#### Updated on 13<sup>th</sup> November, 2018

#### Dr. RANJAN KUMAR

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Date of Birth 19th March, 1974

**Residential Address** E1-67, Sector-14, Panjab University Campus

Chandigarh-160014, India Ph. 0172-2726967

Academic Qualifications: M.Sc. (H.S.) Physics, Ph. D.

**Ph. D. Thesis Title:** Structure and orientational order in pure and

doped C<sub>60</sub> solids.

**Career Profile:** Lecturer: 02-11-1999 to 1-11-2005 (P.U.)

Sr. Lecturer 02-11-2005 to 10-5-2009 (P.U.)

Reader 11-5-2009 to 10-5-2012 (P.U.)

Associate Professor 11-5-2012 to 10-5-2015 (P.U.)

Professor 11-5-2015 to Till date (P.U.)

### **Courses Taught**

- 1. Condensed Matter Physics and material Science (UG)
- 2. Mathematical Physics (PG)
- 3. Electricity and Magnetism and electronics (UG)
- 4. Principles of Physics (Quantum and Statistical Mechanics)
- 5. Physics of Materials and Nanomaterials (M.Tech.)
- 6. Classical Mechanics(PG)
- 7. Statistical mechanics (PG)
- 8. Classical Electrodynamics (PG)
- 9. Condensed Matter Physics (PG)



#### 10. Mathematical Physics -III (UG)

## **RESEARCH**

**Field of specialization:** Theoretical Condensed Matter Physics

#### **Areas of Interest:**

- 1. Model calculations of molecular solids( Fullerenes)
- 2. Edohedral Fullerenes, Nanotobes and graphenes
- 3. Heusler alloys for spintronic applications
- 4. Dilute magnetic semiconductors
- 5. Nanocomposits
- 6. Electronic and Thermoelectric properties of materials
- 7. Conventional superconductors

### Students supervised

S.	Degree	Name of the	Title	status
No.		candidate		
1	Ph. D.	Ms. Devina Sharma	Size effects in cuprate superconductors and AB-initio	Awarded
			study of their electronic properties.	2014
2	Ph.D.	Mr. Nibras Mossa	Effect of endohedral doping on C <sub>60</sub> and carbon	Awarded
		Umran	nanotubes.	2014
3	Ph.D.	Ms. Kumari Seema	Structural and electronic properties of Dilute magnetic	Awarded
			oxides and Heusler Alloys	2014
4	Ph.D.	Ms. Vaneeta Bala	Theoretical and experimental study of semiconductor	Awarded
			/polymer nanocomposites	2015
5	Ph. D.	Ms. Shobhna Dhiman	Theoretical studies of doped C <sub>60</sub> and carbon nanotubes.	Awarded
				2016
6	Ph.D.	Ms. Kulwinder Kaur	Theoretical investigation of thermoelectric materials	Awarded
				2017
7	Ph.D.	Ms. Anita Rani	Study of II-VI and III-V Dilute Magnetic Semiconductors	Awarded
				2017
8	Ph.D.	Ms. Sarita Mann	Thermal and thermodynamic properties of pure and	Awarded
			hetero-graphene	2018
9	Ph.D.	Mr. Anil Sonkusare	Development and characterization of porous silicon gas	Awarded

			sensor	2018
10	Ph.D.	Mr. Gagandeep Singh	Order disorder phenomena in Mn based Heusler	Registered
			compounds	
11.	Ph.D.	Ms. Anuradha	Thermoelectric properties of Li based compounds	Registered
12	Ph.D.	Mr. Surinder Singh	Theoretical Study of Conventional Superconductors	Registered
13	Ph.D.	Mr. Deepak Kumar	Terahertz Metamaterials (Tentative)	Registered
14	Ph.D.	Mr. Gurpal Singh	Transport properties of Graphene(Tentative)	Registerd
		Khosa		
15	Ph.D.	Ms. Preety	Conventional superconductors(Tentative)	Registerd
16	Ph.D.	Mr. Shagun Nag	Two dimensional Thermoelectric materials (Tentative)	Registerd
1	M.Phill.	Ms. Reena Devi	C, Na and H doped Endohedral C <sub>60</sub> : DFT Calculation	Awarded
				2009
2	M.Phill.	Ms. Anita Rani	Structure and electronic properties of doped C <sub>20</sub>	Awarded
			fullerenes.	2010
3	M. Phill.	Ms. Kumari Seema	Structure of alkaline earth and rare earth doped C <sub>60</sub>	Awarded
			solids	2010
4	M.Tech.	Mr. Dheeraj Sharma	A Study of Electronic properties for Zig-Zag, Armchair &	Awarded
	NS&NT		Chiral Carbon-Nanotubes	2011
5	M.Tech.	Ms. Harkiran Kaur	Alkali Metal doped Endohedral Fullerenes	2008
	NS&NT			
6	M.Tech.	Ms. Lavnya Khanna	Density functional theory- A tool for simulation of Nano	2008
	NS&NT	and Harkiran Kaur	systems	
1	M.Sc.	Ms. Rashim	Stability of Na clusters inside C <sub>84</sub>	2008
2	M.Sc.	Ms. Amandeep	Dependence of binding energy and HOMO- LUMO gap	2011
			on shape and size of metal clusters	
3	M.Sc.	Ms. Mandeep Kaur	Structure and electronic properties of Full Heusler Alloy	2012
			Co <sub>2</sub> MnSi	
4	M.Sc.	Ms. Priyanka	Calculation of elastic constants of C <sub>60</sub> solid	2014
5	M.Sc.	Ms. Gurpal Singh	Study of Thermal properties of Mg <sub>2</sub> Si and Mg <sub>2</sub> Ge	2015
6	M.Sc.	Ms. Sofia	Thermoelectric properties of Topological semi-metals	2016
7	M.Sc.	Mr. Sukhwinder Singh	Half Heusler compounds as thermoelectric materials	2016
8	M.Sc	Ms. Chanchal	Magnetism in endohedral doped C <sub>20</sub>	2017
9	MSc.	Ms. Vanisha	Terahertz materials	2018

## **Membership of Professional Societies:**

- 1. Life member of Indian Physics Association (IPA)
- 2. Life Member of Indian Association of Physics teachers (IAPT)
- 3. Local coordinator to conduct NGPE Examination(2016-Till Date)
- 4. Founder member and Secretary of Chandigarh Vigyan Parishad (2016-2018)

## Administrative/Committee Assignments

- 1. Convener UG admissions (Physics) 2015
- 2. Convener UG admissions (Physics) 2016
- 3. Convener UG admissions (Physics) 2017
- 4. Secretary, PGAPMEC, Deptt. of Physics, P U. Chandigarh (Jan, 2015-Dec, 2017)
- 5. Member, PGAPMEC, Deptt. of Physics, P U. Chandigarh (Jan, 2017-Dec, 2019)
- 6. Member IQAC, P U Chandigarh (2017-till date)
- 7. Member RDC Physics (1-1-2018to 31-12-2019)
- 8. Member RDC Chemistry (1-1-2018 to 31-12-2019)
- 9. Coordinatior Exams. CET-UG-2017
- 10. Incharge IQAC, Department of Physics (2018-19)

### RESEARCH PUBLICATIONS

## **Journals**

- Variation of Superconducting Transition Temperature of YSn3 Under Negative Pressure, Surinder Singh and Ranjan Kumar, Journal of Superconductivity and Novel Magnetism, doi.org/10.1007/s10948-018-4811-8
- Ammonia sensing using conducting polymer Polypyrrole-coated silicon wafer, Anil G. Sonkusare, Sachin Tyagi, Sunita Mishra, Mamanpreet Kaur, Ranjan Kumar, International Journal of Applied Environmental Sciences 13(2018)59
- A promising thermoelectric response of HfRhSb half Heusler compound at high temperature: A first principle study, Kulwinder Kaur, Ranjan Kumar and D.P. Rai, Journal of Alloys and Compounds 763 (2018) 1018

- 4. Ab-initio study of (Ga,Cr)N and (Ga,Mn)N DMSs: under hydrostatic pressure, Anita Rani, Ranjan Kumar, Mater. Res. Express 5 (2018) 036104
- 5. Search for thermoelectricity in Li-based half-Heusler alloys: a DFT study, Anuradha, Kulwinder Kaur, Ranber Singh and Ranjan Kumar, Mater. Res. Express 5 (2018) 014009
- High temperature thermoelectric performance of p-type TaRhSn half Heusler compound: A computational assessment, Kulwinder Kaur and Ranjan Kumar, Ceramics International 43 (2017) 15160
- Ti based half Heusler compounds: A new on the screen with robustic thermoelectric performance, Kulwinder Kaur and Ranjan Kumar, Journal of Alloys and Compounds 727 (2017) 1171
- 8. Negative thermal expansion of pure and doped graphene, Sarita Mann, Ranjan Kumar and V. K. Jindal, RSC Adv. 7(2017)22378
- 9. On the possibility of thermoelectricity in half Heusler XRuSb (X = V, Nb, Ta) materials: A first principles prospective, Kulwinder Kaur and Ranjan Kumar, Journal of Physics and Chemistry of Solids 110 (2017) 108
- 10. Strain engineering on thermoelectric performance of Mg<sub>2</sub>Si, Kulwinder Kaur, Shobhna Dhiman and Ranjan Kumar, *Mater. Res. Express* 4 (2017) 075509
- Room Temperature Ammonia Gas Sensing Using Polyaniline Nanoparticles Based Sensor Anil G. Sonkusare, Sachin Tyagi, Ranjan Kumar, Sunita Mishra, Int. J of Materials Science 12(2017)283
- 12. Unraveling the effect of uniaxial strain on thermoelectric properties of Mg<sub>2</sub>Si: a DFT study, Kulwinder Kaur, Ranjan Kumar, *Chin. Phys. B* 26 (2017) 066401
- 13. Sb Substitution effect on thermoelectric properties of Mg<sub>2</sub>Si, Kulwinder Kaur and Ranjan Kumar, Journal of ELECTRONIC MATERIALS. 46(2017)4682
- 14. Hydrostatic Pressure effect on Ga0.75Cr0.25As DMS: DFT Study, Anita Rani and Ranjan Kumar, *J Supecond Novel Mag* 30 (2017)3079
- 15. Optimized interaction parameters for metal doped endohedral fullerenes, Shobhna, Ranjan Kumar, Keya Dharamvir, *Appl Nanosci* 7(2017)137
- 16. Small Al and Ga clusters trapped inside the Bucky-ball (C60) A DFT study, Dhiman Shobhna, Ranjan **Kumar**, Dharamvir Keya, *Int. Journal of Modern Physics B* **30 (2017) 1750092**
- 17. Scrutinize the effect of Ge and Sn doping on electronic and thermoelectric properties of MgSi as thermoelectric material. K. Kaur, S. Dhiman, R. Kumar, *Indian Journal of Physics* 91(2017) 1305
- 18. DFT Study of Hydrostatic Pressure Effect on Cd1–xZxX (Z = Cr, Mn; X = S, Se) DMSs, Anita Rani and Ranjan Kumar, *J Supercond Nov Magn* 30(2017) 2175
- 19. Enhancement of figure of merit (ZT) by doping Bi in Mg2Si for energy harvesting applications Kulwinder Kaur, Ranjan Kumar, *Progress in Natural Science: Materials International* 26 (2016)

- 20. Emergence of thermoelectricity in Half Heusler topological semimetals with strain, Kulwinder Kaur, Shobhna Dhiman and **Ranjan Kumar**, *Physics Letters A* **381 (2017) 339**
- 21. LDA+U Study of Induced Half Metallicity in Cr-Doped GaN, Anita Rani and Ranjan Kumar, J Supercond Nov Magn 30 (2017)1483
- Quest of thermoelectricity in topological insulators: A density functional theory study,
   Sukhwinder Singh, Kulwinder Kaur, Ranjan Kumar, Applied surface science 418 (2017) 232
- 23. Study of half-metallic ferromagnetism and elastic properties of Cd<sub>1-x</sub>Cr<sub>x</sub>Z (Z=S, Se), Anita Rani and Ranjan Kumar, *Appl. Phys. A* (2016) 122:1004 DOI 10.1007/s00339-016-0533-6
- 24. Study of Structural and Electronic Properties of Doped Arm Chair Single-Walled Carbon Nanotubes, Shobhna Dhiman, Ranjan Kumar and Keya Dharamvir, Materials Today: Proceedings 3 (2016) 1820–1827
- 25. DFT Study of Diluted Magnetic Semiconductor Cd<sub>1-x</sub>Cr<sub>x</sub>S at x=3.125, Anita Rani, Ranjan Kumar, *Materials Today: Proceedings* 3 (2016) 1815–1819.
- 26. Electronic and Thermoelectric Properties of Al doped Mg2Si Material: DFT Study, Kulwinder Kaur, Ranjan Kumar, *Materials Today: Proceedings* **3** (2016) 1785–1791.
- 27. Thermodynamic properties of pure and doped (B, N) graphene, Sarita Mann, Pooja Rani, Ranjan Kumar, Girija S. Dubey and V. K. Jindal, *RSC Adv.*, 6(2016) 12158
- 28. Effect of Pressure on electronic and thermoelectric properties of Magnesium silicide: a DFT study, Kulwinder Kaur and Ranjan Kumar, *Chin. Phys. B*, 25, No. 2 (2016) 056401
- 29. First principle investigation of the electronic and thermoelectric properties of Mg2C, Kulwinder Kaur and Ranjan Kumar, *Chin. Phys. B* Vol. 25, No. 2 (2016) 026402
- 30. Effect of Disorder on Electronic, Magnetic, and Optical Properties of Co2CrZ Heusler Alloys (Z = Al, Ga, Si, Ge), K Seema, N. M. Umran and Ranjan Kumar, *J Supercond Nov Magn*, **29** (2016) **401**
- 31. Electrical Properties of pure and (Al, Ga & In) doped CdS/PVA Nanocomposites, Vaneeta Bala, Mamta Rani, Surya Tripathi and Ranjan Kumar, *Mater. Res. Express* 2 (2015) 095016
- 32. DFT study of Cu and Ag clusters inside C<sub>60</sub>, Shobhna Dhiman, **Ranjan Kumar** and Keya Dharamvir, **Journal of Molecular Structure 1100 (2015) 328**
- 33. Stability and electronic properties of Cd<sub>0.75</sub>Mn<sub>0.25</sub>S and Cd<sub>0.75</sub>Mn<sub>0.25</sub>Se in B3 Phase, Anita Rani and Ranjan Kumar, *Appl. Phys. A* **120**, **(2015) 775-784**
- 34. Effect of Dopant Concentration on Electronic and Magnetic Properties of Transition Metal-Doped ZrO<sub>2</sub>, K. Seema and **Ranjan Kumar**, *J Supercond Nov Magn*, **28** (2015) 2735
- 35. Study of endohedral doped C<sub>60</sub> fullerene using model potentials, N M Umran, Narinder Kaur, K Seema and Ranjan Kumar, *Mater. Res. Express* 2 (2015) 055603

- 36. Optical properties of Ga and In doped CdS nanocomposites: An experimental and first principles study, Vaneeta Bala, S.K. Tripathi and Ranjan Kumar, *Material Letters*, **149** (2015) **18-21**
- 37. Effect of encapsulation (Au&Tl) molecule in fullerene  $C_{60}$  on electronic and magnetic properties, Nibras Mossa Umran and **Ranjan Kumar**, **Quantum Matter**, **4** (2015), 1–5.
- 38. Effect of Variation in Dilute Limit on Electronic and Magnetic Properties of Transition Metal doped HfO<sub>2</sub>, K Seema and **Ranjan Kumar**, **Quantum Matter**, **4 (2015)**, **1–6**.
- 39. Electronic structure and magnetic properties of quaternary Heusler alloy Co<sub>2</sub>CrGa<sub>1x</sub>Ge<sub>x</sub> (x=0-1), K Seema, Ranjan Kumar, *J Magnetism and Magnetic Materials*, 377 (2015) 70-76.
- 40. Structural and electronic properties of endohedral doped SWCNTs: A DFT study, Nibras Mossa Umran, Vaneeta Bala, K. Seema and Ranjan Kumar, *Physica E*, 65 (2015) 68-76
- 41. Correlation of photoluminescence quenching with Charge Transport in groupIII (Al,Ga&In) elements doped CdS/PVANCs: Experimental and First Principles Studies, Vaneeta Bala, S.K. Tripathi and Ranjan Kumar, *Materials Letters*,132 (2014) 38–40
- 42. Investigations of Al:CdS/PVA nanocomposites: A joint theoretical and experimental approach, Vaneeta Bala, Mamta Sharma, S.K. Tripathi and Ranjan Kumar, *Matrials Chemistry and Physics*, 146(2014) 523-530
- 43. Cyclic Voltammetry of Doped CdS Nanocomposites: Relation Between Theoretical and Experimental Band Gap, Vaneeta Bala, S. K. Tripathi, and Ranjan Kumar, *Journal of Nanoengineering and Nanomanufacturing*, 4 (2014)1-4
- 44. Theoretical investigation of endohedral complexes of Si and Ge with C<sub>60</sub> molecule, Nibras Mossa Umran and Ranjan Kumar, *Physica B*, 437(2014) 47–52
- 45. Half-metallic behavior of Co<sub>2</sub>YZ (Y = V, Cr; Z= Al, Ga) under pressure: a DFT study, K Seema and Ranjan Kumar, *Appl. Phys. A* 116 (2014) 1199
- 46. Investigation of the electronic, magnetic and optical properties of Co<sub>2</sub>CrZ (Z = Si, Ge) under pressure—a density functional theory study, K Seema and Ranjan Kumar, *Phys. Scr.* 89 (2014) 015801
- 47. First principal study of Fe based Full Heusler Alloys, Kumari Seema and Ranjan Kumar, J. integ. Sci. Technol.,1(2013) 41
- 48. AC and DC susceptibility study of sol gel synthesized Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> Superconductor, Devina Sharma, **Ranjan Kumar** and V.P. S. Awana, **Ceram. Int. 39 (2013) 1143**
- Temperature and field dependence of thermally activated flux flow resistance inBi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> superconductor, Devina Sharma, Ranjan Kumar and V.P. S. Awana, Solid State Communications 152 (2012) 941
- 50. Structure and electronic properties of H<sub>n</sub>@C<sub>20</sub> molecule, **Ranjan Kumar** and Anita Rani, *Physica* **B 406 (2011) 1173**
- 51. Comparative experimental and density functional theory study of the physical properties of MgB<sub>2</sub> and AlB<sub>2</sub>, Devina Sharma, Jagdish Kumar, Arpita Vajpayee, **Ranjan Kumar**, P.K. Ahluwalia and V.P.S. Awana, *J. Supercond. Nov. Magn.* 24 (2011) 1925

- 52. Structure of alkaline-earth and rare earth metal doped C<sub>60</sub> solids, Kumari Seema and **Ranjan Kumar**, **Phys. Scr. 83 (2011) 025603**
- 53. Influence of grain size on the superconductivity of La<sub>1.85</sub>Sr<sub>0.15</sub>CuO<sub>4</sub>, Devina Sharma, **Ranjan Kumar**, H. Kishan and V.P.S. Awana, *J. Supercond. Nov. Magn.* **24 (2011) 205**
- 54. Structure and stability of endohedral  $C_n@C_{60}$ , Reena Devi and **Ranjan Kumar**, Modern Physics Lettres B24 (2010)1255.
- 55. Phonon dynamics and thermodynamical properties of alkalimetal doped MC<sub>60</sub> compounds, D. Varshney, Rajendra K. Jain, **K. Ranjan**, Keya Dharamvir and V. K. Jindal, *Modern Physics Letters* **B** 23 (2009)2557
- 56. Zinc phthalocyanine thin film and chemical analyte interactions studies by density functional theory and vibrational techniques, G S S Saini, Sukhwinder Singh, Sarvpreet Kaur, **Ranjan Kumar**, Vasant Sathe and S K Tripathi, *J. Phys.: Condens. Matter* 21 (2009) 225006
- 57. Stability of Na metal clusters inside  $C_{84}$  and  $C_{60}$ , Ranjan Kumar and Harkiran Kaur, *Materials Science- an Indian Journal*, 5 (2009) 62
- 58. Stability of Na and H atoms inside C<sub>60</sub> Molecule DFT Calculations, Reena Devi and **Ranjan** Kumar, *Pb. Univ. Res. J (Sci.)* 58 (2008)217
- 59. Charge Transfer in endohedral Na doped C<sub>240</sub> molecule, **Ranjan Kumar**, Harkiran Kaur and Keya Dharamvir, **Pb. Univ. Re. J (Sci.)** 58 (2008)207
- 60. Comparative study of alkali doped C<sub>60</sub> solids, **K. Ranjan**, K. Dharamvir and V. K. Jindal, *Physica B*, **371 (2006)232**
- 61. Bulk Properties of alkali doped C<sub>60</sub> solids, **K. Ranjan**, K. Dharamvir and V. K. Jindal, *Indian J. of Pure & Applied Physics*, 43 (2005)654
- 62. Cohesive energy of potassium doped C<sub>60</sub> solids, **K. Ranjan**, K. Dharamvir and V. K. Jindal, *Physica B*, 365 (2005)121
- 63. Orientational ordering and binding in alkali doped C<sub>60</sub> solids, **K. Ranjan**, Sarabpreet Singh, K. Dharamvir and V. K. Jindal *Indian J. of Engineering & Materials Sciences*, **7** (2000)320.

# **Conference Proceedings**

- 1. Binding in doped  $C_{60}$  solids- Effect of Coulomb correlation, **K. Ranjan**, K. Dharamvir and V. K. Jindal, *Proceedings of the DAE- Solid state Physics symposium (India)* (1998) 335
- 2. Madelung constant of some alkali doped  $C_{60}$  systems, **K. Ranjan**, K. Dharamvir and V. K. Jindal, Proceedings of the DAE- Solid state Physics symposium (India) (2002) 359
- 3. Effect of alkali metal (M) on the structure of  $M_nC_{60}$  solids, **K. Ranjan**, K. Dharamvir and V. K. Jindal, Proceedings of the DAE- Solid state Physics symposium India (2005) 561
- 4. Structure and ionicity of Na doped C<sub>60</sub> solids, K. Ranjan, Keya Dharamvir and V. K. Jindal,

- Chandigarh Science Congress (2007)
- Thermodynamics of RbC<sub>60</sub> solid in FCC phase, K. Ranjan, N. Kaurav, D Varshney, K. Dharamvir and
   V. K. Jindal, Proceedings of the DAE- Solid state Physics symposium India (2007) 729
- 6. Stability of Na clusters inside C<sub>240</sub> molecule, Harkiran Kaur, **K. Ranjan** and Keya Dharamvir, *Recent Advances in Innovative Materials (RAIM-08)* Excel India Publishers, (2008) 260.
- 7. Carbon clusters inside  $C_{60}$  molecule- a DFT Calculation, Reena Devi and **Ranjan Kumar**, Proceedings of the DAE- Solid state Physics symposium India (2008).
- 8. Structure of silicon clusters- A DFT calculation, Harkiran Kaur , Lavanya Khanna and **Ranjan Kumar**, *Chandigarh Science Congress* (26-28, Feb, 2009)
- Effect of interaction parameters on the thermodynamics of RbC<sub>60</sub>, Ranjan Kumar, N. Kaurav, D.
   Varshney, Keya Dharamvir and V. K. Jindal, Proceedings of National conference on Recent Advances in Condense Matter Physics, 23-24 May, 2009. pp 51
- 10. Adsorption of H atoms inside  $C_{20}$  molecule, Anita Rani, Shobhna Dhiman and Ranjan Kumar, Proceedings of the DAE- Solid state Physics symposium India (2009) 373
- 11. Bulk Properties of Ba and Sr doped  $C_{60}$  solids, K. Seema and Ranjan Kumar, Proceedings of the DAE- Solid state Physics symposium India (2009) 731
- 12. Stability of nitrogen substituted C<sub>20</sub> fullerene: DFT calculations, Anita Devi, Shobhna Dhiman and Ranjan Kumar, Chandigarh science congress, 2010.
- 13. Influence of grain size on the superconductivity of La<sub>1.85</sub>Sr<sub>0.15</sub>CuO<sub>4</sub> Devina Sharma, Ranjan Kumar, H Kishan and VPS Awana, International Conference on Superconductivity and Magnetism (ICSM), Antalya, Turkey, (April 25-30, 2010)
- 14. Impact of particle size on the magneto-transport properties of La<sub>1.85</sub>Sr<sub>0.15</sub>CuO<sub>4</sub> Devina Sharma, Ranjan Kumar and VPS Awana, International conference on quantum effects in solids of todat (I-CONQUEST), National Physical Laboratory, New Delhi, (20-23 Dec, 2010)
- 15. Density Functional study of provskite superconductor MgCNi<sub>3</sub>, Jagdish Kumar, Devina Sharma, Ranjan Kumar, P K Ahluwalia and VPS Awana, AIP Conference proceedings (ICACNM-2011) 1393, 197-198
- 16. Electronic properties of Carbon nanotubes using density functional theory, Shobhna Dhiman, Dheeraj Kumar, Nibras Mossa Umran and Ranjan Kumar, AIP Conference proceedings (ICACNM-2011) 1393, 357-358
- 17. Strucrural and electronic properties of C20-n Sin (n=1-10), Anita Rani, Seema Rani, Vaneeta Bala and Ranjan Kumar, AIP Conference proceedings (ICACNM-2011) 1393, 231-232
- 18. Inter and intra granular properties of La1.85Sr0.15CuO4 Superconductors as influenced by varying grain size, Devina Sharma, Ranjan Kumar and VPS Awana, AIP Conference proceedings (ICACNM-

- 2011) 1393, 233-234
- Sensing of ammonia based on porous silicon sensor, Anil G. Sonkusare, Amit L Sharma, Ranjan
   Kumar and Sunita Mishra, AIP Conference proceedings (ICACNM-2011) 1393, 359-360
- 20. Structure and Electronic properties of c-HfO<sub>2</sub>, Seema Kumari and **Ranjan Kumar**, International conference on Current Developments in Atomic, Molecular, Optical and Nano Physics, D. U. Delhi( 14-16, Dec, 2011)
- 21. The Structural and Electronic Properties of HfO<sub>2</sub>, K. Seema, **Ranjan Kumar**, AIP Conf.

  Proc. 1447, 1077 (2012). The DAE Solid State Physics Symposium (DAE SSPS 2011), 19-23rd Dec.
  2011, held at SRM university, Chennai.
- 22. Ab-initio Study of Chromium doped Cubic Hafnia, K. Seema, Ranjan Kumar, CHASCON-2012, 26-28<sup>th</sup> Feb.2012, Panjab University, Chandigarh.
- 23. Search for ferromagnetism in transition metal doped monoclinic HfO<sub>2</sub>, K. Seema, Ranjan Kumar, AIP Conf Proc. 1512, 1176 (2013). The DAE Solid State Physics
  Symposium (DAE SSPS 2012), 3-7<sup>rd</sup> Dec. 2012, held at IIT Bombay, Mumbai.
- 24. Study of quaternary Heusler alloy  $Co_2CrAl_{1-x}Si_x$ , K. Seema, **Ranjan Kumar**, AIP Conf Proc. 1512, 1154 (2013). The DAE Solid State Physics Symposium (DAE SSPS 2012), 3-7 Dec. 2012, held at IIT Bombay, Mumbai.
- 25. Study of AlN Nanotubes, Vaneeta Bala, Nibras Mossa Umran and **Ranjan Kumar** in 6<sup>th</sup> Chandigarh Science Congress (CHASCON) held at P.U. Chandigarh. (Feb. 26-28, 2012).
- 26. DFT Study of CdS-PVA film, Vaneeta Bala, S. K. Tripathi and **Ranjan Kumar**, International Conference on Materials Science and Technology (ICMST 2012) held at Department of Physics, St. Thomas College, Pala, Kerala (June 10 14, 2012).
- 27. Effect of sintering temperature on the nature of weak links and flux pinning mechanism in La1.85Sr0.15CuO4 superconductor, Devina Sharma, **Ranjan Kumar** and V P S Awana, *International Conference on Materials Science and Technology (ICMST-2012) held at Department of Physics, St. Thomas College, Pala, Kerala (June 10 14, 2012).*
- 28. Structural and Electronic Properties of N Substituted C<sub>20</sub> Fullerene, Anita Rani, Shobhna Dhiman, and Ranjan Kumar, International Journal of Nanotechnology and Applications ISSN 0973-631X Volume6, Number 3, 11-15 (2012)
- 29. Computational studies of polyvinyl alcohol encapsulated tetrahedral cadmium sulphide cluster, Vaneeta Bala, S. K. Tripathi and **Ranjan Kumar**, AIP Conf. Proc. 1536, 301 (2013).

- 30. An ab-initio study of full Heusler alloy F<sub>e2</sub>CoGa, K. Seema, **Ranjan Kumar**, AIP Conf Proc. 1536, 805 (2013).
- 31. Influence of Al doping on Optical properties of CdS/PVA Nanocomposites: Theory and Experiment, Vaneeta Bala, S. K. Tripathi and **Ranjan Kumar**, to be published in AIP Conf. Proc. 1591, 456(2014)
- Pressure Dependence of Half Metallic Behavior of Co<sub>2</sub>VZ (Z=Si, Ge)-An *ab initio* Study, K. Seema, Ranjan Kumar, AIP Conference Proceedings 1591, 1414 (2014).
- 33. Effect on magnetic properties of germanium encapsulated C<sub>60</sub> Fullerene, Nibras Mossa Umran, Ranjan Kumar, AIP Conf. Proc, , 2013, 1512, 264-265.
- 34. Ab initio Study of Structural and Electronic Properties of Cu<sub>n</sub>@C<sub>60</sub> Shobhna Dhiman, Ranjan Kumar and Keya Dharamvir, AIP Conference Proceedings **1536**, 847 (2013)
- 35. Density functional Study of Structural and Electronic Properties of Al<sub>n</sub>@C<sub>60</sub>, Shobhna Dhiman, **Ranjan Kumar** and Keya Dharamvir, *AIP Conf. Proc* 2014, 1591,1106-1108.
- 36. Ab initio study of nitrogen –multisubstituted neutral and positively charged C<sub>20</sub> fullerene, Anita Rani and Ranjan Kumar, AIP Conf. Proc 2014, 1591, 580-582
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- 38. Thermoelectric properties of Al doped Mg2Si material, Kulwinder Kaur, Anita Rani, and Ranjan Kumar, AIP Conference Proceedings 1675, 030023 (2015)
- 39. Effect of disorder on electronic and magnetic properties of Co2VGa Heusler alloy, K. Seema and Ranjan Kumar, AIP Conference Proceedings 1675, 030036(2015)
- 40. Silver clusters encapsulated in  $C_{60}$ : A density functional study Shobhna Dhiman, **Ranjan Kumar**, and Keya Dharamvir, AIP Conference Proceedings 1675, 020004 (2015)
- 41. DFT study of CdS-PVA film, Vaneeta Bala, S K Tripathi and **Ranjan Kumar**, IOP Conf. Series: Materials Science and Engineering 73 (2015) 012118
- 42. DFT study of Al doped armchair SWCNTs, Shobhna Dhiman, Anita Rani, **Ranjan Kuma**r, Keya Dharamvir, AIP Conference Proceedings **1731**, 050114 (2016).
- 43. Effect of hydrostatic pressure on the structural and electronic properties of Cd<sub>0.75</sub>Cr<sub>0.25</sub>S, Anita Rani, Kulwinder Kaur, Shobhna Dhiman, **Ranjan Kumar**, AIP Conference Proceedings **1731**, 120023 (2016).
- 44. Ab –inito study of thermoelectric properties of Mg<sub>2</sub>Ge, Kulwinder Kaur and **Ranjan Kumar**, AIP Conference Proceedings **1731**, 120017 (2016)
- 45. Thermoelectric properties of ZrNiSn Half-Heusler system: An ab-initio study, Sukhwinder Singh, Kulwinder Kaur, and Ranjan Kumar, AIP Conference Proceedings 1832, 110004 (2017)

# Invited Talks and Extension Lectures

# a) Invited Talks

SN	Title of Lecture/ Academic Session	Title of Conference/Seminar etc	Date(s) of the event	Organised by	Whether International/ National
1	Electronic properties of doped fullerenes using DFT	National seminar on Experimental and computational Techniques in Material Science ( ECTMS-2012)	March 31 to April 02, 2012	Deptt. of Physics, H P U Shimla	National
2	Endohedrally doped fullerenes: a DFT Study	International Conference on Advances in Functional materials	Jan 6-8, 2017	Central Univ. of Tamilnadu and Anna University, Chennai	International
3	CNTs, Graphene and their applications	Faculty development programme on Nanotechnology: Developments and challenges	May 12-16, 2014	Department of applied sciences, National Institute of technical teachers training and research (NITTR)	National
4	Characterizing materials and Nanomaterils with Density Functional Theory	Department Seminar/Colloquium	Feb 06, 2015	Deptt. of Physics, Panjab University Chandigarh	National
5	Carbon based Nanomaterials & their applications	Faculty development programme on Nanotechnology	Nov.16,2015	Department of applied sciences, National Institute of technical teachers training and research (NITTR)	National
6	Nanomaterials & their applications	Faculty development programme on Nanotechnology	Nov.21, 2016	Department of applied sciences, National Institute of technical teachers training and research (NITTR)	National
7	Endohedraly doped fullerenes: A DFT study	International conference on advances in functional Materials (ICAFM-17)	6-8 Jan, 2017	Anna Univ. Chennai	International
8	Exploring	Faculty development	March 10,	Deptt. of Electronic	National

	Nanomaterials using DFT	programme	2017	Sciences, Kurukshetra Univ. Kurukshetra	
9	Carbon based Nanomaterials	Faculty development programme on: Nanotechnology: Developmant & Applications	May 22, 2017	Department of applied sciences, National Institute of technical teachers training and research (NITTR)	National
10	Characterizing materials with Density Functional Theory	Refresher course	Dec. 01, 2017	SCERT Solan HP	State
11	Exploring materials using DFT.	Refresher course in Experimental Physics	Dec 12, 2017	Department of Physics P. U. Chandigarh	National

# b) Extension Lectures

SN	Title of Lecture/ Academic Session	Title of Conference/Seminar etc	Date(s) of the event	Organised by	Whether International/ National
1	General science and its importance	Extension lecture	12-02-2013	Khalsa college for women, Sidhwan Khurd, Ludhiana (Pb.)	National
2	Research methodology in sciences	Refresher course on research methodology in sciences	June 11, 2014 to July 01, 2014	Department of Physics, Kurukshetra University, Kurukshetra (Haryana)	National
3	Condensed Matter Physics	Refresher course	June, 2015	SERC, Solan, HP	State
4	Rotational Motion	In service Course	Dec. 27, 2016	Kendriya Vidyalya 3 BRD AFS Chandigarh	National
5	Research Methodology in Sciences	Refresher Course: Research methodology in Physical and Life sciences	May, 26, 2017	Deptt. of Physics, Panjab University Chandigarh	National
6	Research Methodology	FDPP in Physics	3rd July, 2017	Chandigarh University, Gharuan	

## **Conferences Organised**

- 1. Organized International conference on Advances in condensed and Nanomaterials (ICACNM-2011) as secretary, Feb. 2011
- 2. Member LOC of 1st IAPT national student symposium on Physics (2013)

- 3. Member of Local organizing committee of 2nd IAPT National student symposium on Physics, Deptt. Of Physics, P. U. Chandigarh hel on 17-19 January 2014.
- 4. Member of Local organizing committee of International Seminar on Current Trends in Quantum Gases, BEC and Solitons, Department of Physics, Panjab University, Chandigarh, 3–6 March 2014
- 5. Secretary, Physical Sciences Section CHASCON-2018

#### Conferences/seminars/workshops attended

- 1. DAE solid state physics symposium, K. U. Kurukshetra, Dec, 1998
- 2. National conference on recent developments in disordered materials, Deptt. of Physics, P. U. Chd., 15-16, March 2001
- 3. Seminar on computational techniques in Physics, Deptt. of Physics, P. U. Chandigarh, 6-7, March 2002
- 4. DAE solid state physics symposium, K. U. Kurukshetra, Dec, 2002
- 5. 91st Session of Indian Science Congress association, Panjab Univ. Chandigarh, 3-7, Jan, 2004
- 6. DAE solid state Physics Symposium, BARC Mumbai, 5-9, Dec. 2005
- 7. Ist Chandigarh Science Congress, 10-11 March, 2007
- National conference on Recent advances in innovative materials, NIT, Hamirpur, May, 2008
- 9. National conference on Recent advances in condensed matter Physics, NIT, Hamirpur, 23-24 May, 2009
- 10. 3<sup>rd</sup> Chandigarh science congress, P. U. Chd., 26-28, Feb, 2009
- 11. 54th DAE solid state Physics Symposium, MS Univ. of Baroda, 14-18, Dec, 2009
- 12. 4th Chandigarh Science Congress, 19-20 March 2010
- 13. Seminar cum workshop on First principle and other simulation methods in condensed matter physics, H. P. U. Shimla, 22-29 March, 2010
- 14. Internantional conference on advances in condensed and nano materials, P. U. Chd., 22-26, Feb., 2011
- 15. 5th Chandigarh science Congress, P. U. Chd.26-28 Feb, 2011

- 16. International conference on Frontiers in Nanoscience nanotechnology and their applications, p. U. Chd. 16-18 Feb., 2012
- 17. 6th Chandigarh Science Congress, P. U. Chd. 26-28 Feb., 2012
- 18. National seminar on Experimental & computational techniques in material science, H. P.U. Shimla, 31-3-2012 to 2-4-2012
- 19. 58th DAE solid ate Physics Symposium, Thapar Univ. Thapar, 17-21 Dec, 2013
- National conference on Physics of engineering materials, DCRUST, Murthal, 15-17 March, 2013
- 21. 7th Chandigarh Science Congress, P. U. Chd. 1-3 March, 2013
- 22. 8th Chandigarh Science Congress, P. U. Chd 26-28 Feb, 2014
- 23. Conclave on science Education- A manifesto for India's Future 29 Nov., 2014
- 24. NanoSciTech 2014, P. U. Chd., 13-15 Feb, 2014
- International conference on condensed matter physics, H P U Shimla, 4-6 Nov.,
   2014
- 26. 9th Chandigarh Science Congress, P. U. Chd, 25-27 Feb, 2015
- 27. Workshop on High Performance Computing, deptt. of Physics, P. U. Chd, 16-17 March 2015
- 28. 10th Chandigarh Science Congress, P. U. Chd, 29 Feb- 02 March, 2016
- 29. International conference on advances in functional Materials (ICAFM-17), Anna Univ, Chennai, 6-8 Jan, 2017
- 30. 12th Chandigarh Science Congress, P U Chandigarh 12-14 Feb, 2018.