Engineering and Innovation Research Studentship October 2021

Project title:	**Advanced functional materials for synthesising photocatalytic solar fuel**
Discipline	**Materials Engineering, materials for energy, Energy storage**
Key words:	Photocatalysis, 2D materials, surface engineering, plasma functionalisation, hydrogen energy
Supervisory team:	**Satheesh Krishnamurthy, Sudhagar Pitchaimuthu, Silvia Varangolo and N.S Braithwaite**
URL for lead supervisor's OU profile	http://www.open.ac.uk/people/sk9268

Project Highlights:

- Advanced 2D materials and functionalisation of photo/electrocatalytic materials for textile wastewater treatment
- High end fundamental knowledge development and characterisation for alternative oxidation processes to water oxidation
- Prototype development

Overview:

This research engages with the central concern of synthesis/processing of 2D materials such as mXene, MoS_2 and other similar groups of materials as light-driven catalysts for photocatalytic wastewater treatment.

Thever-increasing population and the continuous thriving economic development have raised the global energy demand by orders of magnitude. As of now, the majority of our energy needs are derived from fossil fuels such as coal, oil, and natural gas. However, the gradual depletion of fossil fuels and the adverse effects fossil fuels pose to the environment have stimulated intense research to develop novel strategies to derive sustainable and clean energy sources. Conversion of solar energy to chemical energy via artificial photosynthesis could be an ideal solution to address these energy and environment issues, providing us with carbon-free energy resources. Water oxidation is the most crucial part of both natural and artificial photosynthesis processes. The major hurdle in achieving high efficiency in artificial photosynthesis is the inherent slow kinetics of the water oxidation reaction. In a practical water-splitting system, oxygen evolution reaction (OER) occurs at the anode and hydrogen evolution reaction (HER) at the cathode. To overcome the energy-demanding bottleneck of OER, developing highly active catalysts have excellent stability, and need low overpotential is crucial. RuO_2 or IrO_2 are currently the leading OER catalysts due to their stable performance in a wide pH range i.e from acidic to alkaline media. But their applications are restricted to a great extent due to their low abundance and high cost. Therefore, it is important to develop highly efficient OER catalysts that are earth-abundant and less expensive. Atmospheric pressure plasma is a novel tool for materials processing and functionalisation of 2D materials. It has been found that atmospheric pressure plasma jets can enhance the crystallinity and charge transport properties of both inorganic and organic materials in-addition to improving hydrophilicity. In this project, atmospheric pressure plasma would be used to functionalise nanostructures i.e nanoparticles and thin films as OER catalysts. The catalysts would be tested for stability in alkaline, neutral and acidic pH conditions. Traditional, metal oxide catalysts fail to show the high activity in pH < 7 conditions. Hence, it is highly desired that the catalyst operates optimally at neutral pH (ideally in lower pH regimes) in comparison to commercial RuO_2 or IrO_2 OER catalysts and hence reducing target pollutants (textile dyes).

The project is an inter-disciplinary with the intention to advance the ways that we design for catalysis using plasma, materials engineering and electrochemistry.

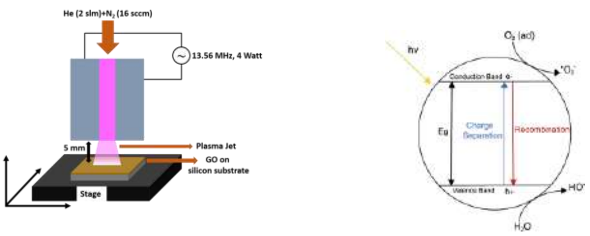

Figure on the left show inhouse atmospheric pressure plasma jet for functionalisation of 2D materials and right is the photocatalytic mechanism. The photo-generated charge carriers (electron and hole) in TiO_2 produce hydroxyl and superoxide radicals which capable to oxidize the target pollutants.

Methodology:

The development of novel photocatalysts/ anodes and to exploit their unique reactivity for the selective oxidation of organic substrates. The objective is to develop highly efficient water oxidation route and to produce high-value chemicals via photooxidation to enable early-stage commercialisation of solar fuel technologies. Ultimately, the light-driven oxidation of organic/inorganic substrates will be coupled to fuel synthesis as the cathodic process.

Chemical and plasma processing facilities to tune the properties of the materials.

Analytical methods include cyclic voltammetry with AM1.5 Solar simulator, chromatography (GC, HPLC, MS) and X-ray Photoelectron spectroscopy to identify electronic properties.

For morphological studies, Scanning Electron Microscopy, Atomic Force Microscopy , Transmission Electron Microscopy. All these facilities are available at OU for the candidate.

Indication of project timeline:

Year 1: Literature survey and selection of new materials synthesis and optimisation
Year 2: Optimisation of selected material and its deeper mechanism. Conference presentation and field trials
Year 3: prototype development with reactor design, dissemination manuscript writing, Complete thesis write-up.

Field visit: Professor Krishnamurthy has recently secured major European Union Horizon funding for textile wastewater treatment. The PhD student will have opportunity to travel to textile industries in Turkey and other institutes in Italy and Spain.

Further reading:

1. Synthesis of MoS 2-TiO_2 nanocomposite for enhanced photocatalytic and photoelectrochemical performance under visible light irradiation, M. Mehta, A. P Singh, S. Kumar, S. Krishnamurthy, B. Wickman, S. Basu, 2018, Vacuum, 6,6
2. Plasma Jet Printing and in situ Reduction of Highly Acidic Graphene Oxide, Avishek Dey, Satheesh Krishnamurthy, James Bowen, Dennis Nordlund, M Meyyappan and Ram P Gandhiraman, 2018, ACS Nano, 5,23
3. Tuning the properties of a black TiO_2-Ag visible light photocatalyst produced by rapid one-pot chemical reduction, Michael Coto, Giorgio Divitini, Avishek Dey, Satheesh Krishnamurthy, Najeeb Ullah, Cate Ducati and R Vasant Kumar, Materials Today Chemistry, 2018 142-149
4. Synthesis of MoS_2-TiO_2 nanocomposite for enhanced photocatalytic and photoelectrochemical performance under visible light irradiation, Manan Mehta, Aadesh P Singh, Sandeeep Kumar, Satheesh Krishnamurthy, Björn Wickman, Suddhasatwa Basu, Vacuum, 2018, 675

Further details:

Students should have (or expect to obtain) at least the equivalent of a UK upper second class honours degree (and preferably a Masters degree) in chemistry, materials science, solid state physics or other relevant scientific disciplines. Knowledge of synthetic and characterisation techniques for inorganic materials and a broad interest in sustainable chemistry would be an advantage.The student will join a well-established team researching on materials functionalisation for solar energy, solar fuels and battery group.

Please contact **Satheesh Krishnamurthy Satheesh.krishnamurthy@open.ac.uk** for further information.

Applications should include:

- A 1000 word cover letter outlining why the project is of interest to you and how your skills match those required
- an academic CV containing contact details of three academic references
- an Open University application form, downloadable from: http://www.open.ac.uk/postgraduate/research-degrees/how-to-apply/mphil-and-phd-application-process
- IELTS test scores where English is an additional language

Applications should be sent to **STEM-EI-PhD@open.ac.uk by 05.03.2021.**