CHAPTER 7

Concluding remarks

7.1 Summary

This chapter summarizes the main results of different thesis chapters and tries to arrive at general conclusions wherever possible. Organic pollutants such as PNP, OG, etc., are stable in an aqueous medium and toxic to human health. Thus, their removal from natural waters is critical. This thesis examines the mechanisms of various techniques of remedying water containing such pollutants. Appropriate computational and experimental studies were conducted to get vital insights into organic pollutant removal/degradation mechanisms by adsorption, Fenton, and photo-Fenton processes. Table 7.1 compares TOF values using different catalysts for photo-Fenton degradation of PNP. The thesis ends with a short discussion on the future scope of this work.

The first investigation is MD simulations of the magnetite nanoparticles' aqueous medium adsorption mechanism towards organic pollutants. RDF results between different atom types in the adsorbent and other molecules (adsorbate and solvent) were used to elucidate the adsorption mechanism. This study delineated the atom-type interactions dominating the investigated adsorption phenomena. The strength of adsorption depends on the hydrophilic nature of solute molecules. The strength of interaction between the solute molecules and adsorbent surface atoms will be higher for less hydrophilic solute molecules and vice-versa.

Next, Fenton activity is found better for PNP degradation in the case of SMNPs than MNPs (Table 7.1). Therefore, it is quite clear that starch stabilization affects the Fenton catalytic properties. MD simulations showed that the presence of starch on the magnetite nanoparticle surface significantly increased its affinity towards H_2O_2 molecules. At the same time, the PNP molecules remain in the vicinity of the MNP surface. The combination of MD simulations and experimental studies gave a crucial stabilizer molecule selection criterion for designing an efficient Fenton nanocatalyst.

The subsequent investigation is about the change in Fenton interfacial phenomena due to MNP surface modification by appropriate composite formation with GO. Prior to that, it was necessary to investigate the Fenton and photo-Fenton activities of GO itself. GO has negligible Fenton PNP degradation activity. But the prepared GO does exhibit Fenton activity towards OG degradation. Furthermore, it also had a visible bandgap and exhibited enhanced photo-Fenton OG degradation activity. The reason was better H_2O_2 adsorption to the epoxy groups on the GO surface. The photo-excited HOMO resides on the epoxy-functional groups. Thus, these functional groups are the excited state nucleophilic centers on the GO surface. Better adsorption of H_2O_2 molecules to these centers facilitates H_2O_2 reduction for optimum hydroxyl radical generation.

Table 7.1 Comparisons of Fenton and photo-Fenton PNP degradation TOF values over different catalysts prepared in this thesis.

Fenton PNP degradation		
Catalyst	**Time(minutes)**	**TOF (moles gram^{-1} min^{-1})**
MNPs	125	1.06×10^{-8}
MGO	125	1.08×10^{-7}
SMNPs	80	2.41×10^{-6}
Photo-Fenton PNP degradation, Light source: 14W cool white LED		
MNPs	50	7.45×10^{-8}
MGO	50	2.17×10^{-7}

As mentioned earlier, GO and MNPs both show negligible Fenton activity towards PNP. But the composite of GO and magnetite (MGO) exhibited substantially better PNP degradation Fenton activity, though it was not superior to SMNPs. Moreover, GO and MNPs have visible range bandgaps. The formation of nanocomposite enhances the charge separation rate in MGO, increasing the photo-Fenton photocatalytic activity towards PNP. Table 7.1 displays the TOF values for Fenton and photo-Fenton PNP degradation over different catalysts prepared in this thesis. The MGO photo-Fenton PNP degradation activity is the best among those investigated.

7.2 Future scope of this work

Future studies should consider the following points.

- The comparative Fenton activity of MNPs stabilized by other polymers or natural macromolecules (such as PVA, PVP, glutathione, etc.) should also be investigated.
- MD studies can further be carried out on other iron oxide phases known for their Fenton reaction activity towards specific organic pollutants.
- Detailed computational studies can be carried on the persulfate-based oxidation process using the prepared catalyst.
- Other support materials (2D materials like carbon derivatives, MoS_2) with visible range bandgaps can be explored for designing improved photo-Fenton catalysts.