. These intense emissions, lying in the ultraviolet and violet region, are accompanied by low intense blue and green emissions respectively. Since the emission peaks are associated with oxygen vacancies, thermal annealing at 800 ºC reduces the intensity of these peaks. The intensity ratio of the emissions of F^+/F and F^+/F_2^{2+} decreases at 800 ºC, whereas F/F_2^{2+} intensity ratio increases at 800 ºC. This is possibly due to the thermal conversion of F^+

and F_2^{2+} to F centers at 800 ºC, which finally results in the enhancement in the emission intensity of F centers at high temperature. Again sincere investigation was carried out on the core-shell TiO_2-MgO nanostructures and it has been established that the core-shell nanostructure is a more efficient photocatalyst for degradation of methylene blue dye under sunlight than core TiO_2. After comparing the characteristics of core-shell TiO_2-MgO with both core TiO_2 and shell MgO individually, it was proved that the core-shell structure resembles very less to the shell but highly matching with the core one. But the shell MgO layer played a vital part in improving the core TiO_2 surface by inducing abundant oxygen vacancies as well as favoring ambient charge separation.

- ✓ After coating core TiO_2 with an insulating layer, next we opted for a near band gap semiconductor SnO_2 as the shell layer. To our surprise, the absorbance spectra of the core-shell structure highly resembles to the shell in contrary to the core. This is an interesting phenomenon we observed, as in general core-shell structures only exhibit modified/deteriorated core characteristics only. This may be due to the fact that a coupling mechanism may occur between core and shell when some of the UV photons excited by the lamp source are absorbed by the outer shell and may b due to high shell thickness the excitation source must have low intensity to penetrate the shell resulting in distinct absorbance peaks resembling the shell. Also we tried to tune the properties of core-shell TiO_2-SnO_2 with three different shell precursor concentrations. While testing the photocatalytic activity, it has been observed that the core-shell with highest shell thickness did not degrade methylene blue dye indicating that a saturation thickness has been attained.

- ✓ In the next chapter we discussed two core-shell structures both of which are TYPE 1 in bulk alignment but converted to TYPE 2 when the size is changed from bulk to nano. First we discussed about TiO_2-ZrO_2 core-shell structures (very few reports are found on this core-shell structure to the best of our knowledge). We found that due to generation of defect related states between the conduction band and valence band of the shell, a quasi TYPE 2 structure is attained in the core-shell particles which favor charge separation resulting in efficient photocatalytic degradation of methylene blue dye under daylight. The noteworthy point which is obtained from analysis of this material is that the crystallite size gets smaller than the core structure resulting in red shift in Raman spectra. Then we worked on another material where TiO_2 was acting as a shell over CdSe nanoparticles. TiO_2-CdSe nanocomposites have been reported widely but we developed the core-shell structure without any surface active agent like Hexane which is very rarely reported. This core-shell structure once again is found to be a better photocatalytic agent than the core counterpart.

- ✓ In our last chapter we fabricated films from already prepared TiO_2 nanopowder through a reported method along with three core-shell films TiO_2-MgO, TiO_2-SnO_2 and TiO_2-ZrO_2. We studied structural, optical and electrical properties and found that as synthesized TiO_2-ZrO_2 film would not be suitable for photovoltaic study because it did not exhibit any better electrical characteristics under illumination than dark. For photovoltaic measurement a simple experiment was performed to find whether the prepared films can be properly act as photoanodes.

- ✓ Finally we can conclude that we synthesized some potentially applicable oxide as well as sulfide core-shell nanostructutres.

During the course of research, care was taken to minimize the time-gap between synthesis and characterization of the synthesized samples.

Future directions

- ✓ We have established in our thesis that Ag_2S-HgS nanostructures can be tuned between TYPE 1 and TYPE 2 by changing the shell thickness. Thus they place themselves as potential candidate for application in LEDs as well as photovoltaic devices. It should be noted that the nanostructure shows very good visible regime absorbance, so they might be a suitable alternative to dye sensitized solar cells.

- ✓ We have found that all the core-shell nanostructures are exhibiting enhanced photocatalytic activity than the core counterpart. Now a days environmental pollution has emerged as a major issue in day to day life and to solve it, quest is started in search of efficient photocatalyst. As our synthesized core-shell nanostructures are showing good photocatalytic activity even under daylight they can be used in degrading industrial wastes or contaminants that pollute water. There is even a scope for using them in hydrogen splitting.

- ✓ We have studied the photovoltaic performance of the materials with very simple laboratory equipments. Still, they are found to act as promising photovoltaic candidate. It is expected that under intense illumination and with use of proper filters, the photovoltaic performance of the materials will be enhanced and they could be caste in solar panels for practical applications a alternative to Si photovoltaics.

- ✓ Very few reports on magnetic properties of core-shell nanostructures have been brought to light. But there is scope in studying the magnetic behavior of these core-shell nanostructures as they possess some amount of lattice mismatch due to different parameters of core and shell. Also improved magnetization can be expected in the core-shell structures compared to bare core particle as the former possess high amount of cationic or anionic vacancies and ferromagnetic interaction of the shell with the core can take place through the vacancies.

List of Publications:

1. P.Basyach and A.Choudhury, Structural and optical properties of core shell Ag_2S /HgS nanostructure, Materials Research Bulletin, 48 (2013) 2543–2548

2. P.Basyach, A.Choudhury, Structural And Optical Properties Of Core-Shell TiO2/MgO Nanostructures at different Annealing Temperatures, IJIRD,vol 1 ,issue 7(special issue),175.

3. Biswajit Choudhury, Priyanka Basyach, Amarjyoti Choudhury, Monitoring F, F^+ and F_2^{2+} related intense defect emissions from nanocrystalline MgO, Journal of Luminescence149(2014)280–286.

4 . Priyanka Basyach, Pawan Chetri, Amarjyoti Choudhury, Enhanced Photocatalytic Activity of Core-Shell TiO2/SnO2 Nanostructures under UV Illumina-tion, IJSER, Volume 4, Issue 12, December-2013

Conferences:

- Oral presentation at ICORE 2011,Tezpur University
- Poster presentation at CMDAYS 2011,Gauhati University
- Poster presentation at NCSN 2011, Tezpur University
- Oral presentation at ISWESD 2012,Sivasagar College
- Oral presentation at NCPS 2013,D.H.S.K College
- Oral presentation at ICETRE 2013,C.V.Raman College of Engineering,Bhubaneswar
- Poster presentation at NSCTPR 2014, Darrang College, Tezpur, Assam