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## CERTIFICATE

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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

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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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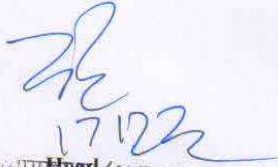
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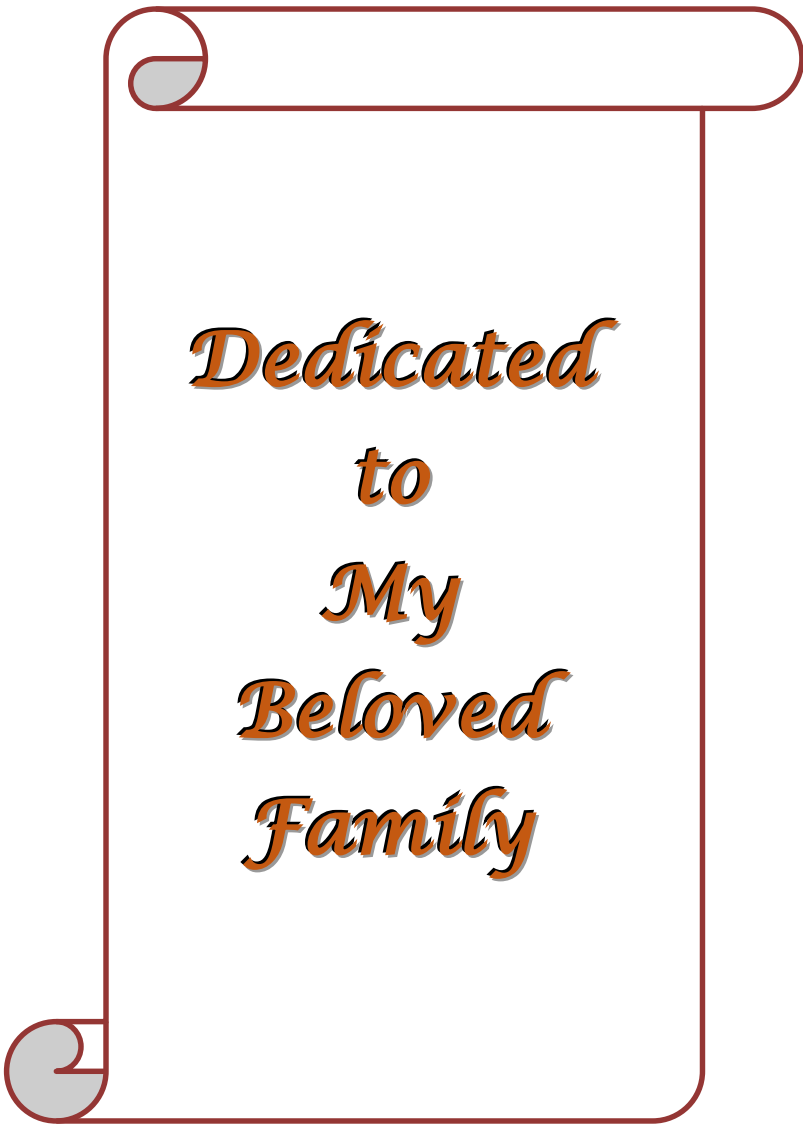
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*Dedicated  
to  
My  
Beloved  
Family*

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**Jyoti Kuntail**

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## ABBREVIATION

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<b>MNPs</b>	Magnetite nanoparticles
<b>SMNPs</b>	Starch functionalized magnetite nanoparticle
<b>GO</b>	Graphene oxide
<b>OG</b>	Orange-G
<b>PNP</b>	<i>p</i> -Nitrophenol
<b>PCP</b>	<i>p</i> -Chlorophenol
<b>AOP</b>	Advanced oxidation process
<b>MAPS</b>	Materials and Process Simulation
<b>MD</b>	Molecular dynamics
<b>RDF</b>	Radial distribution function
<b>LAMMPS</b>	Large-scale Atomic/Molecular Massively Parallel System
<b>SciPCFF</b>	Scientific Polymer Consistent Forcefield
<b>SEM</b>	Scanning electron microscopy
<b>UV-vis</b>	Ultra violet visible Spectroscopy
<b>UV-DRS</b>	Ultra violet diffuse reflectance spectroscopy
<b>XRD</b>	X ray diffractometer
<b>FT-IR</b>	Fourier transforms infrared spectroscopy
<b>TEM</b>	Transmission electron microscopy
<b>TOF</b>	Turn over frequency
<b>HOMO</b>	Highest occupied molecular orbital

<b>LUMO</b>	Lowest unoccupied molecular orbital
<b>TD-DFT</b>	Time-dependent density functional theory
<b>DFT</b>	Density functional theory
<b>H<sub>2</sub>O<sub>2</sub></b>	Hydrogen Peroxide
<b>•OH</b>	Hydroxyl radical
<b>•OOH</b>	Hydroperoxyl radical
<b>OH<sup>-</sup></b>	Hydroxide ion
<b>NaOH</b>	Sodium hydroxide
<b>ROS</b>	Reactive oxygen species
<b>O<sub>2</sub><sup>•-</sup></b>	Superoxide radical
<b>VB</b>	Valence band
<b>CB</b>	Conduction band
<b>MNDO</b>	Modified Neglect of Differential Overlap

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