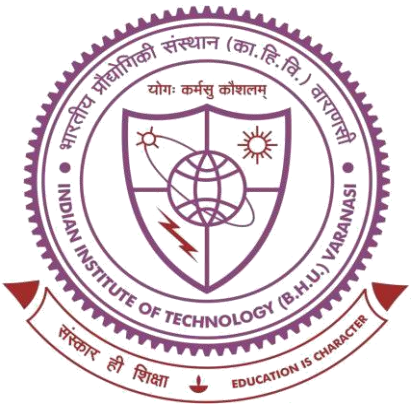
$MoSe_2$ Nanostructures Based Electrocatalysts for Electrolyzer and Zinc-air Battery



Thesis submitted in partial fulfilment

for the Award of

Doctor of Philosophy

By

Prince Kumar Maurya

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It is certified that the work contained in the thesis titled ***"$MoSe_2$ Nanostructures Based Electrocatalysts for Electrolyzer and Zinc-air Battery"*** by **Prince Kumar Maurya** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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Date: 22-04-2024

Place: Varanasi

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DECLARATION BY THE CANDIDATE

I, ***"Prince Kumar Maurya"***, certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of ***"Dr. Ashish Kumar Mishra"*** from ***"July 2018"*** to ***"April 2024"***, at the ***"School of Material Science and Technology"***, Indian Institute of Technology (BHU), Varanasi. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc.*, reported in journals, books, magazines, reports dissertations, theses, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.

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CERTIFICATE BY THE SUPERVISOR

This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

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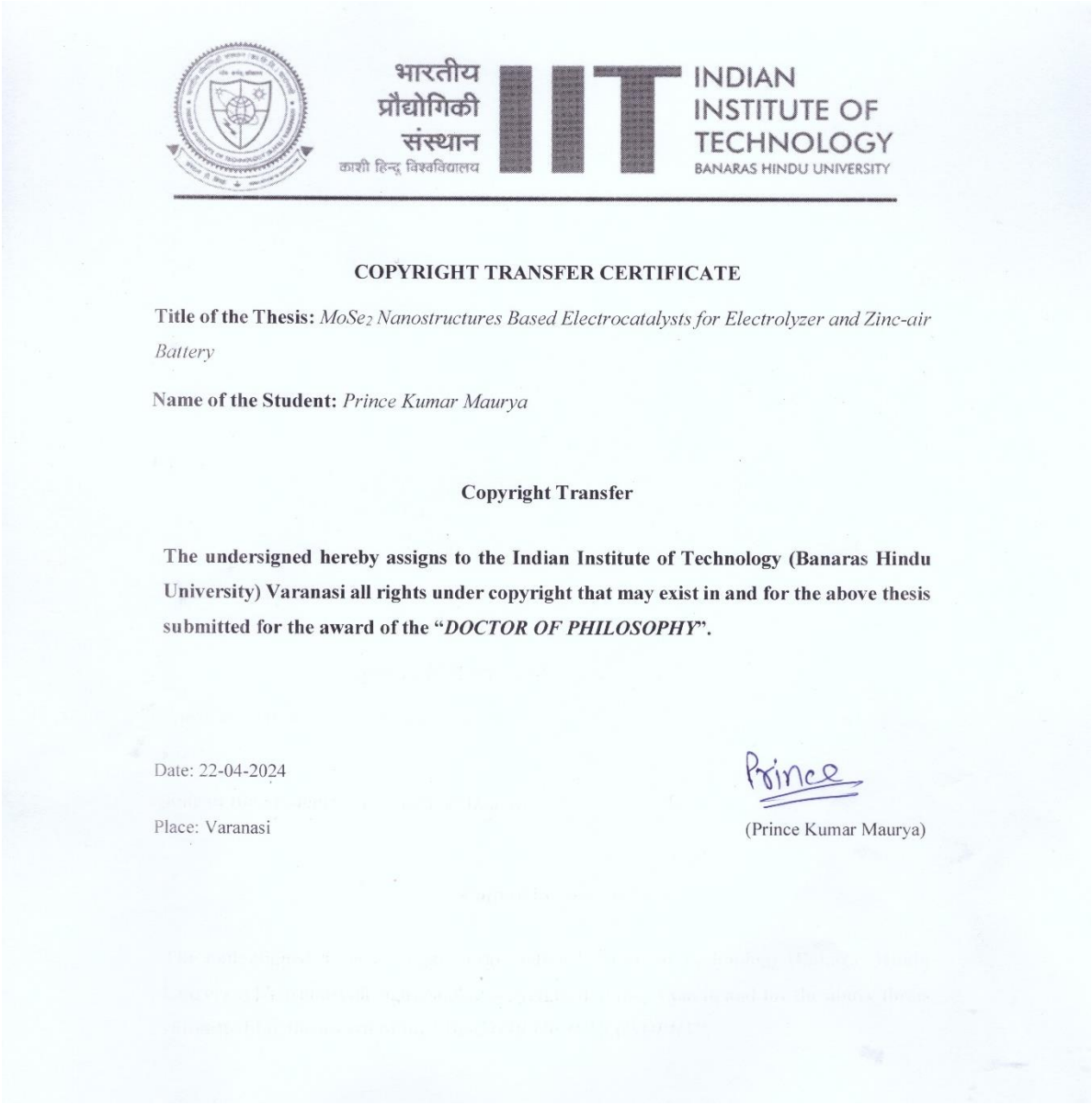

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(Prince Kumar Maurya)

Dedicated to my beloved parents

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List of Abbreviations

$MoSe_2$	Molybdenum Diselenide
MoS_2	Molybdenum Disulfide
TMDCs	Transition metal dichalcogenide
HER	Hydrogen Evolution Reaction
OER	Oxygen Evolution Reaction
RHE	Reversible Hydrogen Electrode
CCP	Conducting carbon paper
MABs	Metal Air batteries
XRD	X-ray Diffraction
SEM	Scanning Electron Microscope
TEM	Transmission Electron Microscope
FTIR	Fourier-transform infrared spectroscopy
LSV	Linear Sweep Voltammetry
CV	Cyclic voltammetry
GCD	Galvanostatic Charge-discharge
EIS	Electrochemical Impedance Spectroscopy
CPE	Constant Phase Element
HR	High Resolution
2D	Two Dimensional
CVD	Chemical vapor deposition
ECSA	Electrochemical active surface area

List of Symbols

η	Overpotential
^{o}C	Degree Celsius
F	Faraday constant
eV	Electron volt
%	Percentage
C_d	Specific capacity
I_d	Discharge current density
mA	Milli ampere
ΔT	Discharge time
m_{zn}	Consumed mass of zinc
E_d	Energy density
WL^{-1}	Watt per litter
$Wh\ kg^{-1}$	Watt hour per kilogram
V	Volt
P_d	Power density
V_d	Discharge working potential
Pt	Platinum
Zn	Zinc
G^{o}	Gibbs free energy
Rs	Series resistance
Rct	Charge transfer resistance
Li	Lithium
E_{op}	Overall potential
E_{rev}	Reversible thermodynamic potential
Ni	Nickle

Table of Contents

Preface

Molybdenum diselenide ($MoSe_2$) is one of the widely studied materials of the transition metal dichalcogenide family, having fascinating properties such as high conductivity, semiconducting characteristics, high surface area, electrocatalytic activity and good stability in acidic/basic medium. These attractive feature characteristics allow $MoSe_2$ nanostructures to be used in energy generation and storage applications. The present thesis entitled "**$MoSe_2$ Nanostructures Based Electrocatalysts for Electrolyzer and Zinc-air Battery"** is focused on the synthesis of pristine $MoSe_2$, bimetal oxides-$MoSe_2$ hybrid nanostructures and Ni decorated $MoSe_2$ nanocomposites via hydrothermal technique for hydrogen evolution reaction (HER), oxygen evolution reaction (OER), Electrolyzer, and zinc-air battery applications. The morphology and structure of the synthesized samples have been confirmed through Scanning electron microscopy (SEM), Transmission electron microscopy (TEM) and X-ray diffraction (XRD) techniques. We have also performed Raman and Fourier transform infrared (FTIR) spectroscopy techniques to confirm the vibrational characteristics of prepared samples. The X-ray photoelectron spectroscopy (XPS) has been performed to analyze oxidation states of different elements in pristine $MoSe_2$, bimetal oxides-$MoSe_2$ hybrid nanostructures and Ni decorated $MoSe_2$ nanocomposite. We have further elucidated the electrocatalytic activity of prepared samples through different electrochemical measurements such as cyclic voltammetry (CV), linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS) and chronoamperometry for HER and OER. Further, we have designed electrolyzer and Zinc air battery cells using prepared electrocatalysts and studied their performance.

In-situ grown $MoSe_2$ over Ni foam ($MoSe_2$-Ni foam) electrode shows low overpotential η_{10} ~100 mV and Tafel slope ~73 mV dec^{-1} in 1M KOH for HER, while in-situ grown $MoSe_2$ over conducting carbon paper ($MoSe_2$-CCP) electrode displays η_{10}~ 143 mV and Tafel's slope ~53 mV dec^{-1} in 0.5M H_2SO_4. The better performance of binder-free $MoSe_2$-Ni foam and