Design and Development of $NiFe_2O_4$ based Nanomaterials for Removal of Organic Pollutants from their Aqueous Solutions

Thesis submitted in partial fulfillment for the
Award of Degree

Doctor of Philosophy

By

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It is further certified that the student has fulfilled all the requirements of the Comprehensive, Candidacy, and SOTA.

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I, ***"Anshu Shrivastava"***, certify that the work embodied in this thesis is my own bona fide work and carried out by me under the supervision of ***"Prof. Indrajit Sinha"*** from ***"July 2019"*** to ***"April 2025"***, at the ***"Department of Chemistry"***, 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 credit to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not wilfully 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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DEDICATED TO MY LOVING PARENTS…

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Anshu Shrivastava

Abbreviations

CIP	Ciprofloxacin
MG	Methyl orange
DW	Double distilled water
MAPS	Materials and Process Simulation
MD	Molecular dynamics
RDF	Radial distribution function
LAMMPS	Large-scale Atomic/Molecular Massively Parallel System
XRD	X-ray diffractometer
VSM	Vibrating sample magnetometry
SEM	Scanning electron microscopy
UV-vis	Ultra-violet visible Spectroscopy
UV-DRS	Ultra-violet diffuse reflectance spectroscopy
BET	Brunauer-Emmett-Teller
FT-IR	Fourier transforms infrared spectroscopy
TEM	Transmission electron microscopy
TOF	Turn over frequency
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
TD-DFT	Time-dependent density functional theory
DFT	Density functional theory
$^{\bullet}$OH	Hydroxyl radical
$^{\bullet}$OOH	Hydroperoxyl radical

OH^-	Hydroxide ion
NaOH	Sodium hydroxide
$O_2^{\bullet-}$	Superoxide radical
VB	Valence band
CB	Conduction band
TC	Tetracycline
EIS	Electrochemical Impedance Spectroscopy
MS	Mott-Schottky
IPA	Isopropyl alcohol
NBT	Nitro blue tetrazolium

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