

Sudhir Kumar



Personal Details

Designation Professor
Place Physics Department, Faculty of Engineering and Technology, M. J. P. Rohilkhand University, Bareilly-244 006, Uttar Pradesh
Date of birth October 06, 1962
Citizenship Indian
Gender Male
Professional Interest Research and Teaching
Research Experience 30 Years
Teaching Experience 25 Years
Last Degree Conferred D. Phil.
Degree University Allahabad University, Year-1992, Topic-Electronic Structure of High Temperature Superconductors

Corresponding Details

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Teaching Experience

Oct. 1993–Feb. 1996 **Thermodynamics and Solid State Physics**, *UG and PG*, in Allahabad University.
Optics, Electromagnetic Theory, *UG (B.Tech.)*, in M. J. P. Rohilkhand University, Bareilly.
1998–Present **Futuristic Materials (Material Science)**, *UG (B.Tech.)*, in M. J. P. Rohilkhand University, Bareilly.
2005–Present **Nano Physics and Technology, Advance Solid State Physics**, *PG(M.Sc.)*, in M. J. P. Rohilkhand University, Bareilly.

Professional Experience

Feb. 1993–Oct. 1993 **Post Doctoral Fellowship**, *Uni. des Saarland, Germany*.
Oct. 1993–Feb. 1996 **Post Doctoral Fellowship**, *Allahabad University, India*.

- 10 June–09 July 2000 **INSA Scientist**, *University of Roorkee*, India.
 25 May–08 July 2010 **Visiting Scientist**, *Technical University*, Germany.
 Feb. 1996–Feb. 2005 **Lecturer**, *M.J.P. Rohilkhand University, Bareilly*, India.
 Feb. 2005–Feb. 2008 **Reader**, *M.J.P. Rohilkhand University, Bareilly*, India.
 Feb. 2008–Feb. 2011 **Associate Professor**, *M.J.P. Rohilkhand University, Bareilly*, India.
 Feb. 2011–Present **Professor**, *M.J.P. Rohilkhand University, Bareilly*, India.
 15 June–15 Sept. 2013 **INSA-DFG Scientist**, *Otto Von Guericke University*, Germany.
 June 2017 **Visiting Scientist**, *University of Reading*, United Kingdom, (not availed).

Administrative/Academic Responsibilities

- 1996–2002 **Assistant Proctor**, *M. J. P. Rohilkhand University*, Bareilly.
 1996–2002 **Assistant Dean Studen Welfare**, *M. J. P. Rohilkhand University*, Bareilly.
 2003–2004 **Member of Executive Council**, *M. J. P. Rohilkhand University*, Bareilly.
 2010–2011 **Member of Executive Council**, *M. J. P. Rohilkhand University*, Bareilly.
 2011–2014 **Head, Applied Physics Department**, *M. J. P. Rohilkhand University*, Bareilly.
 2012–2014 **Board of Studies Coordinator**, *M. J. P. Rohilkhand University*, Bareilly.
 2010–2011 **Member of Executive Council**, *M. J. P. Rohilkhand University*, Bareilly.
 2019–Till date **Board of Studies Coordinator**, *M. J. P. Rohilkhand University*, Bareilly.
 May 2020–Till date **Head, Physics Department**, *M. J. P. Rohilkhand University*, Bareilly.
 Sept. 2020–Till date **Director, Directorate of Research**, *M. J. P. Rohilkhand University*, Bareilly.

National/International Conferences Organized

- 1 **National conference on Materials and Devices 2002**, (*MD-2002*), March 09-10, 2002.
- 2 **National Conference of Simulation and Characterization of Advanced Materials**, (*SICHAM-2010*), April 17-18, 2010.
- 3 **National Conference on Science and Engineering of Materials**, (*NCSE-2014*), April 18-19, 2014.

Projects Sponsered

- 1 **Electronic Structure of Solids**, *Sponsering Agency- UGC*, Amount- 0.12 Lacs, Duration- 1 Year (1997).
Current Status- Completed
- 2 **Electronic Structure of Cooperate HTS**, *Sponsering Agency- AICTE*, Amount- 5.0 Lacs, Duration- 3 Years (1997-2000).
Current Status- Completed

- 3 **Ab-initio study of electronic and optical properties of selected II-VI and III-V semiconductors and its alloys: Pressure Effects**, *Sponsering Agency- DST*, Amount- 4.5 Lacs, Duration- 3 Years (2003-2006).
Current Status- Completed
- 4 **Electronic, optical and structural properties of high pressure stable phases of selected III-V and II-VI compounds**, *Sponsering Agency-UGC*, Amount- 5.87 Lacs, Duration- 3 Years (2005-2008).
Current Status- Completed
- 5 **Electronic and optical properties of chalcopyrite compounds: An ab-initio study**, *Sponsering Agency- DST*, Amount- 14.2 Lacs, Duration- 3 Years (2009-2012).
Current Status- Completed
- 6 **Optical properties of N-based semiconductors and its alloys**, *Sponsering Agency- DRDO*, Amount- 22.44 Lacs, Duration- 3 Years (2010-2013).
Current Status- Completed
- 7 **Electronic and optical properties of transparent conducting oxides (TCO) and it alloys: An Ab-initio Study**, *Sponsering Agency- SERB(DST)*, Amount- 34.13 Lacs, Duration- 3 Years (2014-2017).
Current Status- Completed
- 8 **Enhancing gas adsorption properties of borophene by embedding transition metal atom**, *Sponsering Agency- TEQIP-III*, Amount- 2.0 Lacs, Duration- 2 Years (2014-2017).
Current Status- Completed

Lectures/Seminar

Invited By	Name of University/Institute.
Prof. Bal K. Agrawal	Allahabad University, 1992.
Prof. G. Thummnes	Hamburg, Universität (Germany), 1993.
Prof. S. Hufner	Universität des Saarland (Germany)(2), 1993.
Prof. H. Akbarzadeh	Ishfahan University of Technology (Iran), 2005.
SCSM- 2009	Bareilly College, Bareilly (Invited Talk), 2009.
SCAM- 2010	M. J. P. Rohilkhand University, Bareilly (Invited Talk), 2010.
Prof. Dr. G. Gobsch	Technische Universität, Ilmenau (Germany)(2), 2010.
Prof. Dr. F. Bechstedt	Friedrich-Schiller-Universität, Jena (Germany), 2010.
Prof. Dr. F. Reinert	Julius Maximilian Universität, Würzburg (Germany), 2010.
Prof. Dr. G. Gobsch	Technische Universität, Ilmenau (Germany), 2010.
Prof. O. N. Srivastava	Varanasi Hindu University (Invited Talk), March 23, 2010.
Prof. A. C. Sharma	The M. S. University, Baroda, Vadodara (Invited Talk).
Prof. Goldhahn	Otto Von Guericke University, Magdeburg (2), 2013.
Prof. Dr. F. Reinert	Julius Maximilian Universität, Würzburg (Germany), 2013.

Prof. O. N. Srivastava **Varanasi Hindu University (Workshop/Seminar), March 11-17, 2014.**
Prof. Sabu Thomas **Mahatma Gandhi University, Kottayam, Dec. 11-13, 2015.**
Prof. G. Singh **University of Delhi, Delhi, March 01-04, 2016.**
Prof. A. Srivastava **Atal Bihari Vajpai-IIIT, Gwalior, Nov. 17-20, 2016.**

National Conferences Attended/Paper presented

- 1 **Electronic, and optical properties of InP: Pressure effects, S. Kumar et. al.,** Proc. International Symposium on Advanced Materials and Processing, IIT Kharagpur (India).
Dec. 6-8, 2004
- 2 **DST-PAC Meeting, Condensed Matter Physics and Materials Science, S. Kumar,** University of Pondichery.
Feb. 9, 2004
- 3 **Electronic and Optical properties wz InN, S. Kumar et. al.,** 15th National Symposium on Ultrasonic NSU-XV, Allahabad University, Allahabad, (India).
Nov. 1-3, 2006
- 4 **Optical properties of ordered Be_xZn_{1-x}Se alloys, S. Kumar et. al.,** 15th National Symposium on Ultrasonic NSU-XV, Allahabad University, Allahabad, (India).
Nov. 1-3, 2006
- 5 **Structural, electronic and optical properties of In_xGa_{1-x}As alloys, S. Kumar et. al.,** International Conference on Condensed Matter Physics (ICCPMP-2007), Jaipur (India).
Nov. 25-28, 2007
- 6 **The pressure induced structural phase transitions in ZnTe compounds, S. Kumar et. al.,** International Conference on Condensed Matter Physics (ICCPMP-2007), Jaipur (India).
Nov. 25-28, 2007
- 7 **Calculated structural, electronic and optical properties of zincblende InP under hydrostatic pressure, S. Kumar et. al.,** International Conference on Condensed Matter Physics (ICCPMP-2007), Jaipur (India).
Nov. 25-28, 2007
- 8 **DST-PAC Meeting, Condensed Matter Physics and Materials Science, S. Kumar,** Raman Research Institute, Bangalore.
2008
- 9 **Structural properties of high pressure stable phases of ZnTe, S. Kumar et. al.,** 53rd DAE Symposium, BARC, Mumbai.
Dec. 16-20, 2008
- 10 **Effect of Ga addition to InP on its pressure coefficients and effective mass, S. Kumar et. al.,** 53rd DAE Symposium, BARC, Mumbai.
Dec. 16-20, 2008

- 11 **Electronic and optical properties of InN in wurtzite and cubic phases**, *Tarun K. Maurya, S. Kumar and S. Auluck*, in proc. 2nd National Workshop on Advanced Optoelectronic Materials and Devices (AOMD-2008) .
- 12 **DST-PAC Meeting, Condensed Matter Physics and Materials Science**, *S. Kumar*, K. S. Rangasamy College, Tamilnadu. July 6, 2009
- 13 **Optical Properties of Semiconducting Alloys**, *S. Kumar*, Proceedings of Synthesis and Characterization of Smart Materials (SCSM-2009).
- 14 **Comparative study of structural phase transition of ZnS by First-principle codes**, *S. Kumar, S. K. Gupta, and S. Auluck*, Proceedings of the 54th DAE Solid State Physics Symposium (2009).
- 15 **Pressure Coefficients of the ZnS_{1-x}Te_x Alloys**, *Satyam S. Parashari, S. Kumar*, Proceedings of the 54th DAE Solid State Physics Symposium (2009).
- 16 **High pressure Phase Diagram of ZnSe_xTe_{1-x} (x =0.1,0.2, 0.5 0.8)**, *S. K. Gupta, S. Kumar and S. Auluck*, Proceedings of Simulation and characterization of Advanced Materials, April 17-18, 2010, M.J.P Rohilkhand University Bareilly.
- 17 **Ab-initio study of structural electronic and optical properties of bulk CuAlS₂ Chalcopyrite semiconductors**, *S. Pandey, S. Kumar and S. Auluck*, Proceedings of Simulation and characterization of Advanced Materials, April 17-18, 2010, M.J.P Rohilkhand University Bareilly.
- 18 **Ab-initio study of variation in energy gap and pressure co-efficient of GaP**, *Satyam S. Parashari and S. Kumar*, Proceedings of Simulation and characterization of Advanced Materials, April 17-18, 2010, M.J.P Rohilkhand University Bareilly.
- 19 **Electronic and optical properties of Semiconducting Perovskite CsSnBr₃**, *Tarun K. Maurya, S. Kumar and S. Auluck*, Proceedings of Simulation and characterization of Advanced Materials, April 17-18, 2010, M.J.P Rohilkhand University Bareilly.
- 20 **Workshop organized by UPSC Allahabad for deciding the syllabus for lecturership in U.G. and P.G. Government colleges**, *S. Kumar*, Nov. 4-5, 2011.
- 21 **Optical properties of CuX(Al, Ga, In)S₂**, *Suman Pandey, S. Kumar and S. Auluck*, Proceeding of the National Symposium on Advances in Materials Science and Technology, Gujarat University, ahmadabad. Feb. 3-4, 2012
- 22 **Optical properties of CuIn₅Se₈ and CuIn₃Se₅: An ab-initio study**, *S. Kumar, Suman Pandey*, Proceedings of the National Conference on Advanced in Material Science for Energy Applications (AMSEA-2014), University of Petroleum and Energy studies, Dehradun, Uttarakhand. Jan. 9-10, 2014

- 23 **Electronic properties of $\text{Cu}_2\text{ZnSnS}_4$ in kesterite and stannite phases: An ab-initio study**, *Suman Pandey, S. Kumar*, Proceedings of the National Conference on Advanced in Material Science for Energy Applications (AMSEA-2014), University of Petroleum and Energy studies, Dehradun, Uttarakhand.
Jan. 9-10, 2014
- 24 **Optical properties of CuGaSe_2 -based ordered defect compounds**, *Suman Pandey and S. Kumar*, Proceedings of the National Conference on materials and their energy applications (NCME-2014), S. S. Jain Subodh P.G. College, Jaipur-302 004, Rajsthan.
Dec. 22-24, 2014
- 25 **Compositional dependence thermodynamical and electronic properties of $\text{B}_x\text{Al}_{1-x}\text{N}$ alloys: An ab-initio study**, *Suman Pandey and S. Kumar*, Proceedings of the National Conference on materials and their energy applications (NCME-2014), S. S. Jain Subodh P.G. College, Jaipur-302 004, Rajsthan.
Dec. 22-24, 2014
- 26 **Cr incorporated CuGaS_2 : Intermediate band Semiconductors with better absorption for solar energy**, *Durgesh Kumar Sharma and S. Kumar*, Proceedings of the National Conference on materials and their energy applications (NCME-2014), S. S. Jain Subodh P.G. College, Jaipur-302 004, Rajsthan.
Dec. 22-24, 2014
- 27 **Stability, Electronic and Optical Properties of $\text{ZnO}_{1-3x}\text{N}_{2x}\text{F}_x$** , *S. Kumar and Durgesh Kumar Sharma*, International Conference on Multifunctional Materials for Device Application (ICMDA-2016).
Oct. 26-28, 2017
- 28 **Impact of N and F doping in ZnO: An ab-initio study**, *Durgesh Kumar Sharma, S. Kumar and S. Auluck*, 4th International E-Workshop/Conferences on Computational Condensed Matter Physics and Materials Science.
Nov. 18-20, 2016
- 29 **Earth abundant $\text{Cu}_2\text{Cd}_x\text{Zn}_{1-x}\text{SnS}_4$ alloys: A prospective photovoltaic material**, *S. Kumar and Durgesh Kumar Sharma*, International Conference on Emerging Materials and Applications (ICEMA-2017).
Feb. 20-22, 2017
- 30 **Na_xSn alloys: a promising 2D anode material for Na-ion battery**, *Durgesh Kumar Sharma and S. Kumar*, International Conference on Emerging Materials and Applications (ICEMA-2017).
Feb. 20-22, 2017

International Conferences Attended/paper presented

- 1 **International conferences on HTS**, Bangalore, India.
Jan. 10-14, 1990

- 2 **Workshop on Computational Techniques for strongly Correlated Systems**, ICTP, Trieste, Italy.
June 28 - July 09. 1999
- 3 **Material Research Society Fall 1999 meeting**, held at Boston, USA.
Nov 29 - Dec. 03, 1999
- 4 **First conference of Asian Consortium for Computational Materials science**, held at Bangalore.
Nov. 29 - Dec. 01, 2001
- 5 **International Symposium on Advanced Materials and Processing**, held at IIT KGP.
Dec. 6-8, 2004
- 6 **Electronic structure calculations and their applications in Materials science**, Isfahan, Iran (organized by ICTP).
April 35 - May 06, 2005
- 7 **Summer School on Electronic structure Methods And Applications , and Workshop on computational Materials Theory**, JNCASR, Bangalore, India (Organized by ICTP).
July 13-15 and May 06, 2006
- 8 **International Conference on Materials for Advanced Technologies**, Singapore, Organized by MRS Singapore.
July 01-06, 2006
- 9 **14th WEIN2k Workshop**, Institute of High Performance Computing, Singapore.
July 06-09, 2007
- 10 **International Conference on Condensed Matter Physics (ICCPMP-2007)**, Jaipur India.
Nov. 25-28, 2007
- 11 **International Workshop organized by C-DAC on HPC**, Goa.
Dec. 15-16, 2011
- 12 **Electronic Properties of Cu-based Multinary Semiconductors**, *Suman Pandey, S. Kumar and R. Verma*, Proceedings of the 2nd International Conference Optoelectronic Materials and Thin films for Advanced Technology, Cochin University of Science and Technology, Kochi, India.
Jan 03-05, 2013
- 13 **Optical Properties of ordered defect compounds for CuIn_5Se_8 and CuIn_3Se_5 : An ab-initio study**, *Suman Pandey, S. Kumar and R. Verma*, Proceedings of the 2nd International Conference Optoelectronic Materials and Thin films for Advanced Technology, Cochin University of Science and Technology, Kochi, India.
Jan 03-05, 2013

Ph.D. Awarded/Submitted/Working for

- Awarded in 2009 **Electronic and Optical Properties of III-IV Semiconductors Compounds**, *Mr. Satyam S. Parashari.*
- Awarded in 2009 **Electronic and Optical Properties of Selected Semiconductors and their alloys**, *Mr. Tarun K. Maurya.*
- Awarded in 2012 **Electronic, Optical and Structural properties of high pressure stable phases of selected III-V and II-VI compounds**, *Mr. Swatantra Kumar Gupta.*
- Awarded in 2015 **Structural, electronic and optical properties of Chalcopyrite compounds**, *Mrs. Suman Joshi.*
- Awarded in 2021 **Stability, Electronic and Optical Properties of 2D materials: An ab-initio study**, *Mr. Durgesh Kumar Sharma.*

Research Publication

- 1 Electronic structure of defect complexes in crystalline and a-GaAs.**
S. Kumar, Bal K. Agrawal, S. Agrawal and P. S. Yadav
Philosophical Magazine B, 63(3), 657-676(1991).
- 2 Electronic and Vibrational excitations in layered High T_c Superconductors.**
S. Kumar, Bal K. Agrawal, S. Agrawal and P. S. Yadav, J. S. Negi and Namrata Varshney
Bulletin of Material Science, 14(4), 967-971(1991).
- 3 Effects of Ce and F substitutions on the electronic structure of Nd_2CuO_4 superconductors.**
S. Kumar, Bal K. Agrawal, S. Agrawal and P. S. Yadav
Phys. Rev. B, 43, 1166(1991).
- 4 Theoretical evidence for correlation between hole density and T_c in TI-based Superconductors.**
Sudhir Kumar, Bal K. Agrawal, S. Agrawal and P. S. Yadav
Phys. Rev. B, 48, 7364(1993).
- 5 Theoretical evidence for correlation between hole density and T_c $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ Superconductors.**
Sudhir Kumar, Bal K. Agrawal, S. Agrawal and P. S. Yadav
Applied Superconductivity, 3(6), 351-358(1993).
- 6 Photoemission und hochenergetisch Bremsstrahlung Isochromaten - Spektroskopie (BIS) an $Nd_{2-x}Ce_xCuO_4$ und $La_{2-x}Sr_xCuO_4$.**
R. Zimmermann, **S. Kumar** and P. Steiner
Universitat des Saarlandes(1993).

- 7 **Electronic structure of KMnO_4 by Photoemission and inverse photoemission spectroscopy.**
F. Reinert, **S. Kumar**, P. Steiner, R. Claessen and S. Hufner
Z. Phys. B, 49, 431-438(1994).
- 8 **X-ray irradiation effects on KMnO_4 compound.**
Sudhir Kumar, F. Reinert, P. Steiner, R. Claessen and S. Hufner
Unpublished 1994.
- 9 **First-principle calculation of Ga-based System.**
Sudhir Kumar, Bal K. Agrawal, P. S. Yadav and S. Agrawal
Phys. Rev. B, 52, 4896(1995).
- 10 **Van Hove Singularities and hole concentrations in the Parent superconductor $\text{Ca}_{1-x}\text{Sr}_x\text{CuO}_2$.**
Sudhir Kumar, P. S. Yadav, Savitri Agrawal and Bal K. Agrawal
Physica C, 262, 103-110(1996).
- 11 **Ab-initio calculation of $\text{Ga}_{1-x}\text{Al}_x\text{N}$ alloys.**
Sudhir Kumar, Bal K. Agrawal, P. S. Yadav and S. Agrawal
Journal of Physics: Condensed Matter, 9(8), (1997).
- 12 **First- Principles calculation of physical properties of GaN and AlN.**
Sushir Kumar and P. S. Yadav
Semiconductor Materials, R. K. Bedi (Ed), (1998).
- 13 **A First-principles study of structural and electronic properties of $\text{Ga}_{1-x}\text{Al}_x\text{As}$ alloys.**
S. Kumar, Rekha Srivastava, P. S. Yadav, Savitri Agrawal and Bal K. Agrawal
Solid State Communication, 118(9), 479-484(2001).
- 14 **Electronic and optical Properties of Thorium monpnictides.**
S. Kumar and S. Auluck
Bull. Mater. Sci., 26(1), 165-168(2003).
- 15 **Electronic and Optical properties of ordered $\text{Be}_x\text{Zn}_{1-x}\text{Se}$ alloys by FPLAPW method.**
S. Kumar, Tarun K. Maurya and S. Auluck
J. Phys. Condensed Matter, 20, 75205(2008).
- 16 **Pressure induced electronic, structural and optical properties of zincblende InP.**
S. Kumar, Satyam S. Parashari and S. Auluck
Solid State Electronics, 52, 749755(2008).
- 17 **Structural, electronic and optical properties of $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys by Full Potential Linear Augmented Plane Wave Methods.**
S. Kumar, Tarun K. Maurya and S. Auluck

- Jpn. J. Appl. Phys., 47, 5417(2008).
- 18 **Calculated structural, electronic and optical properties of Ga-based semiconductors under pressure.**
S. Kumar, Satyam S. Parashari and S. Auluck
Physica B, 403, 3177-3788(2008).
 - 19 **Dielectric functions and critical points of $\text{Be}_x\text{Zn}_{1-x}\text{Se}$ alloys.**
S. Kumar, Tarun K. Maurya and S. Auluck
J. Alloys and Compounds, 480, 717-722(2009).
 - 20 **Disorder effects on electronic and optical properties of ternary $\text{Ga}_x\text{In}_{1-x}\text{P}$ ($x = 0.25, 0.50, 0.75$) alloy.**
S. Kumar, Satyam S. Parashari
Phys. Stat sol. B, 246(10), 2294-2300(2009).
 - 21 **Electronic properties of stable high pressure phases of ZnTe.**
S. Kumar, Swatantra K. Gupta
Physica B, 404, 3789-3794(2009).
 - 22 **Ab-initio study of electronic and optical properties of InN in wurtzite and cubic phases.**
S. Kumar, Tarun K. Maurya
Optics Communications, 283, 4655-4661(2010).
 - 23 **Ab-initio study of Structural, electronic and optical properties of ZnS.**
Swatantra K. Gupta, **S. Kumar** and S. Auluck
Optics communications, 284, 20-26(2011).
 - 24 **Band structure and optical properties of hexagonal In-rich $\text{In}_x\text{Al}_{1-x}\text{N}$ alloys.**
S.Kumar, Suman Pandey, Swatantra K. Gupta, Tarun K. Maurya, P.Schely, G.Gobsch, R.Goldhahn
J. Phys.: Condens. Matter, 23, 475801(2011).
 - 25 **Tran blaha modified Becke-johnson potential band structure including spin orbit interaction.**
S.Kumar, Suman Pandey, S. Auluck
Advances in optoelectronic Materials (AOM), 2(1),(2014).
 - 26 **An ab-initio study of CuInSe_2 based ordered defect compounds.**
S. Kumar, Suman Panday and S. Auluck
Material chemistry and physics, DOI 10.1016/j.matchemphys.2015.06.001, (2015).
 - 27 **Ab-initio study of Electronic, optical and thermo dynamical properties of ordered $\text{B}_x\text{Al}_{1-x}\text{N}$ alloy.**
S .Kumar, Suman Joshi, B. Joshi and S. Auluck

- Journal of Physics and Chemistry of Solids, 86, 101-107(2015).
- 28 **Ab-initio Study of CuInSe_2 based ordered defect compounds (ODC).**
S. Kumar, Suman Joshi and S. Auluck
Material Chemistry and Physics, 162, 372-379(2015).
 - 29 **Band gap engineering of ZnO substituted with Nitrogen and Fluorine, $\text{ZnO}_{1-3x}\text{N}_{2x}\text{F}_x$: A Hybrid Density Functional Study.**
S. Kumar, Durgesh Kumar Sharma and S. Auluck
RSC Advances, 6, 99088(2016).
 - 30 **Theoretical insights into kesterite and stannite phases of $\text{Cu}_2(\text{Sn}_{1-x}\text{Ge}_x)\text{ZnSe}_4$ based alloys: A prospective photovoltaic material.**
S. Kumar, Durgesh Kumar Sharma and S. Auluck
AIP ADVANCES, 6, 125303(2016).
 - 31 **Stability, electronic and optical properties of wurtzite $\text{Cu}_2\text{Cd}_x\text{Zn}_{1-x}\text{SnS}_4$ alloys as photovoltaic materials: First principles insight.**
S. Kumar, Durgesh Kumar Sharma and S. Auluck
Physical Review B, 94, 235206(2016).
 - 32 **Magnetism by embedding 3d transition metal atoms into germanene.**
Durgesh Kumar Sharma, **Sudhir Kumar**, and Sushil Auluck
Journal of Physics D: Applied Physics, 51, 225006(2018).
 - 33 **Mono and bi layer germanene as prospective anode material for Li-ion batteries: A first-principles study.**
Durgesh Kumar Sharma, **Sudhir Kumar**, A. Laref, and Sushil Auluck
Computational Condensed Matter, 16, e00314(2018).
 - 34 **Electronic structure, defect properties, and hydrogen storage capacity of 2H- WS_2 : A first principles study.**
Durgesh Kumar Sharma, **Sudhir Kumar**, and Sushil Auluck
International Journal of Hydrogen Energy, 43, 23126-23134(2018).
 - 35 **Theoretical characterization of C doped SiGe monolayer.**
Durgesh Kumar Sharma, **Sudhir Kumar**, and Sushil Auluck
Journal of Applied Physics, 125, 145703(2019).
 - 36 **Enhancing gas adsorption properties of borophene by embedding transition metals.**
Sudhir Kumar, Manoj Singh, Durgesh Kumar Sharma and Sushil Auluck
Computational Condensed Matter, 22, e00436(2020).
 - 37 **Influence of defect pairs in Ga-based ordered defect compounds: A hybrid density functional study.**

- Sudhir Kumar**, Suman Joshi, Durgesh Kumar Sharma and Sushil Auluck
Canadian Journal of Physics, 98, 770 (2020).
- 38 **Strain induced optoelectronic properties of two dimensional MnPSe₃/WS₂ heterostructure.**
Durgesh Kumar Sharma, **Sudhir Kumar** and Sushil Auluck
Journal of Physics : Condensed Matter, 32, 315501, (2020).
- 39 **Anomalous and Topological Hall effect in Cu doped Sb₂Te₃ Topological Insulator.**
A Singh, V. K. Gangwar, Prashant Shahi, Debarati Pal, Rahul Singh, Shiv Kumar, S. Singh, S. K. Gupta, **Sudhir Kumar**, Jinguang Cheng, and S Chatterjee
Applied Physics Letters DOI: <https://doi.org/10.1063/5.00021722> (2020).
- 40 **Role of sintering temperature on electronic and mechanical properties of thermoelectric material: A theoretical and experimental study of TiCoSb half-Heusler alloy.**
Bhasker Gahtori, Ajay Kumar Verma, Kishor Kumar Johari, Kriti Tyagi, Durgesh Kumar Sharma, Pawan Kumar, **Sudhir Kumar**, Sivaiah Bathula, S.R. Dhakate
Materials Chemistry and Physics DOI: <https://doi.org/10.1016/j.matchemphys.2022.125854>
- 41 **In Situ Evolution of Secondary Metallic Phases in Off-Stoichiometric ZrNiSn for Enhanced Thermoelectric Performance.**
Kishor Kumar Johari, Durgesh Kumar Sharma, Ajay Kumar Verma, Ruchi Bhardwaj, Nagendra S. Chauhan, **Sudhir Kumar**, Manvendra Narayan Singh, Sivaiah Bathula, and Bhasker Gahtori
ACS Applied Materials & Interfaces DOI: <https://doi.org/10.1021/acsami.2c03065>
- 42 **The charge carrier density modulation in off-stoichiometric ZrNiSn leads to enhanced thermoelectric performance**
Johari Kishor, Kumar, Ajay Kumar Verma, Upadhyay Naval, Kishor, Shyam Radhey, Sharma Durgesh, Kumar, **Kumar Sudhir**, Gahtori Bhasker
Ceramics International DOI: <https://doi.org/10.1016/j.ceramint.2023.05.190>
- 43 **Progress in theoretical study of lead-free halide double perovskite Na₂AgSbX₆ (X = F, Cl, Br, and I) thermoelectric materials**
Kumari Sunita, Kamlesh Peeyush, Kumar, Kumari Lalit, **Kumar Sudhir**, Kumari Sarita, Singh Rashmi, Gupta Rajeev, S Manendra, Rani Chauhan, Upasana, Verma Ajay, Singh
Journal of Molecular Modeling DOI: <https://doi.org/10.1007/s00894-023-05599-0>

Book Contribution

1 **Condensed Matter Physics**

Invited By-Prof. Bal Krishna Agarwal and Prof. Hari Prakash, Physics Department, Allahabad University, Allahabad-211 002

Publisher- Narosa Publishing House(1999)

2 **Advances in Condensed Matter Physics**

Invited By-Prof. A. H. Reshak, Institute of Physical Biology, South Bohemia University, Nov-Hraday-37333, Czech republic

Publisher- SIGNPOT INDIA(2009)

3 **Simulation and Characterization of Advanced Materials**

Editor: dr. Sudhir Kumar, Applied Physics Department, M. J. P. Rohilkhand University Bareilly-243 006

Publisher- Transworld Reserach Network(2012)