A Project Report On

Photocatalytic Degradation Of Methylene Blue dye using 2-D MXene (Ni- Doped Molybdenum Titanium Dicarbide) as a Photocatalyst

Dissertation submitted to

GOA UNIVERSITY

In partial fulfillment of the award of the degree of

MASTER OF SCIENCE (SEM-IV)

By

Usha S. Gadkar

Under guidance of

Dr. Anjani P.Nagvenkar

To the

DEPARTMENT OF CHEMISTRY,

GOA UNIVERSITY

CERTIFICATE

This is to certify that work incorporated in the project entitled **"Photocatalytic Degradation Of Methylene Blue dye using 2-D MXene (Ni- Doped Molybdenum Titanium Dicarbide) as a Photocatalyst"** is the bonafide work done by **Miss. Usha S. Gadkar** during the period of study under my guidance in partial fulfillment of requirement for the award of Degree of Master of Science in chemistry at the Department of Chemistry, Goa University during the academic year 2021-2022.

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<u>DECLARATION</u>

I declare that matter presented in this project entitled **"Photocatalytic Degradation of Methylene Bluedye using 2-D MXene (Ni- Doped MolybdenumTitanium Dicarbide) as a Photocatalyst"** is the original work done by me at the Department of Chemistry, Goa University, Taleigao Plateau, Goa under the guidance of Dr.Anjani P. Nagvenkar. And to the best of my knowledge similar work has not been submitted elsewhere for the requirement of course of study.

Date : 28 April 2022

Place : Goa University
Taleigao-Goa

Candidate Signature

USHA S. GADKAR
(M.Sc- Part II)

ACKNOWLEDGEMENT

The literature review titled **"Photocatalytic Degradation of Methylene Bluedye using 2-D MXene (Ni- Doped Molybdenum Titanium Dicarbide) as a Photocatalyst"** has been successfully completed under the guidance of Dr.Anjani P. Nagvenkar during the year2021-2022 in the partial fulfilment of the requirements for the degree of Master of Science in Chemistry.

I express my deep sense of gratitude to my guide teacher Dr. Anjani P. Nagvenkar,who showed interest in giving valuable guidance at every step. Her enthusiastic support and constant encouragement has been the source of inspiration for me.

I feel the right occasion to express my heartfelt and sincere thanks to our respected Dean Dr.Vidhyadatta Verenkar. I also thank the entire library faculty for helping me out for searching relevant books with respect to my topic.

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INTRODUCTION

Photocatalysis is a low-cost and environment-friendly technique to purify the wastewater from pollutants such as organic dyes. A class of photocatalysts called semiconductor photocatalysts have also been reported for effective degradation of organic compounds in water[1] (e.g Zno & TiO_2). Several semiconductor particles such a TiO_2 and ZnO2 were reported for photocatalysis..[1,2] However they exhibited lower catalytic activity which is attributed to wide band gaps. . TiO_2 due to its photocatalytic nature is also used in water splitting for the production of hydrogen (H2) but is still impeded due to its inferior visible light absorption and requirement of doping with other materials to increase its performance. In recent years 2D layered materials containing transition-metal elements with carbide and nitride, also called MXene, have attracted considerable attention for their carbon-based 2D layered structures. They are characterized by the formula Mn+1XnTx (n=1, 2, 3) where M corresponds to various transition metals like titanium, chromium, and so on, X corresponds to carbon, nitrogen, and so on.[3]The thickness of a single MXene layer is normally less than 1 nm, while its lateral size ranges from nanometers to micrometers highly depending on the synthetic method. The intact metal atomic layers endow MXenes with unique metallic conductivity, while the abundant surface functional groups (e.g. hydroxyl, oxygen and fluorine) confer MXenes with good hydrophilicity.[4,5]. This new kind of innovative material has been normally synthesised via a selectively etching route using MAX phase as precursor.[6] They have suitable properties : large surface area, high electrical conductivity, abundant and highly active surface sites and good adsorption capabilities which makes them suitable to act as a photocatalyst. MXenes have emerged as a good alternate for improving photocatalytic performance in renewable energy and environmental remediation fields because of their high surface area and suitable fermi level.When Mxenes like TiC_2 are used as photocatalysts there is rapid recombination of light excited carriers which decreases its quantum efficiency and photocatalytic performance. Therefore we propose to use Ni-doped Mo_2TiC_2 (Ni-Molybdenum titanium dicarbide) for the photocatalytic degradation of Methylene Blue dye. Molybdenum carbide doped with Nickel could increase the overall surface area of the catalyst and increase its efficiency. To the best of our literature knowledge, this is the first study on the photocatalytic properties of this material.We expect it to act as a better photocatalyst because it is non-toxic , cost effective, has a large surface area and a good chemical and photostability.

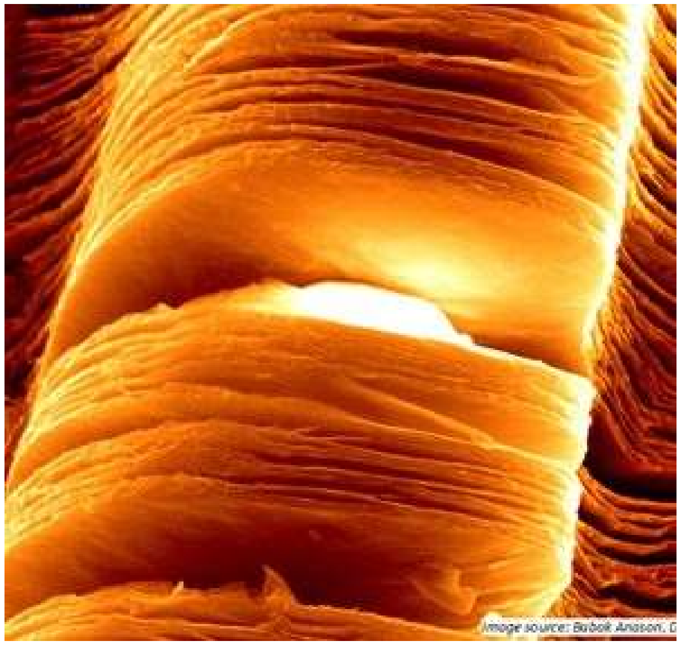

Fig.1 MXene Sheets

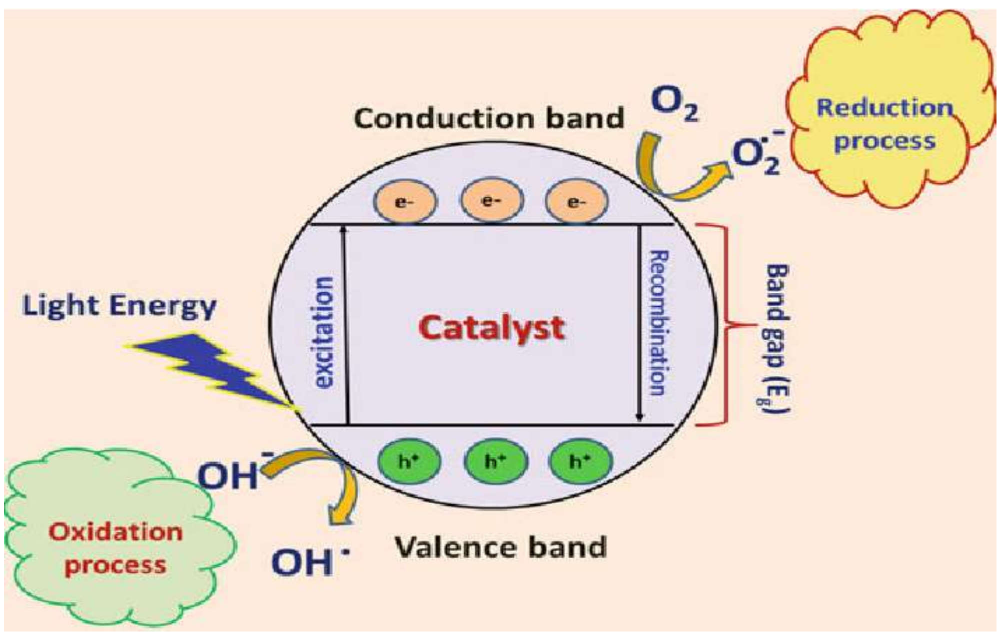

Fig.-2 Photocatalysis Mechanism

IMPORTANCE OF THE PROJECT

Many 2-D MXenes have been widely used as a photocatalyst in many environmental and energy applications due to their efficient photoactivity and high stability. However, their large band gap energies limit their absorption of solar radiation. Their photocatalytic activity is also limited by the rapid recombination of the electron-hole pairs. Some of them have a poor affinity towards the organic pollutants. Therefore there is a need to develop a catalyst which will overcome these shortcomings. Ni-doped Molybdenum titanium dicarbide could act as a more efficient photocatalyst as there is increase in charge separation and there is suppression of rapid charge combination. Doping it with Ni increases its overall surface area so the adsorption capacity also increases. [7,8,9,10]

METHODOLOGY

Methylene Blue was chosen as a target dye for the photocatalytic experiment. It always produces carcinogenic/noxious byproducts by numerous oxidation and hydrolysis reactions in water ecosystems. In this experiment 500ml of Methylene blue aqueous solution will be taken and to that 100mg of powder sample will be added. This solution will be then mechanically stirred for 1 hour in dark. This suspension will be then exposed to sunlight at noon without any agitation. At given time intervals the suspension will be manually agitated with a glass rod. The supernatant solution will be decanted and its residual dye concentration will be measured using UV-Visible spectrophotometer at 662nm to calculate the degradation of dyes. Irradiation with visible light produces electron-hole pairs in the material; the electrons combine with the O_2 and produces O_2^- and the holes combine with the OH^- to produce superoxide and free hydroxyl radicals, respectively. The Mxene sheets quickly trap the electrons and thereby reducing the chances of recombination. These hydroxyl radicals (OH^-) and O_2^- are responsible for the degradation of harmful organic pollutants and produce harmless byproducts likeCO_2 and H_2O.Because they are highly active. Previous reports on dye degradation show the degradation mechanism as shown here..[11–16]

The following equations express the whole photodegradation mechanism:

(1)MXene + hυ $\rightarrow$ $h^+ + e^-$

(2) e^- + MXene → (MXene trapping sites)

(3) e^- (MXene trapping sites) + O_2 → O_2^-

(4) h^+ + H_2O → OH^-

(5) OH^- + MB → CO_2 + H_2O (degradation byproducts)

(6) O_2 + MB → CO_2 + H_2O (degradationbyproducts)

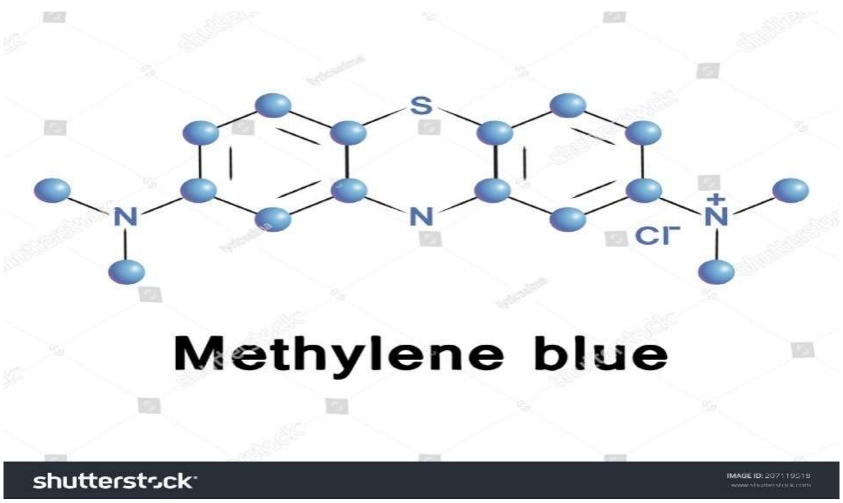

Fig.-3 Structure of Methylene Blue dye

OUTCOME OF THE PROJECT

This study will reveal a new system of a low-cost catalyst with potential application in the photocatalytic degradation of dyes. It will shows a considerable reduction in the final concentrations of the dye solutions. We expect it to act as a better photocatalyst because it is non-toxic , cost effective, has a large surface area and a good chemical and photostability.

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