Chapter VII

Conclusions and future direction

Comprehensive conclusions

Two-dimensional materials (2D) have gained importance due to several unique properties. The wide range of properties and the ability to tune these lead to several potential applications in different fields of electronics, opto-electronics, in energy storage devices etc.[1]. Monolayer TMDCs, due to their direct bandgap are useful in the fabrication of opto-electronic devices, such as LED and solar cells [2]. Apart from these, they exhibit several other important features, which include elastic properties, mechanical properties and so on. Also, they are known to have good photocatalytic efficiency [3]. Despite these interesting aspects, exhibited by 2D materials, yet ample scopes do exist in in different avenues of research. Owing to their technological relevance, there is a need to intensify research in these layered materials.

This thesis is the outcome of processing, modification and characterization of tungsten disulphide (WS_2) nanosystems of different morphologies. A user-friendly hydrothermal method is used for the synthesis of IF-type WS_2 nanoparticles, which was confirmed through TEM imaging. Apart from IF-type WS_2, WS_2 nanopowders have been synthesised following a single step hydrothermal route, and using ultrasonication method, WS_2 nanosheets have been further prepared. The novel, WS_2/C-dot hybrid nanosystem processed by using orange juice as the source of carbon. The fluorescence property of the hybrid system was found to be highly tunable, with the excitation line, thus exhibiting excitation dependent photoluminescence. These features are, unlike size dependent band edge emission characteristics.

The photocatalytic efficiencies of the synthesised systems are investigated under UV and visible light illumination with MG and MO (harmful pollutants) chosen as target dyes. It was revealed that, the presence of IF-type WS_2 nanoparticles can degrade upto 71.2% under visible light as compared to 45% when illuminated by the UV light, while MG dye is considered as the target. The photocatalytic efficiency of the WS_2 nanoheets on MG dyes was found to be 86.6% under visible light illumination and it is 67.4% when illuminated with UV light. As for WS_2/C-dot nanocatalyst, the photodegradation of MG and MO dyes under visible light exposure was observed to be ~81.2% and ~91%; respectively. The WS_2/C-dot nanohybrid system is found to display an apparent enhancement in the photocatalytic activity. This increase in the photocatalytic activity in the hybrid system is attributed to the presence of C- dots which play an important role in enhancing the photoactivity. This phenomenon can be explained by the physiosorption process of the dye onto the WS_2 layers, possessing numerous surface active sites.

The mechanical and wettability characteristics of hydrothermally processed IF-type WS_2 nanoparticles, homogeneously dispersed in a polymer host have been studied. The range of elastic and plastic regions was observed to be dependent on the amount of nanoparticle loading. The nanocomposite films, showed an increased elongation and consequently, Young's modulus of elasticity offering a maximum value for 6 wt% of nano-WS_2 loading. Breaking stress also gives an enhanced value, ranging from 2.7 to 9.7 MPa, without and with 6wt% loading of nano-WS_2. Moreover, tribological studies have revealed a significantly lowered coefficient of friction (COF) with inclusion of nano-WS_2. The wettability of the composite films exhibited a high CA value but reduced CAH and the surface energies of the composite films were found to vary in the range of 24.7 to 37.5 mJ/m^2 by considering contributions from the polar and dispersive parts separately for two reference liquids.

Apart from synthesis, characterisation and the study of basic properties of WS_2 system, we have also employed 80 keV Xe^+ ion irradiation effects on WS_2 nanosheets, the range of fluences being 1×10^{15}- 5×10^{16} ions/cm^2. It has been observed that, the low energy ion irradiation (S_n>S_e) would lead to splitting of nano-WS_2 stacks into smaller, several layered nano-sheets. A subsequent increase in rms roughness has been observed for the irradiated samples along with manifested PL response and enhanced hydrophobicity feature.

The important conclusions drawn from the present study, distributed across six chapters are as highlighted below:-

- ✓ The WS_2 nanosystems has resulted in IF-type nanoparticles, and nanosheets through adequate steps and processing control.
- ✓ The WS_2/C-dot nanohybrid systems are obtained, following a green route by extracting C-dots from orange juice via carbonization at high temperature (120 ^oC).
- ✓ The excitation dependent PL and red-shifting responses are explained using models related to surface traps and electronegativity of heteroatoms.
- ✓ Among the three systems, IF-type WS_2, WS_2 nanosheets and the C-dot/WS_2 hybrid nanosystem, the latter showed maximum photocatalytic degradation of the target dyes.
- ✓ The C-dot is a special class of material which is likely to be used both as a photocatalyst and as an effective fluorescent candidate. This bifunctionality can be explained through electron-transfer and capture properties of the C-dot along with wide absorption range, excitation dependent photoluminescence property.
- ✓ The nanocomposite films (WS_2 dispersed in polymer host) show better mechanical, tribological and enhanced hydrophobic response with increase in WS_2 loading.
- ✓ Under 80 keV Xe^+ ion irradiation, the nanosheets are found to get fragmented and exfoliated, as evidenced from the AFM images and Raman spectra.
- ✓ An increase in electron-phonon coupling parameter (S_p), reveals the strong electron phonon interactions in the irradiated samples.
- ✓ The wetting-dewetting transition has been witnessed with an increasing ion fluence. The de-wetting response is prominent for the irradiated nano-WS_2.

Future scope and direction: Transition metal dichalcogenides (TMDCs) constitute important class of materials, with potential applications in diverse fields. The strong photoluminescence property of monolayer TMDCs makes them a strong candidate for bio-sensing applications. As 2D materials, TMDCs show high surface-to-volume ratio and hence more number of active sites which makes them sensitive to the surrounding environment enabling them to be used as sensors. The unique layered structures of TMDCs are flexible to intercalate or de-intercalate ions in it fulfilling the requirement for energy storage devices. Also, the TMDCs are promising materials for spintronic devices owing to their strong spin splitting property. Among different chalcogenide systems, MoS_2 has been studied quite extensively and the exploration of WS_2 system is in progress. However, the synthesis of pure, defect free, single layered TMDC is still quite challenging. Moreover, the transfer to substrates and making electrical contacts for miniaturized devices though fascinating, involves greater challenges/difficulties. While moving from laboratory to real products, numerous exercises is to be dealt with these materials. Necessity, feasibility and proof of principles to be examined while paying due attention to environment and ecosystem.

References

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