

***To Maa, Papa and Piya, I am deeply grateful for your love and support.***

***Thank you for always being by my side.***



**TEZPUR UNIVERSITY**

(A Central University established by an Act of Parliament)

Napaam-784028, Tezpur, Sonitpur, Assam, India

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**DECLARATION BY THE CANDIDATE**

I, **Mr. Nishant Biswakarma**, hereby, declare that the thesis entitled “**NO oxidation over bare and zeolite supported precious transition metal clusters using quantum mechanical approach**” has been submitted to the Department of Chemical Sciences under the School of Sciences of Tezpur University, in partial fulfilment of the requirements for the award of the degree of **Doctor of Philosophy in Chemistry**. This thesis is a record of original research work carried out by me under the guidance of **Prof. Ramesh Ch. Deka** and the contents of the thesis, in full or in part, has not been previously considered for the award of any degree, diploma, associateship, fellowship or any other similar title or recognition from any University, Institute or other Organization.

I further declare that; I have duly acknowledged all sources of assistance and any text, figures, results or design that are not of my own are appropriately referenced in order to give credit to the original author(s).

Date: 17/09/2025

Place: Tezpur University

*Nishant Biswakarma*  
(Nishant Biswakarma)

Department of Chemical Sciences

**Dr. Ramesh Ch. Deka**

Professor, Department of Chemical Sciences

Tezpur University

Napaam

Tezpur-784028

Assam, India

Mobile: 9435380221

E-mail: [ramesh@tezu.ernet.in](mailto:ramesh@tezu.ernet.in), [rcdekatu@gmail.com](mailto:rcdekatu@gmail.com)



**NAAC Grade A+**

### **CERTIFICATE FROM THE SUPERVISOR**

This is to certify that the thesis entitled “**NO oxidation over bare and zeolite supported precious transition metal clusters using quantum mechanical approach**” has been submitted by **Mr. Nishant Biswakarma** to the Department of Chemical Sciences under the School of Sciences of Tezpur University, in partial fulfilment of the requirements for the award of the degree of **Doctor of Philosophy in Chemistry**. This thesis is a record of bona fide research work carried out by him under my supervision and guidance. He has been registered, completed his PhD course work and the thesis presented is worthy of consideration for the award of PhD degree.

All help received by him from various sources have been duly acknowledged.

The contents of this thesis, in full or in part, have not been submitted for the award of any degree, diploma, associateship, fellowship or any other similar title or recognition from any University, Institute or other Organization.

Date: 17/09/2025

Place: Tezpur University

*Ramesh Ch. Deka*  
(Ramesh Ch. Deka)

Department of Chemical Sciences

*“No one who achieve success does so without  
acknowledging the help of others”*

*- Alfred North Whitehead*

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“प्रेम ईश्वरस्य महत्तमपारितोषीकमस्ति।”

Nishant Biswakarma

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## LIST OF ABBREVIATIONS

Co- $E_{\text{ads}}$	Co-adsorption energy
DFT	Density Functional Theory
EA	Electron Affinity
$E_{\text{ads}}$	Adsorption energy
ECP	Effective core potential
E-R	Eley-Rideal
GGA	Generalized gradient approximations
GTO	Gaussian type orbital
HF	Hartree Fock
HOMO	Highest occupied molecular orbital
IM	Intermediate
IP	Ionization potential
KS	Kohn Sham
LDA	Local density approximations
L-H	Langmuir Hinshelwood
LUMO	Lower unoccupied molecular orbital
MM	Molecular mechanics
MO	Molecular orbital
M06L	Minnesota 06 local functional
NP	Nanoparticle
PES	Potential energy surface
QCE	Quantum confinement effect
QM	Quantum mechanics
SCF	Self consistent field