Ab-initio study of $LiTm_2O_4$ (Tm=V, Mn, Fe, Co & Ni)

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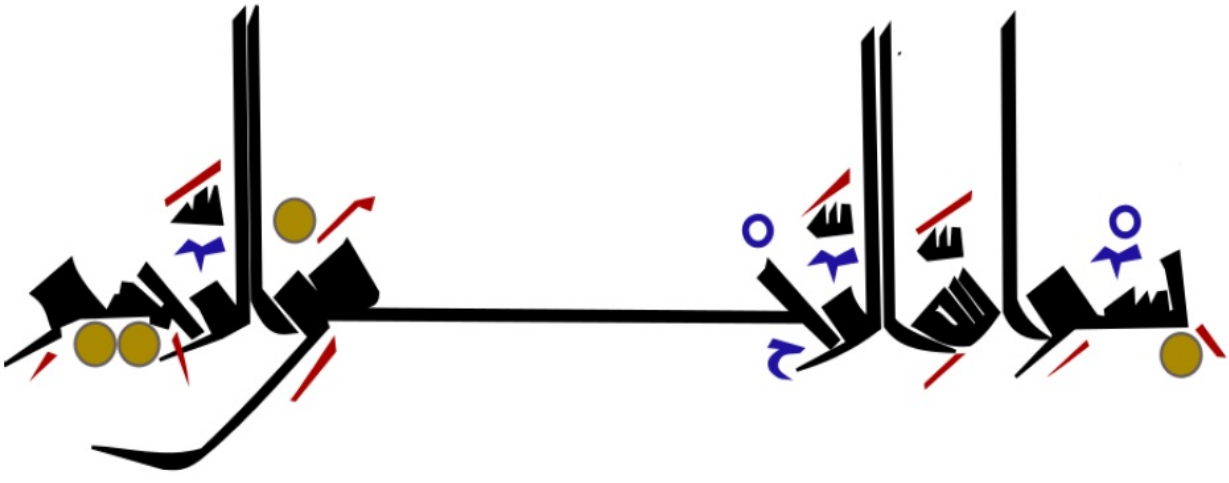

In the Name of Allāh, the Most Gracious, the Most Merciful

RESEARCH COMPLETION CERTIFICATE

Certified that the research work contained in this thesis titled, **"Ab-Initio study of $LiTM_2O_4$ (TM=Vanadium, Chromium, Manganese, Iron Cobalt & Nickel) Structural, Electronic, Magnetic and Thermoelectric properties"** has been carried out and completed by **Saima Mohyuddin, ID: 14004139016**. The quantum and the quality of the work contained in this thesis is adequate for the award of Degree of MS/M.Phil.

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Dedicated

To
My Parents
Who have always
been a source of
Inspiration and
Knowledge
For me

DECLARATION

This thesis which is being submitted for the award of degree of Master of Philosophy in Physics in the University of Management and Technology Lahore does not contain any material which has been submitted for the award of any other degree or diploma in any university and, to the best of my knowledge and belief, neither this thesis contain any material published or written previously by another person, except when due reference to made to the source in the text of the thesis. If any reference is found missing in this thesis, that would completely be unintentional and I do not have any pretension to own the credit for that.

ACKNOWLEDGEMENT

In the name of Allah, most gracious, most merciful

All praises and glory to Almighty Allah, the most gracious, the most merciful, and the creator of all the universe with ideas of beauty, symmetry and Who is supreme authority knowing the ultimate realities underlying all sort of phenomenon going on in this universe who is the benefactor, who guides us in the darkness and difficulties and who gave me courage and the patience to carry out this work.

I offer my humblest thanks to the last prophet, **Hazrat Mohammad** (PBUH), who is forever source of guidance for mankind.

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Saima Mohyuddin

Abstract

The transition metal spinel oxides as the electrode materials for lithium ion batteries have been inspected comprehensively lately with large capacity and high working voltage. The structural, electronic, thermoelectric and magnetic physiognomies of $LiTm_2O_4$ (Tm=V, Cr, Mn, Fe, Co, Ni) have been reconnoitered contained by the framework of density functional theory using the full-potential linear zed augmented plane wave method. The ferromagnetic ground-state energies have been premeditated by using the optimized structures. To compute the precise prophecy of the electronic and magnetic properties of $LiTm_2O_4$ (Tm=V, Cr, Mn, Fe, Co, Ni), the modified Becke-Johnson local density approximation functional is reachable. The half-metallic behavior in these compounds has been exposed by the electronic band structures and density of states plots, which is elucidated in expressions of exchange and crystal field splitting energies and magnetic moments. The key parameters for thermo electric response i.e electrical conductivity, thermal conductivity, see beck coefficient and power factor are studied in detail. The considered compounds of $LiTm_2O_4$ (Tm=V, Cr, Mn, Fe, Co, Ni) have been revealed theoretically that they grow potential spintronic and Li-ions batteries applications.

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List of abbreviations

DFT	Density functional Theory
GGA	Generalized Gradient Approximation
CB	Conduction Band
VB	Valence Band
eV	Electron Volt
TDOS	Total Density Of State
mBJ	Modified Becke Johnson
$LiTm_2O_4$	Lithium transition metal oxide
Tm	Transition Metal
ZT	Figure of merit
APW	Augmented plane wave
LAPW	Linearized Augmented Plane wave

CHAPTER 1

INTRODUCTION

With rapidly growing energy demands, the demand for more efficient and renewable energy resources has been raised. Energy from renewable sources such as wind, water solar, timber and biomass need some storage devices for their effective usage during depilation of time. In this regard the batteries, electro chemical storage devices play vital role in the effective use of renewable energy. Batteries are combination of electrical cells that stores and produce electricity by means of chemical reaction. During this era of development, battery technology has attained massive importance. The rechargeable lithium ion batteries with highest specific energy, cell voltage and small self-discharge, have accomplished greater attention.