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Conclusion

7.1 Summary

The primary focus of the thesis is on developing novel, emerging materials using facile synthesis methods that can be applied to potential applications addressing energy and environmental issues.

The major findings in the thesis are as follows:

1) 2D ZnO-Ti_3C_2 nanohybrid catalysts with varying wt.% of ZnO were synthesized through in situ hydrothermal methods. The experimental data revealed that the MXZnO-10 nanohybrid sample has a high MB degradation capacity of 99.2% after an irradiation time of 60 min with a high level of reproducibility, reusability, and stability through six catalytic cycles. Among the materials, MXZnO-5 shows the lowest overpotential of 495 mV at anodic 10 mA/cm^2 current density, a small Tafel slope of 108 mV/dec, and a contact resistance of 109 Ω. The photo- and electrocatalysis performance of hydrothermally synthesized 2D ZnO-Ti_3C_2 nanohybrids has been confirmed as an excellent nanostructure composition for photocatalytic, and electrocatalytic applications.
2) The Ti_3C_2Tx and ZnO-Ti_3C_2Tx catalysts are used for selective hydrodeoxygenation of methyl oleate as a model compound for bio-oil up-gradation to diesel-grade hydrocarbons. It is found that higher catalytic loading initiates the cracking process while lower catalyst loading gives intermediates aldehyde (-CHO), and alcohol (-OH) with less selectivity towards the desired n-C17 and n-C18 products. We understood that when the ZnO-$Ti_3C_2T_x$ catalyst (at 280°, 30 bar and 13h) was applied for selective HDO reaction, the synergy of metal oxide with 2D MXene resulted in 90.04% selectivity with 100% conversion. Surprisingly, the catalysts showed excellent recyclability without significant drop-in catalytic activity up to 5 test cycles. High HDO selectivity is very promising by reducing carbon dioxide footprint and carbon economy principle regarding future biofuel production via the green chemistry route. Advantageously, the solvent-free condition offers an excellent and green method for diesel-grade hydrocarbon production from biomass.
3) An effective sulphur-free and highly dispersed non-noble metal-based (Fe-doped SiO_2–Al_2O_3) heterogeneous catalyst with high surface area and excellent acidic sites has been developed for bio-jet fuel production. Catalytic hydrotreatment of methyl oleate over 10% Fe/SiO_2–Al_2O_3 demonstrated remarkable selectivity and reusability with complete conversion at 380 °C, 5 bar, and 5 h of reaction period. The maximum conversion and selectivity obtained for the 10 wt% Fe/SiO_2–Al_2O_3 catalyst are 100% and 74.13%, respectively. Furthermore, excellent conversion and selectivity were achieved using FAME of different oils (linseed, rapeseed, neem, and tung oils) under optimised reaction conditions.
4) The Gd-doped LMO was successfully prepared by a one-pot hydrothermal sol-gel route. A detailed analysis of magnetic properties were by correlating with Raman and DFT analysis. The results observed a high coercivity value for the doped LMO compared to pristine LMO, which scales down from 0.57 T to 0.14 T with an increase in Gd concentration. The current study revealed that Gd LMO shows paramagnetic nature at room temperature and undergoes paramagnetic to antiferromagnetic phase transition at very low temperatures owing to ion exchange between Mn and Gd ion. The susceptibility follows the Curie-Weiss law with a negative Weiss constant indicating the dominated antiferromagnetic interaction over paramagnetic. The obtained magnetic moment of the materials is due to the combined effect of Mn^{3+}-Mn^{3+} interaction with 3d-4f election spin coupling. Gd02 showed the highest magnetic moment (6.50μ_B) with Mr of 2.31 emu g^{-1} and Hc of 0.56 T.

7.2 Future scope

The synthesized materials can be further adapted for use in large-scale synthesis and commercial applications. For example, 2D MXene can be incorporated into many applications with repeated usability and easy recovery. Additionally, further studies can be performed for the degraded dye to confirm mineralization and its by-products after degradation. The MXene catalyst also can be used for all pharmaceutical drugs, which will help to reduce pollution. Incorporation of the 2D MXene into biofuel production can also help to reduce the carbon footprint during production. The catalytic activity of MXene and its surface group revealed that these materials can also be tested for possible biofuel and organic transformation applications. Furthermore, the synthesized high availability, low toxicity, and thermal stability $Fe/SiO_2–Al_2O_3$ catalyst can be utilized for jet fuel production from their biomass. Also, the excellent acidic sites can be optimized for bio jet fuel production by varying doping metal, temperature, reaction time, H_2 pressure and catalyst loading. The magnetic material Lithium manganese oxide can be correlated with the discharge capability. Also, the batteries can be tested and utilized under the magnetic field to explore the discharge capability.