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Master Thesis Defense

Entitled

SYNTHESIS, CHARACTERIZATION, ELECTRONIC STRUCTURE OF REDUCED GRAPHENE OXIDE MODIFIED FENBO4, NH2-MIL-125(TI) MODIFIED FENBO4 COMPOSITES AND THEIR PHOTOCATALYTIC ACTIVITIES

by

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Abstract

The production of value-added products through CO_2 utilization using Photocatalysis offers an alternative green route for CO_2 fixation. Wide bandgap photocatalysts allow the absorption of light in the UV region, which represents the lowest percent of the sunlight irradiation. On the other hand, narrow bandgap photocatalysts absorb light in the visible region, though the recombination rate of the generated electron-hole pairs affects their activity. In this thesis, the narrow band gap $FeNbO_4$ was synthesized, studied and efforts were made to reduce the recombination rate and enhancing the photocatalytic activity.

$FeNbO_4$ visible-light-driven photocatalysts were synthesized using various synthetic methods and different pH values and characterized using UV-vis DRS, PXRD, BET, SEM, and EDS. Monoclinic phase was obtained for all different preparation methods, where band gap and surface area varied with synthesizing method and pH value. $FeNbO_4$ prepared via co-precipitation method presented the highest surface area with a band gap value of 1.85 eV.

$FeNbO_4$ prepared via co-precipitation method was further synthesized incorporating rGO. Three different mass ratios of rGO were used, $FeNbO_4$-3%rGO, $FeNbO_4$-5%rGO, and $FeNbO_4$-10%rGO. Results confirm the successful incorporation of rGO into $FeNbO_4$ and the role of rGO in reducing the recombination rate. The prepared composites were examined for the photocatalytic cycloaddition of CO_2 into propylene oxide, where $FeNbO_4$-5%rGO exhibits the highest photocatalytic activity with a percent yield of 57%.

Moreover, three $FeNbO_4$/NH_2-MIL-125(Ti) composites with different mole ratios were prepared, characterized and their photocatalytic activity was evaluated for the same reaction. Obtained data confirms that reaction proceeds photocatalytically. $FeNbO_{4\ (75\%)}$ /NH_2-MIL-125(Ti) $_{(25\%)}$ showed the highest percent yield of 59%, results suggest the cooperative mechanism between $FeNbO_4$ and NH_2-MIL-125(Ti).

Both composites $FeNbO_4$/rGO and $FeNbO_4$/NH_2-MIL-125(Ti) have proven to be effective in increasing photocatalytic activity compared to $FeNbO_4$. As percent rGO increases, the photocatalytic activity increases showing the highest yield for $FeNbO_4$-5%rGO where rGO works as electron trapper, hindering electron-hole pairs recombination. The high percent yield obtained for $FeNbO_{4\ (75\%)}$ /NH_2-MIL-125(Ti) $_{(25\%)}$ is related to the capability of $FeNbO_4$ to absorb more light generating electrons that moves to the (LUMO) of NH_2-MIL-125(Ti), hence reducing the recombination rate. Future work could be directed toward testing various epoxides substrate to compare photocatalysts' effectiveness. Furthermore, different synthesizing methods for preparing composites could be implemented to enhance the interaction of both systems thus improving the photoactivity of the photocatalysts.

Keywords: Photocatalyst, Band gap, $FeNbO_4$, Composites, rGO, LUMO, Recombination, NH_2-MIL-125(Ti).