A density function theory study of the electronic and optical properties of cesium lead halide perovskites for potential application in solar cell

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بسم الله الرحمن الرحيم

A Density Function Theory Study of the Electronic and Optical Properties of Cesium Lead Halide Perovskites for Potential Application in Solar Cell

Submitted to University of Management and Technology Lahore in partial fulfillment of the requirements for the award of degree of

MASTER OF PHILOSOPHY

IN

PHYSICS

By

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I.D

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SESSION: 2014-2016

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RESEARCH COMPLETION CERTIFICATE

Certified that the research work contained in this thesis titled, **"A Density Function Theory Study of the Electronic and Optical Properties of Cesium Lead Halide Perovskites for Potential Application in Solar Cell"** has been carried out and completed by **Muhammad Waqas, ID: 14004139005**. 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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Dated: _____ _____

(Muhammad Waqas)

DEDICATION

I dedicate this research work to my parents, brothers, sisters, students and teachers especially to my supervisor Prof. Dr. Muhammad Azhar Iqbal. Without their guidance, understanding, support, and love, the completion of this research work would not have been possible.

ACKNOWLEDGEMENT

This research is a result of the blessings showered and endowed by Almighty Allah, most beneficent and merciful for which I offer my gratitude to Allah. May the Holy Prophet Muhammad (PBUH) be praised who enabled us to recognize our creator.

I wish to acknowledge with humble gratitude the valuable guidance and assistance rendered to me by my supervisor Professor Dr. M. Azhar Iqbal. I am greatly indebted to him for his valuable help and excellent guidance to achieve my task.

I am much obliged to my parents, brothers, sisters and students whose prayers, support and encouragement enabled me to be a part of this research. This research would not have been possible without their help and moral support.

Author

Dua from Quran

God is the Most High and the True King. (Muhammad), do not be hasty in reading the Quran to the people before the revelation has been completed. "Say, My Lord, grant me more knowledge."

(sūrat ṭā hā, verse114)

Abstract

The current study was planned to use WIEN2k code in order to calculate thestructural, electronic and optical, properties of the lead halide perovskites $CsPbX_3$ (X = Cl, Br, I). Lead halide perovskites had attracted enormous attention as optoelectronic materials, because these materials have power conversion efficiency up to 20 %. So as to calculate the optical, structural, and electronic properties of cubic perovskites $CsPbX_3$ (X = Cl, Br, I), full potential linear augmented plane wave (FP-LAPW) method was opted, that was based on density functional theory (DFT) within LDA, GGA-PBE and mBJ approximation. We have found a good agreement between experimentally measured values and theoretically calculated lattice constants. The perovskite compound $CsPbX_3$ (X = Cl, Br, I) has direct and wide band gap located at point of R-symmetry, while the band gap decreased from 'Cl' to 'I' down the group,. The study of the densities of electrons has revealed strong covalent bonding between Pb and halides, while strong ionic bonding between Cs and halides. The reflectivity, refractive indices, absorption coefficients, real and imaginary parts of dielectric function, optical conductivities, and the other optical properties were calculated. Modeling of these perovskites compounds have direct band gap nature and high absorption power in visible-ultraviolet range that enabled to study the potential applications of these compounds in solar cell application.

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Nomenclature

Abbreviations

$CsPbX_3$(X = Cl, Br, I)	Cesium Lead Halide
DFT	Density Function Theory
BZ	Brillioun Zone
DOS	Density of States
LDA	Local Density Approximation
GGA	Generalized Gradient Approximation
FP-LAPW	Full Potential Linearized Augmented Plane Wave
FP-LAPW+LO	Full Potential Linearized Augmented Plane Wave Plus Local Orbitals
SCF	Self Consistent Field Cycle
R_{MT}	Muffin-Tin radius
mBJA	Modified Becke-Johnson approximation

Symbols

a	Lattice parameter
B	Bulk modulus
E_g	Energy Gap
n	Refractive Index
K	Extinction coefficient
R	Reflectivity
S	Seebeck coefficient

Greek Letters

ε	Dielectric function
ε_1	Real part of dielectric function
ε_2	Imaginary part of dielectric function
σ	Optical Conductivity
ω	Frequency
α	Absorption Coefficient

Chapter 1

Introduction

1.1 Background

The periodic table offers us a basic background to study the periodic behavior of chemical and physical properties of elements as well as their compounds **[1]**. The arrangement of the elements is in ascending order with respect to their atomic numbers, due to which there is repetition in their chemical properties in a periodic manner. The vertical columns in which elements, with similar properties are placed are known as groups **[2]**. These eight groups are usually numbered by Roman numerals ‘I’ to ‘VIII’. These groups are divided into two subgroups named as ‘A’ and ‘B’ followed by roman numerals.