NANYANG TECHNOLOGICAL UNIVERSITY

IITM NTU JDP PROGRAM REPORT 2022

Diamond Jubilee 2018 2019

IIT MADRAS

IITM NTU JDP PROGRAM REPORT – 2022

A Joint doctoral degree programme with two of the prestigious research institutions, IIT Madras and NTU Singapore provides a unique opportunity and international platform to scholars to perform and assess the research work with the utilization of facilities of two of the pioneering institutes. Moreover, the guidance from two expertise faculties combined together gives an overwhelming and prodigious research experience. Such exposure to cutting edge research is a great motivation and helps in growing self-confidence.

So far 8 beneficiaries have been benefitted through this program

Name	Roll no	Beneficiary	Research Topic
Vinothkumar Sundharamoorthi	ME15D048	2020 & 2021	Precision machining of aluminium alloys and effects of quilting on machined surface
Vishnupriya R	AM17D011	2020 & 2021	Brain computer Interface
Gayathri R	PH17D045	2020 & 2021	Femtosecond light transport through wave guiding media
Rakhi Agarwal	AM18D004	2020 & 2021	Motor learning (yet to be completely finalized)
Kavita Devi	CY20D071	2022	Synthesis and characterization of novel main group compounds and their application in catalysis.
Shoumick Mitra	CE20D033	2022	Atmospheric Geochemistry
Divya Thokala	CE20D019	2022	Experimental and Computational Hydraulics
SELVAM R	CY19D053	2022	Design, Synthesis and Application Ion Pair Chiral Halogen Bond Donor Catalysts For Asymmetric Synthesis

Beneficiaries Report:

"SYNTHESES AND CHARACTERIZATION OF NOVEL MAIN GROUP COMPOUNDS AND THEIR APPLICATIONS IN CATALYSIS"

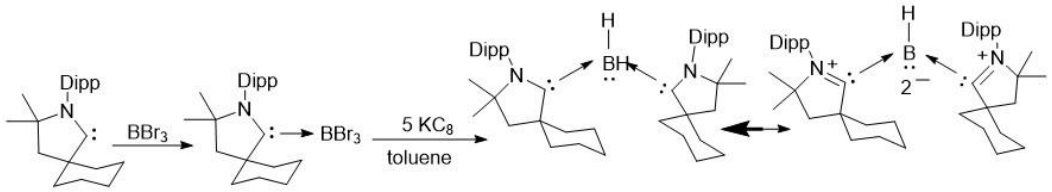
KAVITA DEVI
CY20D071
Ph.D Chemistry

Brief Description about my Research:

In main group elements, the group 13 elements, in general, adopt +3 oxidation states in most of the cases, hence producing electron-deficient compounds. To compensate electron deficiency, they promptly form adducts and undergo hyper-valent bonding, therefore they act as Lewis's acids. In 2005, Bertrand's research group reported the preparation of a new class of stable five-membered carbenes called cyclic(alkyl)(amino)carbenes (or in general, cAACs), which possess better electrophilic and nucleophilic properties compared to NHC carbenes. The comparative reactivity of different stable carbenes has been performed, and cAACs have emerged as important ligands. Due to excellent electrophilic character and smaller singlet-triplet gap, cAACs under mild conditions can activate small molecules such as H_2, CO and P_4 and even enthalpically strong σ-bonds like those of Si-H, P-H, B-H and N-H. Probably, one of the prominent uses of cAACs in boron-chemistry was to synthesize tricoordinate organoboron compound **1a** by the reaction of a parent borylene with the cAAC, in which boron features +1 oxidation state. Recently, more interesting results in borylene (:BR) chemistry, in which unique reactivity of the boron atom in a low oxidation state is explored; have been reported.

Our work focuses on the syntheses and development of cAAC containing Boron compounds which can activate various strong bonds like N-H, O-H and N_2 molecule. This work was inspired from the isolation of compounds containing diborane flanked by two cAAC ligands, which have been used in exotic chemical reactions by various research groups, for instance, the activation of CO, CO_2, acetone and dinitrogen (**2a**). The catalytic activation of these strong bonds has been of major industrial importance and replacement of toxic metals with main group elements can help in achieving a greener chemistry approach.

Figure 1a: Previously reported tricoordinate organoboron compound by the reaction of a parent borylene (:BR) with the cAAC:



My future research work: The proposed research is directed with the aim of developing a suitable system which can be effective in reducing N_2 to NH_3, which is as follows,

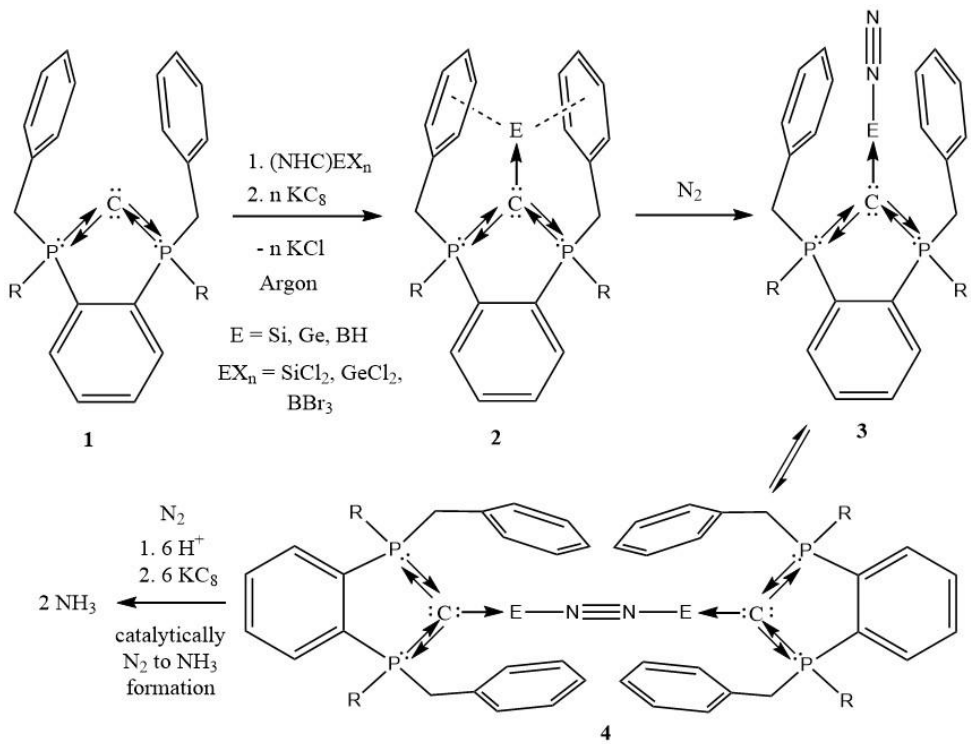


Figure 2a: Effective reduction of dinitrogen to Ammonia catalyzed by carbene stabilized main group elements.

“DESIGN, SYNTHESIS AND APPLICATION ION PAIR CHIRAL HALOGEN BOND DONOR CATALYSTS FOR ASYMMETRIC SYNTHES ”

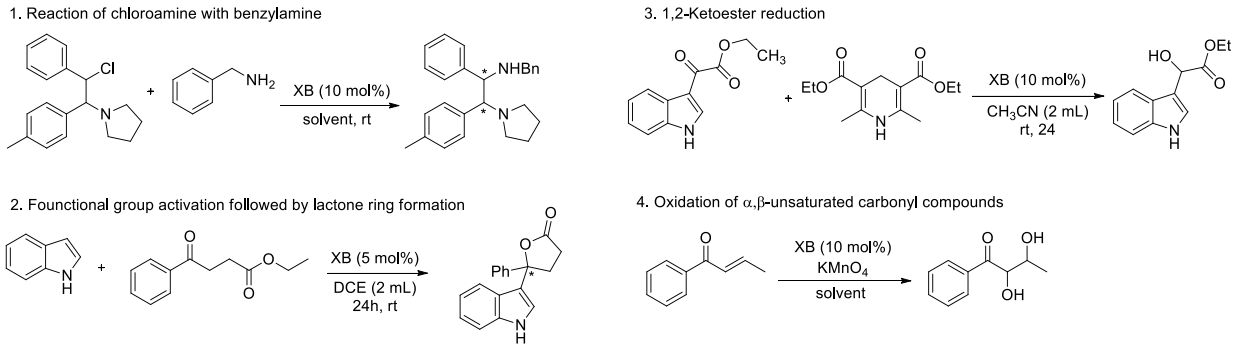
SELVAM R
CY19D053
Ph.D Chemistry

Brief Description of Research

Enantioselective synthesis is a key process in modern chemistry and is particularly important in the field of pharmaceuticals, as the different enantiomers of a chiral molecule often have different activities. Recently, asymmetric organocatalysis has been a key transition from the conventional transition metal-catalyzed enantioselective synthesis since it avoids the use of expensive and toxic transition metals. Halogen bonding is an emerging domain in metal-free organic transformation, and its net attractive interaction between an electrophilic region of the halogen atom in a molecular entity, and a nucleophilic region in another or the same molecular entity.[1] Halogen bonding is similar to other non-covalent interactions. However, it is comparatively less explored to its contemporaries due to the lack of its in-depth studies in the field of organic synthesis. More recently, the hypervalent iodine catalyst has fascinated the organic chemists due to its high electrophilic reactivity over the low valent iodine catalyst.[2]

This research proposal deals with designing and synthesizing of a new class of chiral ion pair catalyst through halogen bonding concept. The proposal has been divided into two parts. The first part deals with cationic iodine (III) stabilized by chiral anion whereas the latter part of the proposal involves chiral iodine (III) cationic catalyst derived from alkaloids and BINAM scaffolds (Scheme 1).[3]The cationic iodine (III) catalyst can be prepared by reacting iodo-compounds with m-CPBA followed by the addition of acids to give the corresponding ion pair catalyst. Further, the desired counter-anions can be attained by anion exchange.[4]The newly synthesized chiral catalyst will be characterized by various techniques. This will be followed by subjecting it with various substrates to study the difference between chiral ion pair catalyst and their reactivity.

Further, we intend to use the new chiral halogen bonding catalyst for the development asymmetric synthesis, such as 1)reaction of chloramine with benzylamine, 2)lactone formation, 3)ketoester reduction, and 4)oxidation of α,β-unsaturated carbonyl compounds (Scheme 2).



(**Scheme 2**)

Also, a detailed and in-depth mechanistic study is crucial to understand the mechanism and asymmetric induction of the proposed asymmetric synthesis. Finding an appropriate favourable diastereomeric transition state which will give the major enantiomer of the product (asymmetric induction) will be pivotal in this proposal. Prof. Choon Hong of NTU has excellent knowledge as well as a full-fledged lab dedicated to the area of asymmetric synthesis using ion-pair organocatalysts and halogen bonding catalysis.[5] Prof. Hong's expertise and guidance will be helpful in executing this research proposal at NTU as a successful research project. This project, if proven successful, will open up a new avenue of chiral halogen-bonding catalysts.

References: 1) Cavallo, G.; *Chem. Rev.* **2016,***116*, 2478-2601. 2) Sutar, R. L.; Huber, S. M., *ACS Catal.* **2019,***9*, 9622-9639. 3) Zhang, Y.; Han, J.; Liu, Z.-J., *RSC Adv.* **2015,***5*, 25485-25488. 4) Huber, S. M.; Weiss, R., *Angew. Chem. Int. Ed.***2018,***57*, 3830-3833. 5) Zhang, X.; *Science* **2019,***363*, 400-404.

"EXPERIMENTAL AND NUMERICAL STUDY OF EFFICACY OF A SUBMERGED SPUR DIKE FOR RIVERBANK PROTECTION DURING FLOODS"

THOKALA DIVYA
CE20D019
Ph.D Civil Engineering

Brief Description of Research

Rivers have been playing a foremost role in the evolution of human civilization. They are exceptionally valued for a variety of reasons including spiritual, ecological, aesthetic, and practical reasons. The effects of riverbank failure are miscellaneous: social, health, economic, and sometimes political. The social impacts are main that include loss of homes, agricultural land. Spur dikes are constructed to protect banks in rivers represent a great impact on flow depths and velocity fields.

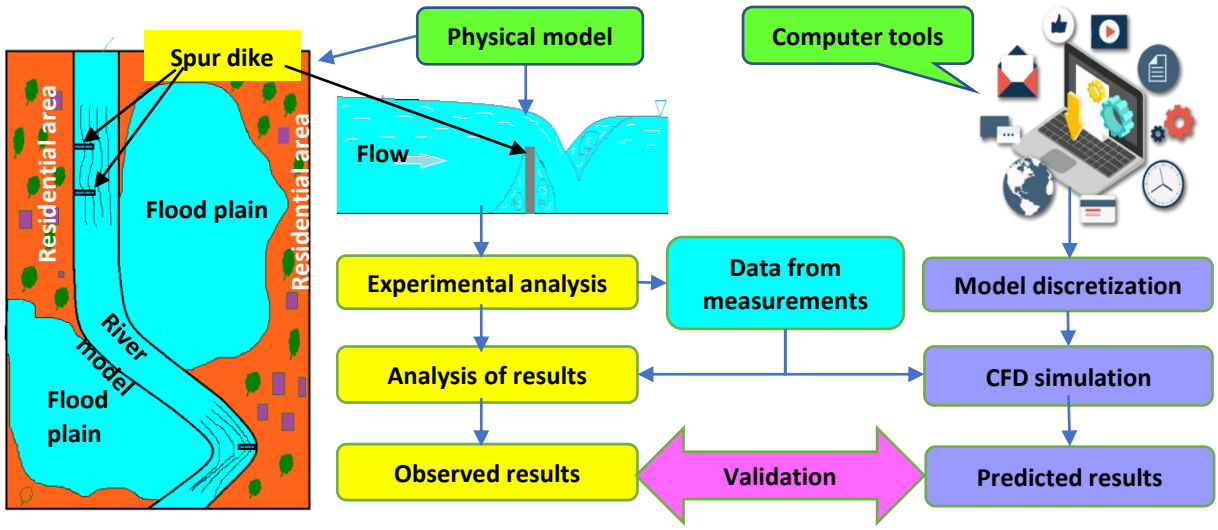
The spur dikes are so far designed considering the maximum flood level so that they can withstand floods. However, this has resulted in siltation on the riverbed over time and many rivers have become vulnerable to floods. A new concept is evolving by designing *submerged spur dikes*, which are found to be a viable option for riverbank protection. This has motivated the investigator to conduct exhaustive experiments and numerical simulations to understand flow and morpho dynamics around a submerged spur dike for various design parameters.

The research on spur dikes is well explored for non-submerged conditions. However, they are non-submerged during low flow conditions and submerged during high flows. The flow mechanism in its vicinity significantly may vary especially during unsteady flood flows. Therefore, it is indispensable to have a study on submerged spur dikes.

Numerical investigations nowadays are more concerned ascribed to their flexibility, time, and simplicity. So, it is necessary to put the research to conduct numerical experiments for various design considerations.

Objectives

- To study the influence of submergence during the steady and unsteady flows for hydro-morpho dynamics using experiments in the spur dike field
- To simulate the flow field and sediment transport around submerged spur dike field under the influence of steady and unsteady flow event using a numerical model



Flowchart of methodology for the proposed research

"HEALTH RISK ASSESSMENT OF PM2.5 BOUND TRACE METALS AND PAHS FROM A MINING & THERMAL POWER PLANT BASED INDUSTRIAL TOWN OF TAMIL NADU, INDIA"

SHOUMICK MITRA
CE20D033
Ph.D Civil Engineering
(Environmental and Water Resources Engineering Division)

Research Area: Atmospheric Geochemistry

Brief Description of Research

For the well-being and sustenance of both humankind and the surrounding ecosystem, clean air is the foremost requirement. However, owing to rampant industrialization and uncontrolled urbanization, the release of various air pollutants has been constantly on the rise. In the present scenario, air pollution is singlehandedly one of the largest environmental and public health challenge which is faced globally (Liu et al., 2019; WHO, 2016; Fuzzi et al., 2015). Recent WHO findings show that a staggering 91% of the world's people dwell in places where the air quality fails to meet the WHO guideline limits and is detrimental to human health. Particulate matter with an aerodynamic diameter ≤ 2.5µm (PM2.5) is considered fine particulate matter (Yang et al. 2018; Callén et al., 2012). Owing to their very small size, the fine particulates (PM2.5) stay much longer in the air and can easily bypass the nasal cavity and penetrate deep into the unciliated and alveolar sections of the lungs (Spengler et al., 1990). In a study published by the Global Burden of Disease about the currently prevailing condition of air pollution, it is estimated that in India alone in 2019, a staggering 1.67 million deaths occurred as a result of air pollution. The majority i.e., around 0.98 million of these deaths were because of ambient particulate air pollution (GBD India State-Level Disease Burden Initiative Air Pollution Collaborators, 2020). Again, according to very recent research from Harvard University, it has been estimated that globally around 10.2 million pre-mature deaths every year can be attributed to PM2.5 generated from fossil fuels alone. In that list, India with an estimated pre-mature mortality of around 2.5 million ranks second only to China which has the highest mortality impact of around 3.9 million annually (Vohra et al., 2021).

To Read more CLICK HERE

Thank you!

We would like to take this opportunity again to express our heartfelt gratitude to all those who made benevolent contributions towards the growth and development of IIT MADRAS

Indian Institute of Technology Madras, Chennai – 600036
www.iitm.ac.in

For more information, please contact:
Office of Alumni and Corporate Relations
T: +91-44-2257 8390 | acr.iitm.ac.in

Stay Connected:

March 2022