



## PhD Project

Project Details	
Project Title	Two Dimensional Molecular Sieves for Post-Emission Carbon Capture
Project Summary	<p>An 100 % increase in atmospheric CO<sub>2</sub> concentration from the year 1750 to 2020 is largely attributed to human activities such as industrialization and burning of fossil fuels<sup>1</sup>. Postemission carbon capture from CO<sub>2</sub> emissions is a rapidly growing technology with several existing commercial installations. Currently, chemical absorption of CO<sub>2</sub> using amines is the widely used technique with high selectivity for CO<sub>2</sub> and reasonable gas flow rates. However, the capture and regeneration processes are extremely energy intensive consuming approximately 20 – 30% of the power plant output. Membrane based gas percolators and molecular sieves are an excellent alternative with very low costs and high energy efficiency. Recently, atomically thin two-dimensional materials are being deployed with the polymer membranes to provide newer ways of molecular permeation control with greater selectivity and flow rates. Here, we propose to develop complete CO<sub>2</sub> segregation solutions using nanochannels in few layer atomic sheets suspended over inexpensive nanopore platforms. The solution is aimed to have good gas selectivity, high permeation rates, low installation and operation costs, and energy efficient. We will strive to have the solution locally manufacturable. Currently, there are no Indian solutions to this extremely pertinent and most glaring environmental challenge. A commercial, cheap and energy efficient solution will have a large market space ranging from large industries to millions of small automobiles.</p> <p>Interdisciplinary nature: The proposed research requires close interaction between physicists doing first principles studies, chemists with molecular dynamics expertise and material scientists with experimental experience with low dimensional materials. The proposed members are already closely working on several research avenues and have an excellent working platform with complementing expertise.</p> <p>Man-power requirements: A full-time PhD candidates is required to conduct experimental and theoretical work in parallel.</p> <p>End Users and Stake-holders: The proposed research has excellent commercial scope. The research is aimed at development of graphene based membrane for desalination and carbon capture which are among the most urgent requirement for the country at present.</p>

**PhD Supervisors (Equal contributions)**

<b>Role</b>	<b>Faculty</b>	<b>Academic Unit in IITD</b>	<b>Email ID</b>
Supervisor 1	Saswata Bhattacharya	Physics	saswata@iitd.ac.in
Supervisor 2	Krishna Balasubramanian	Material Science and Engineering	bkrishna@mse.iitd.ac.in
Supervisor 3	Tarak Karmakar	Chemistry	tkarmakar@iitd.ac.in

**Project requirements (Student qualifications, experience required, etc)**

- MSc/ME in Physics/Chemistry/Materials Engg with background/interest in computational materials
- Interest to learn and conduction research in inter-disciplinary field

**Source of funding (IRD/FITT Project details, if any)**

# We propose to recruit candidates with external funding such as CSIR JRF or use the institute permitted MHRD quota for the research.

**Role of Faculty Members involved:**

S. Bhattacharya: First principles of defect engineering in two dimensional materials for precision molecular permeation.

K. Balasubramanian: 2D material synthesis, experimental membrane fabrication

T. Karmakar: Classical molecular dynamics simulations and Ab-initio calculations