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It is certified that the work contained in the thesis titled ***"Adsorption and Catalysis on Magnetite, Graphene Oxide and their Composites"*** by ***"Jyoti Kuntail"*** has been carried out under my supervision and this work has not been submitted elsewhere for a degree.

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

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DECLARATION BY THE CANDIDATE

I, ***"Jyoti Kuntail"***, certify that the work embodied in this thesis is my own bona fide work and carried out by me under the supervision of ***"Dr. Indrajit Sinha"*** from ***"December 2016"*** to ***"December 2021"***, 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 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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It is certified that the above statement made by the student is correct to the best of my knowledge.

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Dedicated
to
My
Beloved
Family

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Jyoti Kuntail

CONTENTS

ABBREVIATION

MNPs	Magnetite nanoparticles
SMNPs	Starch functionalized magnetite nanoparticle
GO	Graphene oxide
OG	Orange-G
PNP	*p*-Nitrophenol
PCP	*p*-Chlorophenol
AOP	Advanced oxidation process
MAPS	Materials and Process Simulation
MD	Molecular dynamics
RDF	Radial distribution function
LAMMPS	Large-scale Atomic/Molecular Massively Parallel System
SciPCFF	Scientific Polymer Consistent Forcefield
SEM	Scanning electron microscopy
UV-vis	Ultra violet visible Spectroscopy
UV-DRS	Ultra violet diffuse reflectance spectroscopy
XRD	X ray diffractometer
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
H_2O_2	Hydrogen Peroxide
$^{\bullet}OH$	Hydroxyl radical
$^{\bullet}OOH$	Hydroperoxyl radical
OH^-	Hydroxide ion
NaOH	Sodium hydroxide
ROS	Reactive oxygen species
$O_2^{\bullet-}$	Superoxide radical
VB	Valence band
CB	Conduction band
MNDO	Modified Neglect of Differential Overlap

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