

Declaration

I hereby declare that the work presented in this Thesis titled " $\text{Cu}_2\text{HgSn}(\text{Se}_x\text{S}_{1-x})_4$ based Quaternary Chalcogenides for Photovoltaic and Thermoelectric Applications" submitted to the Indian Institute of Technology Jodhpur in partial fulfilment of the requirements for the award of the degree of Doctor of Philosophy, is a bonafide record of the research work carried out under the supervision of Prof. Ambesh Dixit. The contents of this thesis in full or in parts, have not been submitted to, and will not be submitted by me to, any other Institute or University in India or abroad for the award of any degree or diploma.



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Certificate

This is to certify that the thesis titled "*Cu₂HgSn(Se_xS_{1-x})₄ based Quaternary Chalcogenides for Photovoltaic and Thermoelectric Applications*", submitted by *Sumit Kukreti (P19PH015)* to the Indian Institute of Technology Jodhpur for the award of the degree of *Doctor of Philosophy*, is a bonafide record of the research work done by him under my supervision. To the best of my knowledge, the contents of this report, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Ambesh Dixit
Ph.D. Thesis Supervisor

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List of Symbols

Symbol	Description
L_n (L_p)	Diffusion Length for electrons (holes)
D_n (D_p)	Diffusion constant of electrons (holes)
N_a (N_d)	Acceptor (Donor) Carrier concentration
J_F	Forward biased current density
J_{ph}	Photogenerated current density
J_{sc}	Short-circuit current density
V_{oc}	Open circuit voltage
J_m	Maximum power point current density
V_m	Maximum power point voltage
FF	Fill Factor
P_{in}	Input Power
AM	Air Mass
n_o (p_o)	Equilibrium concentrations of electrons (holes)
$g_c(E)$	Conduction band density of states
$f_F(E)$	Fermi-Dirac distribution function
E_F	Energy at Fermi level
N_c (N_v)	Effective density of states in the conduction band (valence band)
E_c	Energy of conduction band
E_v	Energy of valence band
E_g	Band Gap Energy
G_n (G_p)	Generation rate of electrons (holes)
R_n (R_p)	Recombination rate of electrons (holes)
C_{rad}	Radiative recombination coefficient
C_n (C_p)	Auger recombination coefficient of electrons (holes)
τ_n (τ_p)	Lifetime of electrons (holes)
E_T	Energy of Shockley-Read-Hall trap states
ϵ	Permittivity
Φ	Electrostatic potential
J_n (J_p)	Electron (hole) current density
μ_n (μ_p)	Electron (Hole) Mobility
κ_e	Electronic contribution to thermal conductivity
m^*	Effective mass of the carrier
m_d^*	Density of states (DOS) effective mass
κ_l	Lattice contribution to thermal conductivity
v_q	Average phonon velocity
γ	Gruneisen parameter
E_H	Hartree Energy
E_{XC}	Exchange Correlation Energy
$D_{\alpha\alpha'\beta}(q)$	Dynamical Matrix
M_s	Mass of s^{th} atom
C	Specific heat
Λ	Mean Free Path
S	Seebeck Coefficient
τ	Relaxation Time

List of Abbreviations

Abbreviation Full form

IEA	International Energy Agency
IRENA	International Renewable Energy Agency
DLS	Diamond-like structure
1D	One-dimensional
2D	Two-dimensional
PV	Photovoltaics
SRH	Shockley-Read-Hall
T	Terminal
CIGS	Cu(In, Ga) ₂ Se ₂
CZTS	Cu ₂ ZnSnS ₄
CHTS	Cu ₂ HgSnS ₄
SQ	Shockley Queisser
SLG	Soda Lime Glass
VBM	Valence Band Maximum
CBM	Conduction Band Minimum
EQE	External Quantum Efficiency
TE	Thermoelectric
PF	Power Factor
FPLAPW	Full Potential and Linearly Augmented Plane Wave
TB-mBJ	modified Becke-Johnson
DFT	Density Functional Theory
SCF	Self-Consistent Field
GGA	Generalized Gradient Approximation
LDA	local density approximation
XC	Exchange-Correlation
DFPT	Density Functional Perturbation Theory
BTE	Boltzmann Transport Equation
LBTE	Linear Boltzmann Transport Equation
RTA	Relaxation Time Approximation
CRT	Constant Relaxation Time
LO	Longitudinal Optical
SMA	Single-Mode Approximation
SCAPS-1D	One-Dimensional Solar Cell Capacitance Simulator
CL	Characteristic Length
IR	Interface Recombination
CBO	Conduction Band Offset
COHP	Chemical Orbital Hamilton Population
Ph-DOS	Phonon Density of States
MFP	Mean Free Path
ADP	Acoustic Deformation Potential
IMP	Ionized Impurities
POP	Polar Optical Phonons
SRTA	Single Mode Relaxation Time Approximation