Development of multifunctional thermo-photocatalytic materials for carbon dioxide reduction to fuels and photodegradation of persistent organic pollutants

Access to safe drinking water is currently a significant challenge worldwide, 3 in 10 people worldwide, totaling 2.1 billion, lack access to safe, readily available water at home.

Rapid industrialization and uncontrolled population growth contribute to the deterioration of water quality through the discharge of toxic pollutants. The persistent organic and emerging pollutants like personal care products and pharmaceuticals, pesticides, industrial and household chemicals represent a new water quality challenge, with still unknown long-term impacts on human health and ecosystems. A reduction of about one-third of the global biodiversity is estimated to be a consequence of the degradation of freshwater ecosystems, mainly due to pollution of water resources and aquatic ecosystems. The water demand will not decrease. Therefore, improving water treatment technology is the most critical task to increase water quality and lower the risk of further contamination. In this regard, one of the primary challenges that societies will face during the 21st century is improving water quality by reducing pollution, minimizing the release of hazardous chemicals, halving the proportion of untreated wastewater, and substantially increasing recycling and safe reuse globally using the fundamentals of green chemistry and green engineering processes.

The second emerging problem of the present time is global warming due to anthropogenic CO_2 emissions. Carbon dioxide (CO_2) is a primary greenhouse gas, which except the increasing global warming, causes ocean acidification, and as a result, threatens the survival of millions of people, plants, and animals. In this regard, the conversion of carbon dioxide into value-added products is of great industrial and environmental interest. However, carbon dioxide is a relatively stable compound, and the input energy required for its conversion is a significant limiting factor. The conventional industrial processes derive heat from fossil fuel incineration to fulfill the energy demand, further contributing to CO_2 release. In this regard, the photocatalytic conversion of CO_2 is considered a promising approach in developing a carbon-neutral energy system, where solar light and photocatalyst are employed to overcome the kinetic limitations of the CO_2 reduction processes.

The main objectives of the present study are related to (i) design and customizing advanced solar energy-driven photocatalysts for the elimination of persistent organic pollutants and (ii) development of advanced photocatalytic materials for energy applications able to contribute to the reduction of greenhouse gasses. In this regard, we propose systematically studying the problem of photocatalyst modifications with respect to the exposed crystal facets to enhance the efficiency of the photocatalytic process. Moreover, new photocatalytic materials from the group of MXenes and scheelite-type compounds, as well as hybrid inorganic-organic materials based on graphitic carbon nitride, graphene oxide, hexagonal boron nitride, will be applied for thermal photoreduction of CO_2 to valuable compounds and photodegradation of sulfamethoxazole, ofloxacin, triclosan, diclofenac, and carbamazepine belonging to the group of pharmaceutical compounds not susceptible to biodegradation.

Both proposed objectives will be synergistically addressed, firstly through theoretical-computational approaches to evaluate and analyze relevant physicochemical parameters of the photocatalytic materials, such as band structure, excitations, or optical properties that enhance the photocatalytic activation under visible light. Moreover, the model for quantitatively describing the relationship between the structure and the properties of photocatalysts will be developed and allow to optimize the photocatalytic process.