Role of Mn on the magnetic and electronic properties of magnetically frustrated Ising $Dy_2Ti_2O_7$ and XY $Er_2Ti_2O_7$ pyrochlores

Thesis submitted in partial fulfilment
For the Award of Degree

DOCTOR OF PHILOSOPHY

In

Materials Science and Technology

By

Rajnikant Upadhyay

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Dedicated to my parents

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It is certified that the work contained in the thesis titled **"Role of Mn on the magnetic and electronic properties of magnetically frustrated Ising $Dy_2Ti_2O_7$ and XY $Er_2Ti_2O_7$ pyrochlores"** by **Mr. Rajnikant Upadhyay** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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I, "**Rajnikant Upadhyay**", certify that the work embodied in this thesis is my own bonafide work and was carried out by me under the supervision of "**Dr. Chandan Upadhyay**" from July 2018 to December 2023 at the School of Materials Science & Technology, Indian Institute of Technology (Banaras Hindu University), 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 work, paragraphs, text, data, results, etc., reported in journals, books, magazines, reports dissertations, thesis, 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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LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS

AFM	Antiferromagnetic
BE	Binding energy
CB	Conduction band
CTT	Charge transfer transition
CF	Crystal field
DFT	Density functional theory
D_{nn}	Nearest neighbor dipolar interaction
DOS	Density of states
DSIM	Dipolar spin ice model
emu/g	Electron mass unit per gram
eV	Electron volt
FC	Field cooled
FM	Ferromagnetic
GGA	Generalized gradient approximation
GSA	Ground state absorption
GP	Griffith Phase
H	Magnetic field
HRXRD	High resolution x-ray Diffraction
J_{nn}	Nearest neighbor exchange interaction

K	Kelvin
keV	Kilo electron volt
kOe	Kilo Oersted
LDA	Local density approximation
LMCT	Ligand to metal charge transfer
M	Magnetization
M-H	Magnetization versus magnetic field
M-T	Magnetization versus temperature
MPMS	Magnetic Property Measurement System
M_s	Saturation magnetization
RE	Rare earth
RRKJ	Rappe-Rabe-Kaxiras-Joannopoulos
SQUID	Superconducting Quantum Interference Device
SXRD	Synchrotron x-ray diffraction
UPS	Ultraviolet photoelectron spectroscopy
UV-Vis	Ultraviolet-Visible
VB	Valence band
VESTA	Visualization for electronic structural analysis
XPS	x-ray photoelectron spectroscopy
ZFC	Zero field cooled