




रुहेलखण्ड विश्वविद्यालय, बरेली

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

Title Dr.	First Name Sudhir	Last Name Kumar	Photograph
Designation	Associate Professor		
Department	Applied Physics Department		
Address (Campus)	Institute of Engineering & Technology,		
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Education			
Subject	Institution	Year	Details
D. Phil	Allahabad University, Allahabad	1992	<i>Electronic properties of High Temperature Superconductors</i>
M.Sc.	Magadh University, Bodh Gaya	1986	Subjects: <i>Physics</i>
B. Sc.	Magadh University, Bodh Gaya	1984	Subjects: <i>Physics (Honors), Chemistry, Maths</i>
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
University of Roorkee, U.A.	INSA Visiting Fellowship	10 June- 09July 2000	Research
M. J. P. Rohilkhand University	Reader	Feb. 96 – Feb. 2005	Teaching and Research
Technical University Ilmenau Germany	Visiting Scientist	25 May-08July 2010	Research
M. J. P. Rohilkhand University	Associate Professor	Feb. 2005 – Onwards	Teaching and Research
<u>Research Interests / Specialization:</u>			

Tools available with us

FP-LAPW (Wien2k code), FPLO, PWscf, SAX, VASP5.2

RESEARCH EXPERIENCE:

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 in identifying the underlying mechanism of various physical processes. First principles methods based on Density Functional Theory, in particular have unprecedented predicting power because they do not 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 FP-LAPW, VASP5.2 methods along with PWscf and FPLO state of art methods.

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	
”	UG (B.Tech.)	Futuristic Material (Material Science)	1998 onwards
”	M.Sc. (Physics)	Solid State Physics (P) Nano Physics and	2005 onwards

Honors & Awards

<u>Name of the Scholarship/Fellowship</u>	<u>Awarding Agency</u>
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. Short Term Research Fellowship:	DAAD (GERMANY) (2010)

Publications:

Books / Monographs

<u>Year of Publication</u>	<u>Title</u>	<u>Publisher</u>
1999	“ <i>Condensed Matter Physics</i> ”	Narosa Publishing House

Invited by: Prof. Bal Krishna Agarwal & Prof. Hari Prakash,
Physics Department, Allahabad University,
Allahabad – 211 002

2009	“ <i>Advances in Condensed Matter Physics</i> ”	SIGNPOST INDIA
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Invited by: Prof. A. H. Reshak, Institute of Physical Biology,
South Bohemia University, Nov-Hraday –37333,
Czech Republic.

In Indexed/ Peer Reviewed Journals:

- Title:** Electronic structure of defect complexes in crystalline and a-GaAs.
Journal: *Philosophical Magazine B*, 1991, Vol. 63, No.3, 657-676.
Authors: Bal K. Agrawal, S. Agrawal and P.S. Yadav, J.S. Negi and S. Kumar.
- Title:** Electronic and Vibrational excitations in layered High Tc Superconductors,
Journal: *Bulletin of Materials Science*, Vol.14,. 4, August - 1991, pp 967-971.,
Authors: Bal K. Agrawal, S. Agrawal, P.S. Yadav, S.Kumar, J.S. Negi and Namrata Varshney
- Title:** Effects of Ce and F substitutions on the electronic structure of Nd₂CuO₄ 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 T_c $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ 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 Bremsstrahlung Isochromaten- Spektroskopie (BIS) an $Nd_{2-x}Ce_xCuO_4$ and $La_{2-x}Sr_xCuO_4$

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: . *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: *Rev.B52*, 4896 (1995).

Authors: 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* (1996) 103-110

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, No. 8, 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 118(9) 2001 PP 479-484.*
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, No. 1, January 2003, pp.165-168.*
Authors: S. Kumar and S. Auluck
15. **Title:** Pressure induced electronic, structural and optical properties of
zinblende InP.
Journal: *Solid State Electronics Vol. No. 52, 749 –755, 2008.*
Authors: S. Kumar, Satyam S. Parashari and S. Auluck
16. **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,.*
Authors: S. Kumar, Tarun K. Maurya and S. Auluck
17. **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
18. **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
19. **Title:** Disorder effects on electronic and optical properties of the
ternary $Ga_{1-x}In_xP$ ($x = 0.25, 0.50, 0.75$) alloy,
Journal: *Phys. Stat. Solidi (b,) 2009*
Authors: S. Kumar, Satyam S. Parashari, S. Auluck, *accepted*
20. **Title:** Electronic properties of stable high pressure phase of ZnTe,
Journal: *Physica B 4043789-3794 (2009)*
Authors: S. Kumar, Swatantra K. Gupta, S. Auluck
21. **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,

22. **Title:** Ab-initio study of electronic and optical properties of InN in wurtzite cubic InN phases,
Journal: *Optics Communications*, 2010 (accepted)
Authors: Tarun K. Maurya, S. Kumar, S. Auluck.
23. **Title:** Ab-initio study of Structural, electronic and optical properties of ZnS.
Journal: *Optics Communications*, 2010, accepted.
Authors: Swatantra K. Gupta, S. Kumar and S. Auluck.
24. **Title:** Analysis of dielectric function and critical points for wurzite In-rich $\text{In}_x\text{Al}_{1-x}\text{N}$ alloys
Journal : *Phys. Conden. Matter (under prepn.) 2010.*
Author: S.Kumar, S.K.Gupta, T.K.Maurya, S.Pandey , P. Schely, R.Goldhahn and G. Gobsch.
25. **Title:** Structural ,electronic and optical properties of $\text{InAs}_{1-x}\text{N}_x$ alloys.
Journal : *Journal Applied Physics (under perpn.. 2010)*
Author: S.Kumar, P.Schely, R Goldhahn and G. Gobsch
26. **Title:** Structural ,electronic and optical properties of $\text{CuX}(\text{Al}, \text{Ga}, \text{In})\text{S}_2$ chalcopyrite. semiconductor.
Journal : *Condensed Matter Physics (under perpn. 2010)*
Author: S.Kumar, S.Pandey, S.Auluck (under preparation) 2010.

Total Publication Profile

Books

02 Books as Contributed Chapters

In Indexed/ Peer Reviewed Journals

26 Publications in Journals

Articles

NA

Conference Presentations

29 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. *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 Ultrasonics NSU-XV 2006 between November 1-3 , 2006 at Allahabad University Allahabad (India)*
4. *Optical properties of ordered $\text{Be}_x\text{Zn}_{1-x}\text{Se}$ alloys S. Kumar et. al. 15th National Symposium on Ultrasonics NSU-XV 2006 between November 1-3 , 2006 at Allahabad University Allahabad (India).*
5. *Structural, electronic and optical properties of $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys S. Kumar et. al International Conference on Condensed Matter Physics “ICCPMP-2007”, 25th -28th November 2007, Jaipur, India.*
6. *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.*
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”, 25th -28th November 2007, Jaipur, India.*
8. *DST-PAC Meeting, Condensed Matter Physics and Materials Science, S. Kumar , Raman Research Institute, 2008, Bangalore.*
9. *Structural properties of high pressure stable phases of ZnTe, S. Kumar et al. 53rd DAE Symposium between 16-20 Dec 2008, BARC Mumbai.*
10. *Effect of Ga addition to InP on its pressure coefficients and effective mass, S. Kumar et al. 53rd DAE Symposium between 16-20 Dec 2008, BARC Mumbai.*
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), BHU, Varanasi.*
12. *DST-PAC Meeting, Condensed Matter Physics and Materials Science, S. Kumar K.S. Rangasamy College, Tamilnadu 6 July (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 $\text{ZnS}_{1-x}\text{Te}_x$ Alloys: Satyam S. Parashari†, and S. Kumar *Proceedings of the 54th DAE Solid State Physics Symposium (2009)*.
16. High pressure Phase Diagram of $\text{ZnSe}_x\text{Te}_{1-x}$ ($x = 0.1, 0.2, 0.5, 0.8$): S. K. Gupta, S. Kumar, and S. Auluck: *Proceedings of Simulation and characterization of Advanced Materials, 17-18 April, 2010, M.J.P Rohilkhand University Bareilly*.
17. 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 April, 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, 17-18 April, 2010, M.J.P Rohilkhand University Bareilly*.
19. Electronic and optical properties of Semiconducting Perovskite CsSnBr_3 : Tarun K. Maurya, S. Kumar and S. Auluck,; *Proceedings of Simulation and characterization of Advanced Materials, 17-18 April, 2010, M.J.P Rohilkhand University Bareilly*.

B: International: 10

1. International conferences on HTS between 10-14 Jan.90, Bangalore (India) .
2. ICTP, Trieste, ITALY Workshop on Computational Techniques for strongly Correlated Systems during 28 June-09 July 99.
3. Material Research Society Fall 1999 meeting held at Boston, USA during 29 Nov.-03Dec. 1999.
4. First conference of Asian Consortium for Computational Materials science held at Bangalore between 29 Nov.-01 Dec.2001.

5. International Symposium on Advanced Materials and Processing, at *IIT KGP* 6-8 Dec. 2004
6. Electronic structure calculations and their applications in Materials science, 25 April –06 May 2005, *Isfahan, Iran* (organized by ICTP).
7. Summer School on Electronic structure Methods And Applications , and Workshop on computational Materials Theory July 13-15 –06 May 2006, *JNCASR , Bangalore* (organized by ICTP) .
8. International Conference on Materials for Advanced Technologies 01-06 July 2007, *Singapore* organized by MRS Singapore.
9. 14th WEIN2k Workshop 06th -09th July 2007, Institute of High Performance Computing, *Singapore*.
10. International Conference on Condensed Matter Physics “ICCPMP-2007”, 25th -28th November 2007, Jaipur, India.

Public Service / University Service / Consulting Activity

NA

Professional Societies Memberships

Material Research Society, Singapore

Projects (Major Grants / Collaborations)

Project	Sponsoring Agency	Amount	Duration	Current Status
1. Electronic Structure of Solids	UGC	0.12 Lacs	One Year	Completed
2. Electronic Structure of cuprate HTS	AICTE	5.0 Lacs	Three Years	Completed
3. Ab-initio study of electronic and optical properties of selected II-VI and III-V semiconductors & its alloys: Pressure effects.	DST	4.5 Lacs	Three Years	Completed
4. Electronic, optical and structural properties of high pressure stable phases of selected III-V and II-VI compounds.	UGC	5.87 Lacs	Three Years	Ongoing

5. Electronic and optical properties of chalcopyrite compounds: An ab-initio study.	DST	14.2 Lacs	Sanctioned in Nov. 2009	Ongoing
6. Electronic and optical properties of N-based semiconducting compound and alloys	DRDO	25.0 lacs	-----	Under consideration

Other Details

Ph. D. Supervision:

Name of the Scholar	Title	Status
Stayam S. Parashari,	Electronic and Optical Properties of III-V Semiconductors compounds	Awarded in 2009
Tarun K. Maurya	Electronic and Optical Properties of Selected Semiconductors and their alloys	Awarded in 2009
Swatantra Kumar Gupta	Electronic, Optical and Structural properties of high pressure stable phases of selected III-V and II-VI compounds	Writing Thesis
Mrs S. Pandey	Optical properties of Chalcopyrite compounds	On going