

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

PROJECT TITLE	RATIONAL DESIGN OF MATERIALS FOR ENERGY APPLICATIONS
PROJECT CODE	UQIDAR 00171
PROJECT DESCRIPTION	In search for a sustainable supply of energy, development of green and renewable processes is desirable for mitigating climate change. Towards fulfilling this goal, design of nanoscale materials with desirable level of catalytic and/or electrocatalytic properties, essentially holds the key to success. In this proposal, a bottom-up approach is adopted, wherein quantum mechanical ab initio density functional theory (DFT) simulations of reactions occurring on the material surface are guiding the rational design of the materials. Classical molecular dynamics (MD) simulations are further applied to dictate material design with desired functionalities. Overall, the ab initio level theory and classical molecular simulations provide us a mechanistic insight into the reaction, which in-turn offers us an opportunity to engineer the material itself. This is often implemented in experiments by changing the material surface, morphology and the characteristic length scales. The project proposal aims to identify well-defined materials for energy and catalytic applications.
PROJECT OUTCOMES	<ol style="list-style-type: none"> 1. Materials for energy and catalytic applications with desired functionalities 2. Understanding on reaction mechanisms, active sites and reactivity of the material. 3. Principles for materials design, structure-function relationships. 4. Development of theoretical methods and protocols for material design.
ADVISORY TEAM	<p>Professor Debra Bernhardt http://www.aibn.uq.edu.au/profile/2001/debra-bernhardt d.bernhardt@uq.edu.au Australian Institute for Bioengineering and Nanotechnology (AIBN) The University of Queensland</p> <p>Associate Professor M. Ali Haider http://web.iitd.ac.in/~haider haider@iitd.ac.in Department of Chemical Engineering Indian Institute of Technology Delhi</p>
TYPE OF STUDENT DISCIPLINE BACKGROUND OF STUDENT	<p>Applications are open to i/a students who meet eligibility criteria.</p> <p>Ideally, this project requires students with a background in chemistry, chemical engineering, physics, material science and engineering, nanotechnology</p>
IDEAL CANDIDATE	<p>Essential capabilities:</p> <ul style="list-style-type: none"> • Strong undergraduate background in science or engineering; • Excellent analytical skills; • Ability to work in a team; • Self-motivated; • Excellent written English; • Interest in computational screening of materials <p>Desirable capabilities:</p> <ul style="list-style-type: none"> • Some computational experience; Communication skills, CSIR/JRF fellow (for i-student)

APPLICATION
PROCESS

Expected qualifications (courses, degrees, etc):

- BSc or B.Eng. with majors in Chemistry, Chemical Engineering, Material Science, Physics or related areas. M.Tech degree (for i-student) or
- M.Sc. degree with CSIR/JRF fellowship. B.Tech degree (preferably from IITs, NITs and other reputed institutes). BSc (Hons 1) or equivalent (for a-student)

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