# The University of Queensland - IIT Delhi Academy of Research Joint PhD Project

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| **PROJECT TITLE** | **STRUCTURAL AND COMPOSITIONAL CONTROLLED CARBON-BASED ELECTROCATALYSTS FOR EFFICIENT OXYGEN REDUCTION REACTION** |
| **PROJECT CODE** | **UQIDAR 00187** |
| **PROJECT DESCRIPTION** | Polymer electrolyte membrane fuel cells (PEMFCs) convert chemical energy generated by the electrochemical reaction between hydrogen and oxygen to electrical energy with high conversion efficiency and low/zero emissions. PEMFCs typically employ the highly active platinum (Pt)-based electrocatalysts. Despite their high activity, Pt-based electrocatalysts suffer from the high cost, low abundance, susceptibility to carbon monoxide and methanol poisoning, and poor long-term stability. Furthermore, the slow kinetics of the cathodic oxygen reduction reaction (ORR) becomes the limiting half-reaction in PEMFCs. Therefore, it is important to develop inexpensive, earth-abundant, and stable non-precious metal-based electrocatalysts with high activities toward ORR. This project aims to develop high-performance carbon-based electrocatalysts for accelerating the ORR kinetics by using elaborately designed metal-organic framework precursors. The key concept lies on the thermal exfoliation of two-dimensional metal-organic frameworks (2D MOFs) to prepare carbon-based electrocatalysts with desirable features for ORR, such as controlled structures, rich defect sites, and heteroatomic doping. This project will involve the preparation of various 2D MOF precursors by wet-chemical methods (e.g., low-temperature precipitation, hydrothermal/solvothermal, etc.). This is followed by the thermal exfoliation of these 2D MOF precursors under inert atmosphere in the presence of metal chlorides as exfoliators to generate 2D carbon-based with desirable features for ORR. The developed 2D MOF precursors and the corresponding carbon-based electrocatalysts will be characterised by various techniques, including X-ray diffraction (XRD), scanning/transmission electron microscopy (SEM/TEM), X-ray photoelectron spectroscopy (XPS), BET surface area analysis, etc. The ORR performances of these carbon-based electrocatalysts will be evaluated using an electrochemical workstation with a three-electrode system. Important performance parameters, such as activity, kinetic current density, electron transfer number, long-term stability will be evaluated. The mechanisms for ORR will be studied by in-situ techniques or theoretical calculations. |
| **PROJECT OUTCOMES** | (1) Novel methods for generating defect-rich, heteroatom-doped carbon-based electrocatalysts via the thermal exfoliation of 2D MOFs will be developed.<br>(2) New knowledge on the rational design of high-performance carbon-based electrocatalysts for ORR, especially in terms of structure and composition, will be generated.<br>(3) Greater mechanistic understanding on the effects of heteroatomic doping, lattice defects, and morphology on the ORR activities of carbon-based electrocatalysts will be achieved through the use of in-situ techniques and/or theoretical simulations.<br>(4) Joint publications between AIBN and IITD in high-impact materials science and chemistry journals, such as ACS Nano, Nano Energy, Angewandte Chemie International Edition, ACS Catalysis, Advanced Materials, Nature Communications, etc. |
| **ADVISORY TEAM** | **Professor Yusuke Yamauchi**<br>Australian Institute for Bioengineering and Nanotechnology (AIBN), UQ<br>https://aibn.uq.edu.au/profile/4422/yusuke-yamauchi |

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| | **Professor Ashok Ganguli**<br>Chemistry, IITD<br>http://web.iitd.ac.in/~ashok/home.html |
| **TYPE OF STUDENT** | Applications are open to **i or q student**s who meet eligibility criteria. |
| **DISCIPLINE BACKGROUND OF STUDENT** | Ideally, this project requires students with a background in: Materials science and engineering, inorganic chemistry, organic chemistry, electrochemistry, chemical engineering, nanotechnology |
| **IDEAL CANDIDATE** | **Essential capabilities:** Nanomaterials synthesis, materials characterisation<br><br>**Desirable capabilities**: Scientific writing experience, electrode fabrication, electrochemical analysis, theoretical simulations (such as density functional theory simulations)<br><br>**Expected qualifications** (courses, degrees, etc): Bachelor or Master degree in Materials Science and Engineering, Chemistry, Nanotechnology, Chemical Engineering, Environmental Science |
| **APPLICATION PROCESS** | Apply online by the due date: https://www.uqidar.org/students/how-to-apply/ |