रूहेलखण्ड विश्वविद्यालय, बरेली

Applied Physics Department,
F.E.T., M.J.P.R.U.

Title	First Name	Last Name	Photograph
Dr.	**Sudhir**	**Kumar**	

Designation	**Reader**
Department	**Applied Physics Department**
Address (Campus)	**Institute of Engineering & Technology, M. J. P. Rohilkhand University, Bareilly-243**
(Residence)	**62, Ashish Royal Park, Pilibhit Road, Bareilly-**
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Education

Subject	Institution	Year	Details
D. Phil	**Allahabad University, Allahabad**	**1992**	***Electronic properties of High Temperature Superconductors***

Professional Qualification

Organization / Institution	Designation	Duration	Role
Uni. des Saarland Saarbrucken (Germany)	**PDF**	Feb. 93-Oct.93	**Research**
Allahabad University, Allahabad	**PDF**	Oct 93 - Feb 96	**Research and Teaching**
M. J. P. Rohilkhand University	**Lecture**	Feb. 96 – Feb. 2005	**Teaching and Research**
M. J. P. Rohilkhand University	**Reader**	Feb. 2005 - Onwards	**Teaching and Research**
University of Roorkee, U.A.	**INSA Visiting Fellowship**	10 June- 09July 2000	**Research**
Technical University Ilmenau Germany	**Visiting Scientist**	25 May-08July 2010	**Research**
Otto-von-Guericke-University Magdeburg	**Visiting Scientist**	15 June- 15Sep 2013	**Research**

Research Interests / Specialization:

Tools available with us

FP-LAPW (Wien2k code), VASP 5.2, FPLO, PWscf, SAX

The central theme of my research group is to determine the electronic and optical properties of materials through a non-empirical description. It usually starts with computational solutions of electronic motion with a quantum mechanical density Functional Theory (DFT). With the advances in computer and algorithms, it is usually possible to characterize and design new materials by such simulations.

We apply a range of computational methods & techniques to investigate fundamental properties of various types of materials and to design new materials. Computational approach is playing an ever-increasing role in studies of materials for advanced technologies and in design of new functional materials. Computation bridges the gap between traditional theoretical and experimental methodologies in the field of science. It is able to provide the theoretical understandings to physical properties of various types of materials and is useful misidentifying the underlying mechanism of various physical processes. First principles methods based on Density Functional Theory, in particular have unprecedented predicting power because they do require experimental input and all physical quantities are computed self consistently by solving quantum mechanical equation. It is the state of the art approach for investigating properties of new materials and for designing new functional materials.

We are using different methods as and when required as per material of investigation. We are mainly using FPLAPW method along with VASP and other state of art techniques.

Teaching Experience (Subjects/Courses Taught)

Name of Institution	UG/PG	Name of Courses	Duration
Allahabad University	UG and PG	Thermodynamic and Solid State Physics Lab	Oct. 1993 to Feb. 1996
MJP Rohilkhand University	UG (B.Tech.)	Optics, Electromagnetic Theory	1998 onwards
MJP Rohilkhand University	UG (B.Tech. Final Year)	Futuristic Material (Material Science)	
MJP Rohilkhand University	M.Sc. (Applied Physics)	Solid State Physics (Prev.) Nano Physics and Technology (Final Year)	2005 Onwards

Honors & Awards

Name of the Scholarship/Fellowship	Awarding Agency
1. Merit Scholarship:	State Government (1980-82)
2. Merit Scholarship:	India Government (1982-84)
3. Merit Scholarship:	India Government (1984-86)
4. Research Fellowship:	Dept. of Sci. & Tech. (1986-92)
5. Research Fellowship:	DAAD (GERMANY) (1992-93)
6. Research Fellowship:	AICTE (INDIA) (1993-96)
7. INSA Visiting Fellowship	INSA, N. Delhi, 1999
8. Research Fellowship:	DAAD (GERMANY) 2010
9. Visiting Scientist :	INSA-DFG (2013)

Total Publication Profile

Books

02 Books as Contributed Chapters (1999, 2009)
01 Book as a Editor (2012)

Books / Monographs

Year of Publication	Title	Publisher
1999	***" Condensed Matter Physics"***	**Narosa Publishing House**
Invited by:	Prof. Bal Krishna Agarwal & Prof. Hari Prakash, Physics Department, Allahabad University, Allahabad – 211 002	
2009	***"Advances in Condensed Matter Physics"***	**SIGNPOST INDIA**
Invited by:	Prof. A. H. Reshak, Institute of Physical Biology, South Bohemia University, Nov-Hraday –37333, Czech Republic.	
2012	***"Simulation and Characterization of Advanced Materials"***	**Transworld Research Network INDIA**
Editor:	Dr. Sudhir Kumar, Applied Physics Department, M. J. P. Rohilkhand University Bareilly-243006, INDIA.	

In Indexed/ Peer Reviewed Journals:

1. **Title:** Electronic structure of defect complexes in crystalline and a-GaAs
   Journal: *Philosophical Magazine B, Vol. 63, No.3, 657-676 (1991)*.
   Authors: Bal K. Agrawal, S. Agrawal and P.S. Yadav, J.S. Negi and S. Kumar

2. **Title:** Electronic and Vibrational excitations in layered High Tc Superconductors,
   Journal: ***Bulletin of Materials Science, Vol.14, No. 4, August - 1991, pp 967-971.,***
   Authors: Bal K. Agrawal, S. Agrawal, P.S. Yadav, ***S.Kumar*** ,J.S. Negi and Namrata Varshney

3. **Title:** Effects of Ce and F substitutions on the electronic structure of Nd_2CuO_4 Superconductors
   Journal: ***Phys. Rev., B43, 1166 (1991).***
   Authors: Bal K.Agrawal, S. Agrawal, P.S. Yadav and ***S.Kumar***

4. **Title:** Theoretical evidence for correlation between hole density and T_c in Tl-based Superconductors
   Journal: ***Phys. Rev., B48, 7364 (1993)***.
   Authors: ***Sudhir Kumar*****,** Bal K.Agrawal, P.S. Yadav***, Sudhir Kumar*** and S. Agrawal

5. **Title:** Theoretical evidence for correlation between hole density and Tc $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ Superconductors,
   Journal: ***Applied Superconductivity Vol. Nos 3-6, pp. 351 – 358 (1993).***
   Authors: Bal K.Agrawal, ***Sudhir Kumar***, S. Agrawal and P.S. Yadav

6. **Title:** Photoemission und hochenergetisch Bremsstrahulung Isochromaten - Spektroskopie (BIS) an $Nd_{2-x}Ce_xCuO_4$ und $La_{2-x}Sr_xCuO_4$
   Authors: R. Zimmermann, ***S. Kumar***, P. Steiner, Universitat des Saarlandes (Unpublished) 1993.

7. **Title:** Electronic structure of $KMnO_4$ by Photoemission and inverse photoemission spectroscopy,
   Journal: ***Z. Phys. B94, 431-438 (1994).***
   Authors: F.Reinert, ***S.Kumar***, P. Steiner, R. Claessen and S. Hufner,

8. **Title:** X-ray irradiation effects on $KMnO_4$ compound,
   Authors: ***Sudhir Kumar***, F.Reinert, P. Steiner, R. Claessen and S. Hufner,

9. **Title:** First - principle calculation of Ga-based System,
   Journal: ***Phys. Rev.B52, 4896 (1995)***.
   Authors: Bal K. Agrawal, P.S.Yadav***, Sudhir Kumar***, and S. Agrawal

10. **Title:** Van Hove Singularities and hole concentrations in the Parent superconductor $Ca_{1-x}Sr_xCuO_2$,
Journal: ***Physica C 262, 103-110 (1996).***
Authors: ***Sudhir Kumar***, P.S.Yadav, Savitri Agrawal and Bal K. Agrawal

11. **Title:** Ab-initio calculation of $Ga_{1-x}Al_xN$ alloys,
Journal: ***Journal of Physics: Condensed Matter Vol. 9, 1763 (1997)***.
Authors: ***Sudhir Kumar***, Bal K. Agrawal, P.S. Yadav, and S. Agrawal

12 **Title:** First- Principles calculation of physical properties of GaN and AlN,
Authors: **Sudhir Kumar** and P.S. Yadav, Semiconductor Materials , R.K. Bedi(Ed) 1998.

13 **Title:** A First-principleS study of structural and electronic properties of $Ga_{1-x}Al_xAs$ alloys
Journal: ***Solid State Communication, Vol. 118(9, 479-484 (2001).***
Authors: **S. Kumar**, Rekha Srivastava, P. S. Yadav, Savitri Agrawal, B.K. Agrawal

14. **Title:** Electronic and optical Properties of Thorium monopnictides,
Journal: ***Bull. Mater. Sci. Vol. 26, 165-168 (2003)***.
Authors: **S. Kumar** and S. Auluck

15. **Title:** Electron and Optical properties of ordered $Be_xZn_{1-x}Se$ alloys by FPLAPW method
Journal: ***J. Phys Condensed Matter Vol. No. 20, 75205 (2008).***
Authors: **S. Kumar**, Tarun K. Maurya and S. Auluck

16. **Title:** Pressure induced electronic, structural and optical properties of zincblende InP.
Journal: ***Solid State Electronics Vol. No. 52, 749 –755 (2008)***.
Authors: **S. Kumar**, Satyam S. Parashari and S. Auluck

17. **Title:** Structural, electronic and optical properties of $In_xGa_{1-x}As$ Alloys by Full Potential Linear Augmented Plane Wave methods.
Journal: ***Jpn. J. Appl . Phys Vol. 47. 5417 (2008).***
Authors: **S. Kumar**, Tarun K. Maurya and S. Auluck

18. **Title:** Erratum Structural, electronic and optical properties of $In_xGa_{1-x}As$ Alloys by Full Potential Linear Augmented Plane Wave methods.

19. **Title:** Calculated structural, electronic and optical properties of Ga-based semiconductors under pressure.
Journal: ***Physica B Vol. 403, 3177-3188 (2008).***
Authors: **S. Kumar,** Satyam S. Parashari and S. Auluck

20. **Title:** Optical properties and critical points of $Be_XZn_{1-X}Se$ alloys
Journal: ***J. Alloys & Compd, Vol. 480, 717-722 (2009).***
Authors: S. Kumar, Tarun K. Maurya and S. Auluck,

21. **Title:** Electronic properties of stable high pressure phases of ZnTe,
Journal: ***Physica B, 404, 3789-3794 (2009).***
Authors: S. Kumar, Swatantra K. Gupta, S. Auluck

22. **Title:** Disorder effects on electronic and optical properties of the ternary $Ga_xIn_{1-x}P$ (x = 0.25, 0.50, 0.75) alloy,
Journal: ***Phys. Stat. Solidi (b,)Vol 246, 2294-2300 (2009).***
Authors: **S. Kumar,** Satyam S. Parashari and S. Auluck,

23. **Title:** Ab-initio study of electronic and optical properties of InN in wurtzite cubic InN phases,
Journal: ***Optics Communications, Vol. 283, 4655-4661 (2010).***
Authors: Tarun K. Maurya, **S. Kumar,** S. Auluck,

24. **Title**: Electronic and Optical properties of high pressure stable phases of ZnS: A comparative study of FPLAPW and PW-PP
Journal: ***Solid State Communications, Vol. 284, 20-26 (2011).***
Authors: Swatantra K. Gupta, **S. Kumar** and S. Auluck

25. **Title**: Band Structure and optical properties of hexagonal In –rich $In_xAl_{1-x}N$ Alloys.
Journal: ***Journal of Physics : Condensed Matter, Vol 23, 47508 (2011)***
Authors: S. Kumar, Suman Pandey, S. K. Gupta, Tarun K Maurya, P.Schley, G. Gobsch and R. Goldhahn.

26. **Title:** Tran Blaha Modified Beck -Johnson Potential, Band Structure Including Spin Orbit Interaction.
Journal: ***Advances in optoelectronic materials(in press 2013).***
Authors: Sudhir Kumar, Suman Pandey and S. Auluck

27. **Title:** An ab-initio study of $CuInSe_2$ based ordered defect compounds .
Journal: ***Computational Material Science (communicated 2014)***
Authors: S. Kumar , Suman Pandey and S. Auluck

28. **Title:** Tuning of electronic and optical properties of CuGaSe ordered defects compounds : An ab-initio study

Journal: ***Journal of Applied Physics (Communicated 2014)***

Authors: **S. Kumar ,** Suman Pandey

29. **Title:** Optical properties of low index surface of Ru: A combined Theoretical and experimental study:

Journal: ***Under preparation (2014)***

Authors: **S. Kumar ,** S. K. Gupta

30. **Title:** Optical properties of oxides semiconductors.

Journal: ***Under preparation (2014)***

Authors: **S .Kumar**, Suman Pandey, Swatantra K. Gupta and R. Goldhahn 2013

31. **Title:** Stacking sequence dependent electronic properties of graphene: An ab-initio study.

Journal: ***Computational Material Science (communicated 2014)***

Authors: Swatantra K. Gupta**,** **S. Kumar** and S. Auluck

32. **Title:** Ab-initio study of structure,electronic and optical properties of ordered $B_xAl_{1-x}N$ alloy.

Journal: **under preparation (2014)**

Authors: **S .Kumar**, Suman Pandey and R. Verma

33. **Title** : Electronic and optical properties of $InAs_{1-x}N_x$

Journal: **under discussion (2014)**

Authors: **S .Kumar**, Suman Pandey and R. Goldhahn 2013

Conference Presentations

24 Conference Presentation

A: National:

1. Electronic, and optical properties of InP: Pressure effects. ***S. Kumar*** *et. al , proc. International Symposium on Advanced Materials and Processing, at* ***IIT Kharagpur*** *6-8 Dec. 2004 (India).*
2. Electronic and Optical properties wz InN ***S. Kumar*** *et. al. 15th National Symposium on Ultrasonics NSU-XV 2006 between November 1-3 , 2006 at Allahabad University* ***Allahabad India.***
3. Optical properties of orderd $Be_xZn_{1-x}Se$ alloys ***S. Kumar*** *et. al. 15th National Symposium on Ultrasonics NSU-XV 2006 between November 1-3 , 2006 at Allahabad University* ***Allahabad India.***
4. Structural, electronic and optical properties of $In_xGa_{1-x}As$ alloys ***S. Kumar*** *et. al International Conference on Condensed Matter Physics "ICCPMP-2007", 25th -28th November 2007,* ***Jaipur, India****.*
5. The pressure induced structural phase transitions in ZnTe compounds ***S. Kumar*** *et. al International Conference on Condensed Matter Physics* "ICCPMP-2007",25th -28th November 2007, **Jaipur, India.**
6. Calculated structural, electronic and optical properties of zincblende InP under hydrostatic pressure, *S. Kumar* et. al. International Conference on condensed Matter Physics "ICCPMP-2007" 25-28th November 2007, ***Jaipur, India.***
7. Structural properties of high pressure stable phases of ZnTe, ***S. Kumar*** et al. *53rd DAE Symposium between 16-20 Dec 2008,* ***BARC Mumbai****.*
8. Effect of Ga addition to InP on its pressure coefficients and effective mass, ***S. Kumar*** et *53rd DAE Symposium between 16-20 Dec 2008,* ***BARC Mumbai***.
9. 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****),* ***BHU, Varanasi***.
10. Ab-initio study of structural electronic and optical properties of bulk $CuAlS_2$ chalcopyrite semiconductors: S. Pandey, ***S. Kumar***, and S. Auluck: Proceedings of Simulation and characterization of Advanced Materials, **17-18 Apr.(2010),** M.J.P Rohilkhand University Bareilly (U.P.).
11. Elecrtronic and optical properties of Semiconducting Perovskite $CsSnBr_3$ **, *S. Kumar***, et. al. Proceedings of Simulation and characterization of Advanced Materials, **17-18Apr.(2010),** M.J.P Rohilkhand University Bareilly (U.P.).
12. Ab-initio study of variation in energy gap and pressure coefficients of GaP, ***S. Kumar,*** et. al. Proceedings of Simulation and characterization of Advanced Materials, **17-18Apr.(2010),** M.J.P Rohilkhand University Bareilly (U.P.).
13. High pressure phase diagram of $ZnSe_xTe_{1-x}$ alloys (where x = 0.1, 0.2, 0.5, 0.8) ***S. Kumar***, et. al. Proceedings of Simulation and characterization of Advanced Materials, **17-18Apr.(2010),** M.J.P Rohilkhand University Bareilly (U.P.).

Technology, Kochi.

14. Optical properties of Cu X (Al, Ga, In)S_2; ¸Suman Pandey, **S. Kumar,**, and S. Auluck Proceeding of the National Symposium on Advances in Materials Science and Technology **3-4 Feb (2012),** Gujarat University, Ahmadabad.
15. Electronic Properties of Cu-based Multinary Semiconductors; Suman Pandey, ***S. Kumar,*** and R. Verma, Proceedings of the 2nd International Conference on Optoelectronic Materials and Thin films for Advanced Technology, **3-5 Jan (2013),** Cochin University of Science and Technology, Kochi.
16. Optical Properties of ordered defect compounds for $CuIn_5Se_8$ and $CuIn_3Se_5$:An ab- inito study, Suman Pandey, ***S. Kumar,*** and R. Verma, Proceedings of the 2nd International Conference on Optoelectronic Materials and Thin films for Advanced Technology, **3-5 Jan (2013),** Cochin University of Science and Technology, Kochi.
17. Recent Trends in Material Science -2013 (RTMS-13), **21 Nov. (2013),** M.J.P Rohilkhand University Bareilly (U.P.).
18. 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, **9-10th Jan. (AMSEA-2014),** University of Petroleum and energy studies Dehradun Uttarakhand.
19. Electronic properties of Cu_2ZnSnS_4 in kesterite and stannite phases: An ab-initio study, Proceedings of the National Conference on Advanced in Material Science for Energy Applications, **9-10th Jan. (AMSEA-2014),** University of Petroleum and energy studies Dehradun Uttarakhand.

B. International

1. Electronic structure of InP under pressure **S. Kumar** et. al. Electronic structure calculations and their applications in Materials science, 25 April –06 May 2005, Isfahan**, Iran (organized by ICTP, Italy)**
2. Structural, Electronic and Optical Properties of ordered $Be_xZn_{1-x}Se$ Alloys, **S. Kumar** et al. International Conference on Materials for Advanced Technologies 01-06 July 2007, **Singapore** organized by **MRS Singapore**

Public Service / University Service / Consulting Activity

NA

Professional Societies Memberships

Material Research Society, Singapore

Projects (Major Grants / Collaborations)

Name of the Project	Sponsoring Agency	Amount	Duration	Current Status
Electronic Structure of Solids	UGC unassigned grant 1997	0.12 Lacs	One Year	Completed
Electronic Structure of cuperate High Temperature Superconductors	AICTE 1997 – 2000	5.0 Lacs	Three Years	Completed
Ab-initio study of electronic and optical properties of selected II-VI and III-V semiconductors & its alloys: Pressure effects.	DST 2004-2007 Six months ext.	4.5 Lacs	Three Years	Completed
Electronic, optical and structural properties of high pressure stable phases of selected III-V and II-VI compounds	UGC 2007-2010	5.87 Lacs	Three Year	Completed
Electronic and optical properties of Chalcopyrite compounds: An ab-initio study	DST 2010-2014 Six month ext.	14.40 Lacs	Three Year	Ongoing
Analysis of electronic and optical properties of N based semiconductors and their alloys: A first principle study	DRDO 2011-2014	22.00 Lacs	Three Year	Ongoing

Ph. D. Supervision:

Name of the Scholar	**Title**	**Year of Ph. D Submission /awarded**	**Publications**
1. Satyam S. Parashari,	Electronic and Optical Properties of III-V Semiconductors compounds	**2009**	Published- **03**
2. Tarun K. Maurya	Electronic, Structural and Optical properties of selected semiconductor compounds and their alloys	**2009**	Published- **05**
3. Swatantra K. Gupta	Structural, Electronic and Optical properties of stable high pressure phases of semiconducting compounds	**2012**	Published-**03** Communicated–**01**
4. Suman Pandey	Structural, Electronic and Optical properties of Chalcopyrite Compounds	Working	Published-**01** Communicated–**03**