

Iron group metal oxide, specially, hematite ($\alpha\text{-Fe}_2\text{O}_3$) being highly abundant, low cost and non-toxic, material with a low bandgap of 2.1–2.2 eV has attracted immense attention in the recent past. It is widely used in a variety of applications such as lithium ion batteries, production of magnetic materials, visible light photocatalytic, water treatment, gas sensors, electromagnetic devices, paints and pigments, etc. However, there are certain drawbacks that limits the use of $\alpha\text{-Fe}_2\text{O}_3$ in solar energy harvesting such as low mobility of carriers ($< 0.1 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$) high recombination rates, short diffusion length (2–4 nm), short excited state lifetime ($< 10 \text{ ps}$), poor light absorption, improper band position for unassisted water splitting. Moreover, the nonmagnetic nature of $\alpha\text{-Fe}_2\text{O}_3$ restricts for microwave application. There is lot of impetus in improving its properties by structural modification, variation in morphology and by doping. Surface fluorination is reported to increase surface electric conductivity and charge density. Surface property has significant impact on any electrochemical process as the transport of electron and hole occurs through surface. The recombination rate of photogenerated electrons and holes can greatly reduce by F^- ions due to their strong electro-negativity. Actually, F^- ion acts as electron-trapping sites on the surface to trap the photogenerated electrons.

In this thesis work, a facile yet effective hydrothermal strategy has been developed for in-situ preparation of surface fluorinated $\alpha\text{-Fe}_2\text{O}_3$ by using N-Chloromethyl-N'-fluorotriethylenediammoniumbistrifluoroborate (tetrafluoroborate) or F-TEDA as a fluorinating agent that gives electrophilic fluoronium ion in solution as the reactive species. In order to understand the interaction and effect of fluorine with $\alpha\text{-Fe}_2\text{O}_3$ we focused on the interplay between the fluorine content (varying F-TEDA concentration 0% to 40%) and resulting structural, optical, photoelectrochemical and magnetic properties together with study on its application in visible light photocatalysis, dye sensitized solar cells, microwave absorption and uranium removal from waste water. Reaction of F-TEDA with $\alpha\text{-Fe}_2\text{O}_3$ precursor resulted in preferential growth of $\alpha\text{-Fe}_2\text{O}_3$ along (110) orientation by $\sim 35\%$, which is important for enhanced charge transport. On increasing fluorination, the dendritic leaf type $\alpha\text{-Fe}_2\text{O}_3$ converts to a snow-flake type structure (F-TEDA-20%) anisotropically growing along the six directions. Therefore, F-TEDA acted as a fluorinating as well as growth directing agent. However, at higher F-TEDA concentrations (above 30%), loosely held particulate aggregates are seen. The X-Ray Photoelectron Spectroscopy (XPS) suggest the maximum fluorination of $\alpha\text{-Fe}_2\text{O}_3$ at 1.21 atomic % in 30% F-TEDA.

Surface fluorinated $\alpha\text{-Fe}_2\text{O}_3$ was investigated for application of solar water splitting, magnetic & microwave absorption and uranium removal from waste water. Screen-printed films of fluorinated $\alpha\text{-Fe}_2\text{O}_3$ on FTO in photoelectrochemical cell exhibited an enhanced current density on illumination of $\sim 100 \text{ W/m}^2$. The increase in photoelectrochemical activity seems to be due to the combination of two factors namely preferentially growth of $\alpha\text{-Fe}_2\text{O}_3$ along (110) direction resulting in improved charge transfer efficiency and reduced recombination losses due to presence of fluorine. A photoanode made by 30% fluorinated $\alpha\text{-Fe}_2\text{O}_3$ in a ratio of 10:90 with respect to nano $\text{TiO}_2(\text{P}25)$ showed improved performance in dye sensitized solar cells with an increase in efficiency by $\sim 16\%$ in comparison to that of pure nano TiO_2 . Furthermore, upon fluorination with Selectfluor, the coercivity decreases and saturation magnetization increases systematically with increasing fluorine wt% due to transition from antiferromagnetic to ferromagnetic nature. Further, the material was evaluated for microwave absorption. The imaginary part of permeability (μ''_r) and magnetic loss tangent value ($\tan \delta_\mu$) of surface fluorinated Fe_2O_3 are found to be superior to pristine $\alpha\text{-Fe}_2\text{O}_3$. The maximum reflection loss in surface fluorinated Fe_2O_3 is observed at different frequencies as a function of sample's thickness; for example, RL -18 dB at 7.5 GHz ($t = 3.5 \text{ mm}$), -12 dB at 9 GHz ($t = 3 \text{ mm}$), respectively. These characteristics make this material a potential candidate, in fact better than pristine $\alpha\text{-Fe}_2\text{O}_3$, as radar absorbing material (RAM) both in C-band and X-bands. Fluorinated $\alpha\text{-Fe}_2\text{O}_3$ was also studied for uranium removal from waste water. The adsorption capacity of F- $\alpha\text{-Fe}_2\text{O}_3$ was affected by the pH, contact time and initial concentration of uranium. The optimal adsorption was achieved at around pH 5. The adsorption capacity of F- $\alpha\text{-Fe}_2\text{O}_3$ was found excellent (Langmuir $q_m = 79 \text{ mg/g}$) as compared to pristine hematite/ hematite composite and the equilibrium achieved in 1 h time.

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