Abstract

The present study focused on developing material having both electrocatalytic oxygen evolution property and Photo-electrochemical property. Several material were fabricated so as to find the experimental and theoretical determination of their physical properties. First of all, silver doped titanate nanosheets was fabricated with different atomic percent of silver doping in the lattice. Physical properties such as crystallinity, morphology, optical, electronic and electro-chemical properties were determined using different experimental techniques. Lattice volume expansion due to silver intercalation in titanate nanosheets were explored by TREOR and DICVOL algorithm. Titanate nanosheets with 2 atomic percent of silver doping shows optimum performance for both the electrocatalytic oxygen evolution and visible light photocatalytic degradation of methyl orange and phenol.

Afterwards, a novel n-type semiconductor, silver nitroprusside was fabricated by ion-exchange route. First principle calculation was employed with the help of density functional theory. Electronic band structure and density of states were calculated by an abinitio quantum chemistry calculation package, Quantum ESPRESSO. Ten least lying spin permitted transitions were deduced with the help of time dependent density functional theory calculation. Theoretically calculated properties of the material were compared with the experimental observation so as to see the concurrency of the result. Material was found to be efficient catalyst for both electrocatalytic oxygen evolution and photocatalytic degradation of an antibiotic drug chloramphenicol.

Afterwards, nano silver nitroprusside were fabricated using surfactant assisted self assembly of Ag^{+}. A faceted nano silver nitroprusside were also fabricated using the similar route with the help of hexamine addition in the precursor solution. For comparison purpose, nano silver phosphate was also fabricated using the same technique. Faceted nano silver nitroprusside shows highest performance for both the electrocatalytic oxygen evolution and visible light photocatalytic degradation of clioquinol. Afterwards, all the catalyst were employed for visible light photodegradation of clioquinol to compare the performance as both electrocatalyst and photocatalyst. Faceted nano silver nitroprusside shows optimum result for both electrocatalytic oxygen evolution reaction and photodegradtion of clioquinol.

Next, a novel semiconductor, copper nitroprusside nanosheet was fabricated using surfactant assisted self assembly. Electronic band structure and density of state were calculated with the help of first principles density functional theory calculation. Experimental observation was also compared with the theoretical calculation to check whether they are in good agreement or not. Material was found to be efficient for electrocatalytic oxygen evolution. Material photocatalytic properties were also observed using methylene blue as target pollutant but it shows some limitation due to weak optical absorbance in visible light.

Lastly, a novel polyoxometalate compound, ferric phosphotungstate was hydrothermally fabricated in nanoscale. Morphology, crystallinity, opto-electronic property and defect density of the ferric phosphotungstate microflower were estimated by several experimental calculation. It was observed that several defects in the material act as a electron trapper in conduction band of the material and thus hinder the electron-hole recombination. Photodegradation of neurotoxic drug amphetamine and electrocatalytic oxygen evolution were observed using this material, which shows efficient catalytic performance.

All the designed catalyst were used to degrade chloramphenicol to compare the optimum performance with respect to dual catalytic activity. Based on the result, a brief conclusion was drawn.

keywords: Photocatalysis, Electrocatalysis, Oxygen evolution reaction, Titanate, Nanosheet, Silver nitroprusside, copper nitroprusside, Methyl orange, Phenol, Chloramphenicol, Clioquinol