Title of the Project: Development of $Ti_3C_2T_x$ MXene composites with metal oxyphosphides/phosphides for electrocatalysis applications: Evaluation of structure-activity relationship

Abstract: The United Nations estimated that the world population will reach 12 billion by 2100. This estimation gives rise to a serious question- Is it possible to meet the energy demands of these 12 billion people? If yes, then do we have enough renewable energy resources/infrastructure to fulfil the need?

Climate change is one of the major challenges that the world is going through. There are many factors responsible for the climate change, burning of fossil fuels for energy requirement is one of them. To overcome this problem, the inclination of scientific community towards clean energy sources has increased. Out of many alternatives, hydrogen (H_2) can also be a clean and an environment friendly source. H_2 can be utilized directly in vehicles or in fuel cells to provide energy. At present, there are various possible sources for the generation of H_2, such as water, fossil fuels and biomass. Production of H_2 using fossil fuels or biomass is not beneficial as these leads to environment pollution but H_2 generation by water is a good and eco-friendly technique. The technique adopted for generation of H_2 from water is called water splitting where water (H_2O) is split up into H_2 and Oxygen (O_2). This technique has gained significant interest as it does not produce any unwanted side products. Both end products of splitting reaction are useful i.e., H_2 is used for energy production and O_2 is good for environment. The production of H_2 from water has been studied by various approaches like electrochemical, thermochemical, photochemical, and photoelectrochemical routes. Since, water splitting is an energy-demanding process so this requires a positive change in the Gibbs free energy ($\Delta G° = 237$ kJ/mol), for reaction to be successful. If the energy demand is not met then the water splitting (generation of H_2 and O_2) remains unsuccessful.

All the approaches, as mentioned above for generation of H_2 are successful enough but they have one or more limitations when applied to water splitting reaction. Thermochemical approach for water splitting demands a temperature of more than 400 °C which sometimes become challenging. Photochemical process can be successful in presence of light only and its efficiency is very low. In photoelectrochemical technique, photoelectrode stability is an issue. Thus, electrochemical approach is chosen in our work for water splitting. The electric current will be used for overcoming the reaction barrier of water splitting reaction. When an electric current runs through water, the chemical decomposition of water into H_2 and O_2 occurs at the respective electrodes. Electrocatalytic water splitting has grown a significant importance in recent years as a means of increasing efficiency and cost-effectiveness of splitting reaction. Electric energy has the greatest potential to meet future energy demands under the rules of sustainability.

This water splitting energy system basically relies on three fundamental reactions to meet these demands: oxygen evolution reaction (OER), hydrogen evolution reaction (HER), and oxygen reduction reaction (ORR). The kinetics of these fundamental reactions are slow, limiting their energy efficiency and broad applicability. Highly efficient and stable electro-catalysts are required to improve the efficiency of the aforementioned processes so electrochemical approach is adopted and efforts will be made for the development of electro-catalyst. The primary purpose of this project will be to develop a high-efficiency electrocatalyst for cleaner energy production. Most catalysts are only active in a single electrochemical system, it is challenging to develop appropriate bifunctional/trifunctional catalysts for OER, HER, and ORR simultaneously. As a result, the focus of this research is on designing bifunctional/trifunctional catalysts that aid in increasing the performance of this sector's self-powered water-splitting process. MXenes, or transition metal carbides and nitrides, are two-dimensional (2D) inorganic compounds made up of a few atomic layers of transition metal carbides, nitrides, or carbonitrides. MXenes are being touted as a new class of catalytic materials. It's a desirable 2D material for a variety of reasons, including, chemical and mechanical stability, single- and multilayered structure and synthesis from heavier and lighter transition metals, which aid in valence electron tuning. MXenes' surfaces can also be functionalized with a variety of chemical groups. These features distinguish MXenes as effective 2D materials. The proposed study seeks to synthesize $Ti_3C_2T_x$ MXene with finely regulated surface characteristics and assess its structure-activity relationship.