Dedicated to.....

My beloved parents

# **Declaration of Academic Integrity**

"I declare that this written submission represents my ideas in my own words and where other's ideas or words have been included, I have adequately cited and referenced the original sources. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above will be cause for disciplinary action as per the rules and regulations of the Institute."

Date: 21-11-2023 Place: Tezpur University Suman Lalkar (Suman Lahkar)

Regn No. TZ156024 of 2015

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Prof. Sunjus, Stans Dalah

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तेजपुर विश्वविद्यालय / TEZPUR UNIVERSITY (संसद के अधिनियम द्वारा स्थापित केंद्रीय विश्वविद्यालय) (A Central University established by an Act of Parliament)

Swapan Kumar Dolui Professor Department of Chemical Sciences Mobile: +91-9957198489 Email: dolui@tezu.ernet.in

# **CERTIFICATE FROM SUPERVISOR**

This is to certify that the thesis entitled "*Development of Electrocatalysts for Hydrogen Evolution Reaction in Acidic Medium*" submitted to the School of Sciences, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in Chemical Sciences is a record of research work carried out by **Ms. Suman Lahkar** under my supervision and guidance. She has been duly registered (Registration No. TZ156024 of 2015), and the thesis presented is worthy of being considered for Ph.D. Degree.

All help received by her from various sources have been duly acknowledged. No part of this thesis has been submitted elsewhere for award of any other degree.

Date: 21-11-2023 Place: Tezpur University

Dates 21 df 2013

**(Prof. Swapan Kumar Dolui)** Supervisor



तेजपुर विश्वविद्यालय / TEZPUR UNIVERSITY (संसद के अधिनियम द्वारा स्थापित केंद्रीय विश्वविद्यालय) (A Central University established by an Act of Parliament)

Panchanan Puzari Professor Department of Chemical Sciences

Mobile: 91-8486872235 Phone: 0-3712-275061 Email: pancha@tezu.ernet.in

### **CERTIFICATE FROM CO-SUPERVISOR**

This is to certify that the thesis entitled entitled "*Development of Electrocatalysts for Hydrogen Evolution Reaction in Acidic Medium*" submitted to the School of Sciences, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in Chemical Sciences is a record of research work carried out by **Ms. Suman Lahkar** under my supervision and guidance. She has been duly registered (Registration No. TZ156024 of 2015), and the thesis presented is worthy of being considered for Ph.D. Degree.

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o-Supervisio

Date: 21-11-2023 Place: Tezpur University

(Prof. Panchanan Puzari) Co-Supervisor

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Suman Lahkar

## ABBREVIATIONS AND SYMBOLS USED

Ag/AgCl	silver/silver chloride
As	arsenic
А	area
APS	ammonium persulfate
A g <sup>-1</sup>	Ampere per gram
В	boron
BET	Brunauer-Emmett-Teller
BJH	Barrett–Joyner–Halenda
CO <sub>2</sub>	Carbon dioxide
СО	carbon monoxide
СВ	conduction band
CoS	cobalt sulphide
$CoS_2$	cobalt disulphide
Со	cobalt
Cu	copper
Cd	cadmium
CoP	cobalt phosphide
С	carbon
CV	cyclic voltammetry
С	capacitance
CA	chronoamperometry
C1	resistance between two parallel circuits composed of
	resistors and constant phase elements
CPE	constant phase elements
$C_{dl}$	electrochemical double-layer capacitance ( $C_{dl}$ )
$C_{sc}$	capacitance of the space charge layer
СООН	carboxylic acid
CH <sub>3</sub> OH	methanol
$C_6H_5NH_2$	aniline
CH <sub>3</sub> COOH	acetic acid
D	dimensional
DFT	density functional theory

eV	electron volt
e	electron
ECSA	electrochemical surface area
EDLC	electric double-layer capacitor
EG	expanded graphite
EDX	elemental dispersive X-ray spectrometry
EIS	electrochemical impedance spectroscopy
$\Delta E(\mathrm{H}^*)$	energy change of hydrogen adsorption
$E_{fb}$	flat band potential
FeS	iron sulphide
F	Faraday constant
FTIR	Fourier transform infrared spectroscopy
FESEM	field emission scanning electron microscopy
Fe(NO <sub>3</sub> ) <sub>3</sub> .9H <sub>2</sub> O	iron (III) nitrate nonahydrate
GCE	glassy carbon electrode
$\Delta G_{Hads}$	free energy of adsorbed hydrogen
GCD	galvanostatic charge-discharge
HER	hydrogen evolution reaction
$\mathrm{H}^+$	proton
H <sub>2</sub> O	water
$H_2$	hydrogen
h	hour
H <sub>ads</sub>	adsorbed hydrogen
$H_2SO_4$	sulphuric acid
HDS	hydrodesulphurization
Hz	hertz
$H_2PtCl_6$	chloroplatinic acid
$H_2O_2$	hydrogen peroxide
НСНО	formaldehyde
IEA	International Energy Agency
IRENA	International Renewable Energy Agency
io	exchange current density
Ir	iridium
i	current

j	current density
J	current density
$J_0$	exchange current density
J-V plot	current-voltage plot
КОН	potassium hydroxide
kHz	kilohertz
KSCN	potassium thiocyanate
KMnO <sub>4</sub>	potassium permanganate
kW kg <sup>-1</sup>	kilowatt per kilogram
LSV	linear sweep voltammetry
Li	lithium
Mt	megatonne
Μ	active metal site
$MoS_2$	molybdenum disulphide
Mo	molybdenum
MoSe <sub>2</sub>	molybdenum selenide
mA cm <sup>-2</sup>	milliampere per centimeter square
mV	millivolt
Mo <sub>2</sub> C	molybdenum carbide
MOF	metal-organic framework
$MoB_2$	molybdenum boride
MWCNT	multi-walled carbon nanotube
$Mo_2N$	molybdenum nitride
mV dec <sup>-1</sup>	millivolt per decade
MnO <sub>2</sub>	manganese dioxide
mHz	millihertz
mV sec <sup>-1</sup>	millivolt per second
M-S	Mott-Schottky
mM	millimole
М	molar
NADPH	nicotinamide adenine dinucleotide phosphate hydrogen
nm	nanometer
NHE	normal hydrogen electrode
NiS <sub>2</sub>	nickel disulphide

Ni	nickel
Ni <sub>5</sub> P <sub>4</sub>	penta nickel phosphide
$Ni_3S_2$	tri nickel disulphide
NiP	nickel phosphide
Ν	nitrogen
n	number of electrons transferred
$Na_2SO_4$	sodium sulphate
$N_D$	charge carrier density
NaDDBS	sodium dodecylbenzenesulfonate
NaBH <sub>4</sub>	sodium borohydride
NaOH	sodium hydroxide
NaNO <sub>3</sub>	sodium nitrate
Na <sub>3</sub> PO <sub>4</sub>	sodium hypophosphate
Na <sub>2</sub> CO <sub>3</sub>	sodium carbonate
Na <sub>3</sub> PO <sub>4</sub> .12H <sub>2</sub> O	sodium phosphate dodecahydrate
$(NH_4)_2S_2O_8$	ammonium peroxodisulfate
OER	oxygen evolution reaction
0	
$O_2$	oxygen
O <sub>2</sub> P	oxygen phosphorous
_	
Р	phosphorous
P Pt	phosphorous platinum
P Pt P	phosphorous platinum power density
P Pt P PANI	phosphorous platinum power density polyaniline
P Pt P PANI PPY	phosphorous platinum power density polyaniline polypyrrole
P Pt P PANI PPY PDOS	phosphorous platinum power density polyaniline polypyrrole Projected density of states
P Pt PANI PPY PDOS q	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge
P Pt PANI PPY PDOS Q	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge
P Pt PANI PPY PDOS Q RDS	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge rate-determining step
P Pt PANI PPY PDOS Q RDS Ru	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge rate-determining step ruthenium
P Pt PANI PPY PDOS Q RDS Ru RGO	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge rate-determining step ruthenium reduced graphene oxide
P Pt PANI PPY PDOS Q RDS Ru RGO R	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge rate-determining step ruthenium reduced graphene oxide resistance
P Pt PANI PPY PDOS Q RDS Ru RGO R RHE	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge rate-determining step ruthenium reduced graphene oxide resistance reversible hydrogen electrode
P Pt PANI PPY PDOS Q RDS Ru RGO R RGO R HE RHE RHE Rct	phosphorous platinum power density polyaniline polypyrrole Projected density of states charge charge rate-determining step ruthenium reduced graphene oxide resistance reversible hydrogen electrode charge-transfer resistance

$R_{f}$	roughness factor
rpm	rotation per minute
S	sulphur
SWCNT	single-walled carbon nanotube
SEM	scanning electron microscopy
$\Delta S$	entropy change of adsorption H
SCE	standard calomel electrode
SCN <sup>-</sup>	thiocyanate ion
Se	selenium
sec	second
TOF	turn over frequency
TMSes	transition metal selenides
TMSs	transition metal selenides
Ti	titanium
TiO <sub>2</sub>	titanium dioxide
Ti <sub>2</sub> O <sub>3</sub>	titanium (III) dioxide
TMD	transition metal dichalcogenide
Т	temperature in kelvin
TOF	Turn Over Frequency
TEM	transmission electron microscopy
TMPs	transition metal phosphides
ТОР	trioctylphosphine
TiOOH	titanium (oxy)hydroxides
TTIP	titanium tetraisopropoxide
TEABF <sub>4</sub>	tetraethyl ammonium tetrafluoroborate
UV	ultraviolet
V	volt
VB	valence band
V <sub>hexane</sub>	volume of hexane
Vethanol	volume of ethanol
W	tungsten
W h kg <sup>-1</sup>	watt hour per kg
XRD	X-ray diffraction
XPS	X-ray photoelectron spectroscopy

Zn	zinc
ΔΖΡΕ	zero-point energy change
γ	gamma
η	overpotential
α	symmetry factor
ε <sub>0</sub>	permittivity of free space
Er	relative permittivity of the dielectric medium
λ	wavelength
θ	angle between the individual atomic planes
$\alpha_c$	charge transfer coefficient for the cathodic potential
Ω	ohm
v	scanning rate
μF	microfarad
<sup>0</sup> C	degree Celsius

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