

Harnessing a clean, affordable, and inexhaustible source of energy, its storage, and addressing environmental pollution necessitates extensive scientific attention. The depletion of these limited resources and their impact on the environment has motivated using alternative energy. Renewable energy sources are abundant and undependable. Renewable energy from solar and wind sources are irregular in nature, and diurnal and seasonal variations motivate the storage of renewable energy in a biomass-derived fuel, hydrogen, for later use. A greener, more attractive solution to this problem would be catalytic hydrocracking to produce biofuels and an electrocatalytic process to produce Hydrogen fuel. The main objectives laid out in this thesis are focused on the synthesis and engineering of materials with different morphological, structural, physical and chemical properties. The studies undertaken in this thesis attempt to address some of these issues.

MXenes have a general formula of $M_{n+1}X_nT_x$, where M represents an early transition metal (Ti, V, Nb, Ta, Cr, Mo, etc.), T refers to the surface terminating functional groups such as oxygen, fluorine, and hydroxyl group, X represent C or N and $n = 1, 2$ or 3 . MXene was synthesized in 2011 by the selective etching process of the Al from the MAX phase. This material exhibits remarkable properties such as metallic conductivity, hydrophilicity, redox activity, good dispersibility, and photochemical stability. Our study includes bandgap engineering of ZnO-MXene for Photocatalytic pollutant degradation and electrocatalytic hydrogen evolution reaction. The maximum photodegradation efficiency was demonstrated by the 10 wt % ZnO- Ti_3C_2 composite, which degraded the methylene blue (MB) dye by 76.4 % within 10 minutes of the reaction and by 99.2 % within 60 minutes. Excellent HER performance was demonstrated by the 5 wt % ZnO- Ti_3C_2 nanocomposite with overpotential of 495 mV at 10 mA/cm² and a Tafel slope of 108 mV/dec. Herein, $Ti_3C_2T_x$ and ZnO- $Ti_3C_2T_x$ catalysts were also demonstrated for selective hydrodeoxygenation reaction (HDO) of methyl oleate (MO) as the model compound. The synthesized ZnO- $Ti_3C_2T_x$ catalyst showed 100% conversion of MO with >90% selectivity for HDO product (n-C18). Additionally, the pure $Ti_3C_2T_x$ demonstrated 100% conversion with a selectivity of 67% for n-C17 hydrocarbon via the decarboxylation route.³

As a part of sustainable energy production, thesis work also focuses on solvent-free bio-jet fuel generation (C8 to C15) from the model substrate methyl oleate as well as various oils feedstocks (Linseed, Rapeseed, Neem and Tung oils) using Fe-loaded $SiO_2-Al_2O_3$ as solid acid catalyst. The acidic sites rendered by the Fe metal and $SiO_2-Al_2O_3$ support reveal that the catalyst is suitable for low pressure hydrocracking of methyl oleate into bio-jet fuel with excellent selectivity (>74 %) and complete conversion at 380°C, 5 bar H_2 pressure with 10% iron loading in five hours.

Additionally, the magnetic properties of LMO (lithium manganese oxide) and Gd-doped LMO were correlated with each other. The magnetic properties can easily identify the minor variations that SEM, TEM, FITR, and XRD cannot detect. Therefore, magnetism is also one of the essential tools for material properties. As a result of the Mn^{+2} or Mn^{+3} ions being replaced by Gd^{+3} ions from the octahedral 16d lattice location, the samples displayed a paramagnetic (at 300K) to antiferromagnetic (at 5K) transition and fluctuation in the magnetic moment. The superexchange process is revealed to be responsible for the phase changes that were detected in the hysteresis curve below the Neel temperature (TN) at 5K.

