

# Sudhir Kumar



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## 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	34 Years
Teaching Experience	27 Years
Last Degree Conferred	D. Phil.
Degree University	Allahabad University, Year-1992, Topic-Electronic Structure of High Temperature Superconductors

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## Corresponding Details

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Mobile	+91-9411472815

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## Teaching Experience

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

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## 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).

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## 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 of Applied Physics**, *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.

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## 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.

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2020-till date Head Physics, Department, M.J.P.R.U, Bareilly

2020-till date Co-ordinator, Research M.J.P. Rohilkhand University, Bareilly

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## 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- Ongoing

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## Lectures/Seminar

Invited By	Name of University/Institute.
Prof. Bal K. Agrawal	<b>Allahabad University</b> , 1992.
Prof. G. Thummme	<b>Hamburg</b> , <i>Universität (Germany)</i> , 1993.
Prof. S. Hufner	<b>Universität des Saarland (Germany)(2)</b> , 1993.
Prof. H. Akbarzadeh	<b>Ishfahan University of Technology (Iran)</b> , 2005.
SCSM- 2009	<b>Bareilly College, Bareilly (Invited Talk)</b> , 2009.
SCAM- 2010	<b>M. J. P. Rohilkhand University, Bareilly (Invited Talk)</b> , 2010.
Prof. Dr. G. Gobsch	<b>Technische Universität, Ilmenau (Germany)(2)</b> , 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.**

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### 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., 15<sup>th</sup>** National Symposium on Ultrasonic NSU-XV, Allahabad University, Allahabad, (India).  
Nov. 1-3, 2006
- 4 **Optical properties of ordered Be<sub>x</sub>Zn<sub>1-x</sub>Se alloys, S. Kumar et. al., 15<sup>th</sup>** National Symposium on Ultrasonic NSU-XV, Allahabad University, Allahabad, (India).  
Nov. 1-3, 2006
- 5 **Structural, electronic and optical properties of In<sub>x</sub>Ga<sub>1-x</sub>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.**, 53<sup>rd</sup> 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.**, 53<sup>rd</sup> 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. 2<sup>nd</sup> 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 54<sup>th</sup> DAE Solid State Physics Symposium (2009).
- 15 **Pressure Coefficients of the ZnS<sub>1-x</sub>Te<sub>x</sub> Alloys, Satyam S. Parashari, S. Kumar**, Proceedings of the 54<sup>th</sup> DAE Solid State Physics Symposium (2009).
- 16 **High pressure Phase Diagram of ZnSe<sub>x</sub>Te<sub>1-x</sub> (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 CuAlS<sub>2</sub> 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 CsSnBr<sub>3</sub>, 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  $\text{CuX}(\text{Al, Ga, In})\text{S}_2$** , *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  $\text{CuIn}_5\text{Se}_8$  and  $\text{CuIn}_3\text{Se}_5$ : 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  $\text{CuGaSe}_2$ -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  $\text{CuGaS}_2$ : 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*, 4<sup>th</sup> 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 photo-voltaic material**, *S. Kumar and Durgesh Kumar Sharma*, International Conference on Emerging Materials and Applications (ICEMA-2017).  
Feb. 20-22, 2017
- 30  **$\text{Na}_x\text{Sn}$  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

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### 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**, JN-CASR, 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 **14<sup>th</sup> 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 2<sup>nd</sup> 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<sub>5</sub>Se<sub>8</sub> and CuIn<sub>3</sub>Se<sub>5</sub>: An ab-initio study**, Suman Pandey, **S. Kumar** and R. Verma, Proceedings of the 2<sup>nd</sup> International Conference Optoelectronic Materials and Thin films for Advanced Technology, Cochin University of Science and Technology, Kochi, India. Jan 03-05, 2013

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### Ph.D. Awarded/Submitted/Working for

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

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### 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<sub>c</sub> 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<sub>2</sub>CuO<sub>4</sub> 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<sub>c</sub> 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  $T_c$  in  $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$  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  
Universität 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. Hüfner  
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. Hüfner  
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  $Ca_{1-x}Sr_xCuO_2$ .**  
Sudhir Kumar, P. S. Yadav, Savitri Agrawal and Bal K. Agrawal  
Physica C, 262, 103-110(1996).
  - 11 **Ab-initio calculation of  $Ga_{1-x}Al_xN$  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  $Ga_{1-x}Al_xAs$  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 mononictides.**  
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<sub>2</sub> 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 B<sub>x</sub>Al<sub>1-x</sub>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<sub>2</sub> 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, ZnO<sub>1-3x</sub>N<sub>2x</sub>F<sub>x</sub>: 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 Cu<sub>2</sub>(Sn<sub>1-x</sub>Ge<sub>x</sub>)ZnSe<sub>4</sub> 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 Cu<sub>2</sub>Cd<sub>x</sub>Zn<sub>1-x</sub>SnS<sub>4</sub> 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<sub>2</sub>: 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 MnPSe<sub>3</sub>/WS<sub>2</sub> 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 Sb<sub>2</sub>Te<sub>3</sub> 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).

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## 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)