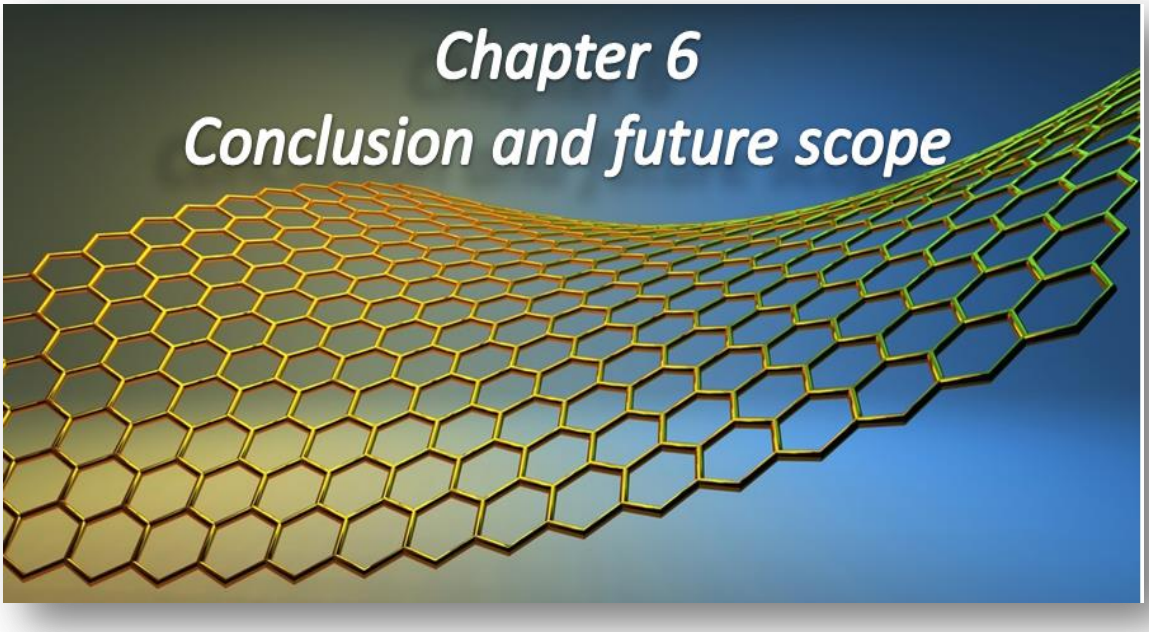
Chapter 6
Conclusion and future scope

6.1 Conclusion

Since its discovery graphene has come a long way. It has opened a new area for the use of 2D carbon materials in catalysis. Due to its unique structure and properties it has become a promising building block in functional materials. Graphene based nanocomposites can be applied to fabricate various unique catalysts due to their high electrical and thermal conductivities, high mechanical strength, huge specific surface area and high adsorption capacities. Graphene is used as catalysts or catalyst support for various chemical, electrochemical and photochemical reactions showing promising results compared to conventional catalysts.

This thesis shows the successful functionalization of various graphene based nanocomposites with CuO, Ni-polypyrrole, ZrO_2-chlorosulfonic acid and *p*-phenylenediamine-MWCNT. The synthesized nanocomposites showed the enhanced catalytic properties compared to their precursors and other reported catalysts. They were used as catalyst for reduction reaction, electro-catalyst for fuel cells and photo-catalyst in photochemical reaction. Functionalized graphene based nanocomposites were also used as supercapacitor and adsorbent for water treatment.

The important outcomes of the thesis are summarized as follows:

1. **Synthesis of copper oxide/reduced graphene oxide nanocomposite and its enhanced catalytic activity towards reduction of 4-nitrophenol and methanol electro-oxidation.**
    - Copper oxide supported on reduced graphene oxide (CuO-rGO) has been successfully synthesized by a facile hydrothermal method from GO and CuCl without using any reducing agents. In this process simultaneous reduction of GO and functionalization of rGO occurred by a redox reaction, where GO was reduced to rGO and CuCl was oxidized to CuO.
    - CuO-rGO showed excellent catalytic activity towards reduction of 4-NP to 4-AP in presence of $NaBH_4$.
    - The reaction followed pseudo-first-order kinetics and then maximum value of the rate constant was 13.951 min^{-1}, which is greater than the other reported works.
    - The catalyst can be easily regenerated by washing with DI water and reused with good reclyability.

- After calcinations at 400 °C, the nanocomposite showed higher electro-catalytic activity towards methanol oxidation.
- The nanocomposite undergoes irreversible methanol oxidation in alkaline medium with lower onset potential and higher peak current density in forward scan compared to bare CuO nanoparticles. The nanocomposite also showed higher durability and stability for 100 continuous cycles.

2. **Multifunctional ternary nanocomposites of Ni/polypyrrole/reduced graphene oxide as supercapacitor and electrocatalyst in methanol oxidation.**
   - A ternary nanocomposites of Ni nanoparticles supported on polypyrrole-reduced graphene oxide (Ni/PPy/rGO) was successfully synthesized by a simple method from PPy/rGO and $NiCl_2.6H_2O$ in basic medium.
   - The nanocomposite was used as a multifunctional electrode material. It showed high electro-catalytic activity and stability towards methanol electro-oxidation in alkaline medium. Its anodic current density (32.94 mA/cm^2) was much higher than that of Ni/rGO (22.1 mA/cm^2) and PPy/rGO (20.35 mA/cm^2).
   - The nanocomposite was also used as supercapacitor materials. It showed high specific capacitance value (763.49 Fg^{-1} at 1.31 Ag^{-1}) with capacity retention of 96.75 % after 200 continuous cycles.
   - EIS Study revealed that the nanocomposite have efficient charge transfer and better capacitive nature than that of PPy/rGO.
3. **Photocatalytic degradation of dye over zirconium oxide supported on sulfonated graphene under visible light.**
   - Monoclinic ZrO_2 supported on sulfonated graphene (*m*-ZrO_2/SG) was synthesized by a simple solution based method.
   - Formation of single crystalline monoclinic phase ZrO_2 without any phase impurities was confirmed by XRD studies.
   - The nanocomposite showed higher photo-catalytic activity compared to SG and *m*-ZrO_2/rGO under visible light.
   - The photocatalytic activity of the *m*-ZrO_2/rGO catalyst was increased with increased annealing temperature.

- The photo-catalyst can be easily recycled and reused after washing with absolute alcohol and DI water.

4. **Selective dye adsorption by pH modulation on amine functionalized reduced graphene oxide-carbon nanotube hybrid.**
    - Graphene was successfully functionalized with *p*-phenylenediamine and MWCNT (rGO-CNT-PPD) where simultaneous functionalization, reduction and hybridization occurred.
    - The nanocomposite selectively adsorbed dye by modulating the pH from their mixture. At pH 7.0, it removed 99.5% methyl violet selectively, while at pH 3.0, it removed methyl orange selectively having 98% removal efficiency.
    - The maximum adsorption capacity (q_m) of the nanocomposite for MV and MO are 298 mg/g and 294 mg/g respectively, which are higher than several previously reported q_m values.
    - The kinetics data for both dyes was well fitted with the pseudo-second-order kinetic model and the adsorption of both the dyes followed Langmuir adsorption isotherm.
    - The adsorbent could be easily regenerated and reused and its activity remained unchanged even after five adsorption-desorption cycles.

6.2 Future scope of the present investigation

Graphene based catalysts has the potential in replacing conventional catalysts. Although considerable improvement has been made, the large-scale synthesis of high quality, controllable layer thickness and controllable nanoparticles size functionalized graphene based catalyst at relatively low cost are still challenging. Thus, there is still a long way ahead before the catalytic applications of functionalized graphene based catalysts at the industrial scale.

Some future scopes on the basis of the present studies are:

- Developing effective strategies for synthesis of new low cost functionalized graphene based nanocomposites for high performance electro-catalyst and photo-catalyst.

- Synthesis of graphene based nanocomposite catalysts with uniform morphologies and controllable nanoparticles size.
- Synthesis of covalently functionalized graphene based catalysts.
- Study the catalyzation mechanisms of graphene catalysts.