



Dr. Ashok Kumar

Assistant Professor

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Education

Ph. D – 2013: Himachal Pradesh University Shimla

M. Sc – 2008: Himachal Pradesh University Shimla

Academic Employment

Assistant Professor – July 2015 to present: Central University of Punjab, Bathinda

UGC-D S Kothari Post-Doctoral Fellow – May 2014-Jul. 2015: Panjab University Chandigarh

Visiting Instructor – August 2013- December 2013: Michigan Technological University, MI, USA

Area of Research

Condensed Matter Physics: Theoretical and Computational Materials Science-Materials
Modelling using Density Functional Theory: Properties and Predictions

Awards/Scholarships/Grants

Research Award-2018: Central University of Punjab, India

UGC-BSR Start-up Grant-2017: University Grants Commission, New Delhi, India

Young Scientist Award – 2015: Punjab Academy of Sciences, Punjab, India

D S Kothari Post-Doctoral Fellowship – 2014: University Grant Commission, New Delhi

International Travel Award – 2012: Department of Science and Technology, Govt. of India

Senior Research Fellowship – 2012: Council of Scientific and Industrial Research, New Delhi

Junior Research Fellowship – 2010: Council of Scientific and Industrial Research, New Delhi

CSIR – NET – 2009

GATE – 2009

Peer Recognitions

Visiting Scientist-2019: Michigan Technological University, MI, USA (May-June, 2019)

Resource Person/Invited Talks

1. **Resource Person:** Workshop on “*Materials Modeling for Device Applications*” organized by Shri Shankaracharya Technical Campus-SSGI, Bhilai, Chhattisgarh (Feb. 18-23, 2019).
2. **Resource Person:** National Workshop on “*In Silico Approach for Modelling of New Materials: Methodology & Applications*” organized by Department of Physics and Astronomical Sciences, Central University of Himachal Pradesh (Jan. 14-20, 2019).
3. **Invited Talk:** “*Two-dimensional Materials Beyond Graphene: Transition Metal Dichalcogenides*” in National Conference on Reaching the Unreached through Science and Technology (ISCA-2018) at Himachal Pradesh University, Shimla, India.
4. **Resource Person:** National Workshop on “*Transport Phenomenon in Low Dimensional Systems and First Principles Simulation of Condensed Matter Systems*” at Post-graduate Department of Physics, DAV College Jalandhar, Punjab (Sept. 29-Oct. 05, 2016).
5. **Invited Talk:** “*MoS₂: A Promising Layered Material beyond Graphene*” in International Conference on Transport Properties in Low Dimensional Systems: Experiment and Simulation (TransLES 2014), DST Institute of Advanced Study in Science and Technology (IASST), Guwahati, Assam, India.
6. **Invited Talk:** “*Ultrathin Metallic Nanowires on Monolayer MoS₂*” in International Workshop on Materials Modeling and Simulations (IWMMS-2014), Budelkhand University Jhansi, M. P., India.

Technical Reviewer

Chemical Society Reviews; Nature Communications; Nano Letters; Nanoscale; Journal of Physical Chemistry Letter; ACS Applied Materials and Interfaces; Journal of Materials Chemistry C; Journal of Physical Chemistry C; Journal of Chemical Physics; Physical Chemistry Chemical Physics; Nanotechnology; RSC Advances; Journal of Alloys and Compounds; Applied Surface Science; Journal of Materials Science; Journal of Physics and Chemistry of Solids, Journal of Physics: Condensed Matter.

Research Guidance

Ph. D – 01 (completed), 02(ongoing)

M.Phil. – 02

M. Sc. – 14

Courses Taught

PG Level: Quantum Mechanics-I; Quantum Mechanics-II; Statistical Mechanics; Nuclear Physics; Advanced Solid State Physics; Computational Methods in Physics, Quantum, Atomic and Molecular Physics

Ph. D Level: Condensed Matter Physics, Density Functional Theory and Applications

Publications

Publications in SCI Journals (h-index: 18; i-10 index: 22; Citations: > 1200; CIF: ~130) Google Scholar Link: https://scholar.google.co.in/citations?user=i59k6UcAAAAJ&hl=en		Impact Factor (2018)
Year-2019		
1. “Electronic Transport and Thermoelectric Performance of Defected Monolayer MoS ₂ ” Munish Sharma, Ashok Kumar , P. K. Ahluwalia <i>Physica E</i> 107 117 (2019)		3.176
Year-2018		
2. “Si and Ge based Metallic Core/Shell Nanowires for Nano-electronic Device Applications” Prabal Dev Bhuyan, Ashok Kumar , Yogesh Sonvane, P. N. Gajjar, Reeta Magri and Sanjeev K. Gupta, <i>Sci. Rep.</i> 8 16885 (2018).		4.011
3. “Two Dimensional Allotropes of Arsenene with a Wide Range of High and Anisotropic Carrier Mobility” Pooja Jamdagni, Anil Thakur, Ashok Kumar , P. K. Ahluwalia and Ravindra Pandey, <i>Phys. Chem. Chem. Phys.</i> 20 29939 (2018).		3.567

4. "Monolayer, Bilayer, and Heterostructures of Green Phosphorene for Water Splitting and Photovoltaics" Sumandeep Kaur, Ashok Kumar , Sunita Srivastava, K. Tankeshwar, Ravindra Pandey, <i>J. Phys. Chem. C</i> 122 26032 (2018).	4.309
5. "Free-standing Pt and Pd Nanowires: Strain-modulated Stability and Magnetic and Thermoelectric Properties" Shivam Kansara, Sanjeev K. Gupta, Yogesh Sonvane, Ashok Kumar , <i>Phys. Chem. Chem. Phys.</i> 20 28114 (2018).	3.567
6. "Highly Infrared Sensitive VO ₂ Nanowires for a Nano-optical Device" Prabal Dev Bhuyan, Sanjeev K. Gupta, Ashok Kumar , Yogesh Sonvane, P. N. Gajjar, <i>Phys. Chem. Chem. Phys.</i> 20 11109 (2018).	3.567
7. "Stability and Carrier Transport Properties of Phosphorene-based Polymorphic Nanoribbons" Sumandeep Kaur, Ashok Kumar , Sunita Srivastava, Ravindra Pandey, K. Tankeshwar, <i>Nanotechnology</i> 29 155701 (2018).	3.399
8. "Alloyed Monolayers of Cu, Ag, Au and Pt in Hexagonal Phase: A Comprehensive First Principles Study" Pooja Kapoor, Arun Kumar, Munish Sharma, Jagdish Kumar, Ashok Kumar , P. K. Ahluwalia, <i>Materials Science & Engineering B</i> 228 84-90 (2018).	3.507
Year-2017	
9. "Stability and Electronic Properties of Hybrid SnO Bilayers: SnO/Graphene and SnO/BN" Qing Guo, Gaoxue Wang, Ashok Kumar , Ravindra Pandey <i>Nanotechnology</i> 28 475708 (2017).	3.399
10. "Tunnelling Characteristics of Stone-Wales Defects in Monolayers of Sn and Group-V Elements" Pooja Jamdagni, Ashok Kumar , Anil Thakur, Ravindra Pandey, P. K. Ahluwalia <i>Journal of Physics: Condensed Matter</i> 29 395501 (2017).	2.711
11. "van der Waals Heterostructures based on Allotropes of Phosphorene and MoSe ₂ " Sumandeep Kaur, Ashok Kumar , Sunita Srivastava, K. Tankeshwar <i>Physical Chemistry Chemical Physics</i> 19 22023-22032 (2017).	3.567
12. "Size Dependent Tunnel Diode Effects in Gold Tipped CdSe Nanodumbbells" Deepashri Saraf, Ashok Kumar , Dilip Kanhere, Anjali Kashirsagar <i>Journal of Chemical Physics</i> 146 054703 (2017)	2.997
13. "Ultra-narrow Blue Phosphorene Nanoribbons for Tunable Optoelectronics" Ram Swaroop, P. K. Ahluwalia, K. Tankeshwar, Ashok Kumar <i>RSC Advances</i> 7 2992 (2017)	3.049
14. "Electronic Properties and STM Images of Vacancy Clusters and Chains in Functionalized Silicene and Germanene" Pooja Jamdagni, Ashok Kumar , Anil Thakur, Munish Sharma, P. K. Ahluwalia <i>Physica E</i> 85 65-73 (2017)	3.176
15. "Electronic, Mechanical and Dielectric Properties of Two-Dimensional Atomic Layers of Noble Metals" Pooja Kapoor, Jagdish Kumar, Arun Kumar, Ashok Kumar , P. K. Ahluwalia, <i>Journal of Electronic Materials</i> 46 651 (2017)	1.676
Year-2016	
16. "2D-HfS ₂ as an Efficient Photocatalyst for Water Splitting" Deobrat Singh, Sanjeev Kumar Gupta, Yogesh Kumar Sonvane, Ashok Kumar , Rajeev Ahuja, <i>Catalysis Science & Technology</i> 6 6605 (2016)	5.726
17. "Tunable Electronic and Dielectric Properties of β -phosphorene Nanoflakes for Optoelectronic Applications" Pradeep Bhatia, Ram Swaroop Ashok Kumar <i>RSC Advances</i> 6 101835 (2016)	3.049
18. "Electronic Structure Engineering of Various Structural Phases of Phosphorene" Sumandeep Kaur, Ashok Kumar , Sunita Srivastava, K. Tankeshwar, <i>Physical Chemistry Chemical Physics</i> 18 18312 (2016).	3.567
19. "Optical Fingerprints and Electronic Transport Properties of DNA Bases Adsorbed on Monolayer MoS ₂ " Munish Sharma, Ashok Kumar , P. K. Ahluwalia, <i>RSC Advances</i> 6 60223 (2016)	3.049
Year-2015	
20. "Pressure and Electric Field Induced Metallization in Phase Engineered ZrX ₂ (X = S, Se, Te) Bilayers" Ashok Kumar , Haiying He, Ravindra Pandey, P. K. Ahluwalia, K. Tankeshwar <i>Physical Chemistry Chemical Physics</i> 17 19215 (2015)	3.567
21. "Electronic, Dielectric and Mechanical Properties of MoS ₂ /SiC Hybrid Bilayer: A First Principle Study" Munish Sharma, Pooja Jamdagni, Ashok Kumar , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> 71 49 (2015)	3.176
22. "Stability and Electronic Properties of SiGe-based 2D Layered Structures" Pooja Jamdagni, Ashok Kumar , Anil Thakur, Ravindra Pandey, P. K. Ahluwalia <i>Materials Research Express</i> 2 016301 (2015)	1.449
Year-2014	
23. "Electronic Stability and Transport Properties of Atomic wires Anchored on the MoS ₂ Monolayer" Ashok Kumar , Douglas Banyai, P. K. Ahluwalia, Ravindra Pandey Shashi P. Karna <i>Physical Chemistry Chemical Physics</i> 16 20157 (2014)	3.567

24. "Electronic and Optical Properties of Silicene under Uni-axial and Bi-axial Mechanical Strains: A First Principle Study" Brij Mohan, Ashok Kumar , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> 61 40 (2014)	3.176
25. "Strain and Electric Field Induced Electronic Properties of Two-Dimensional Hybrid Bilayers of Transition-metal Dichalcogenides" Munish Sharma, Ashok Kumar , P. K. Ahluwalia <i>Journal of Applied Physics</i> 116 063711 (2014)	2.328
26. "Topology Dependent Electronic and Dielectric Properties of Free Standing Alloyed Ultrathin Nanowires of Noble Metals" Arun Kumar, Ashok Kumar , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> 62 136 (2014)	3.176
27. "Strain Engineering of Dirac Cones in Graphyne" Gaoxue Wang, Mingsu Si, Ashok Kumar , Ravindra Pandey <i>Applied Physics Letters</i> 104 213107 (2014)	3.521
28. "Electronic and Dielectric Properties of Silicene Functionalized with Monomers, Dimers and Trimers of B, C and N Atoms" Brij Mohan, Ashok Kumar , P. K. Ahluwalia <i>RSC Advances</i> 4 31700 (2014)	3.049
29. "Electronic Transport and Dielectric Properties of Low-Dimensional Structures of Layered Transition Metal Dichalcogenides" Ashok Kumar , P. K. Ahluwalia <i>Journal of Alloys and Compounds</i> 587 459 (2014)	4.175
Year-2013	
30. "A First Principle Calculation of Electronic and Dielectric Properties of Electrically Gated Mono and Bilayer Silicene" Brij Mohan, Ashok Kumar , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> 53 233 (2013)	3.176
31. "Effect of Quantum Confinement on Electronic and Dielectric Properties of NbX ₂ (X= S, Se,Te)" Ashok Kumar , P. K. Ahluwalia, <i>Journal of Alloys and Compounds</i> 550 283 (2013)	4.175
32. "Mechanical Strain Dependent Electronic and Dielectric Properties of Two-Dimensional Honeycomb Structure of MoX ₂ (X=S,Se,Te)" Ashok Kumar , P. K. Ahluwalia <i>Physica B: Condensed Matter</i> 419 66 (2013)	1.874
33. Semiconductor to Metal Transition in Bilayer Transition Metal Dichalcogenides MX ₂ (M=Mo,W; X=S,Se,Te) Ashok Kumar , P. K. Ahluwalia <i>Modeling and Simulation in Materials Science and Engineering</i> 21 065015 (2013)	1.826
Year-2012	
34. "Ab-initio Study of Structural, Electronic and Dielectric Properties of Free Standing Nanowires of Noble Metals" Arun Kumar, Ashok Kumar , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> 46 259 (2012)	3.176
35. "First Principle Study of Interband Transitions and Electron Energy Loss in Mono and Bilayer Graphene: Effect of External Electric Field" Brij Mohan, Ashok Kumar , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> 44 1670 (2012)	3.176
36. "Tunable Dielectric Response of Transition Metal Dichalcogenides MX ₂ (M = Mo, W; X= S, Se,Te)" Ashok Kumar , P. K. Ahluwalia <i>Physica B: Condensed Matter</i> 407 4627 (2012)	1.874
37. "A First Principle Comparative Study of Electronic and Optical Properties of 1H-MoS ₂ and 2H-MoS ₂ " Ashok Kumar , P. K. Ahluwalia <i>Materials Chemistry and Physics</i> 135 755 (2012)	2.781
38. "Electronic Structure of Transition Metal Dichalcogenides Monolayers 1H-MX ₂ (M=Mo,W; X=S,Se,Te) from Ab-initio Theory: New Direct Band Gap Semiconductors" Ashok Kumar , P. K. Ahluwalia <i>European Physical Journal B</i> 85 186 (2012)	1.440
Year-2011	
39. "Ab-initio Study of Platinum Induced Reconstructions on Ge(001)-(1×2) Surface" Ashok Kumar , P. K. Ahluwalia <i>Physica B: Condensed Matter</i> 406 4691 (2011)	1.874
Publications as Review Articles	
1. "2D Layered Transition Metal Dichalcogenides (MoS ₂): Synthesis, Applications and Theoretical Aspects" Arun Kumar Singh, P. Kumar, D. J. Late, Ashok Kumar , S. Patel, Jai Singh <i>Applied Materials Today</i> 13 242 (2018)	8.013
Publications as Book Chapters	
1. "Tunable Electronic and Dielectric Properties of Molybdenum Disulfide" Ashok Kumar , P. K. Ahluwalia Vol. 21 of the series Lecture Notes in Nanoscale Science and Technology, pp 53-76 Publisher: Springer International Publishing Switzerland ISBN: 978-	

Publications in AIP Conference Proceedings

1. "Stability and Electronic Properties of Two Dimensional Pentagonal Layers of Palladium Chalcogenides", **Ashok Kumar**, Mukesh Jakhar, Sunita Srivastava, K. Tankeshwar, *AIP Conference Proceedings* **2115** 030387 (2019).
2. "Stability, Electronic and Optical Properties of In-plane WSe₂ Heterophase Nano-ribbons", Ankush Bharti, Neha Katoch, **Ashok Kumar**, Raman Sharma, P K Ahluwalia *AIP Conference Proceedings* **2115** 030360 (2019).
3. "Stability and Electronic Structure of Tricycle-type Allotropes of Pnictogen Monolayers", Pooja Jamdagni, Anil Thakur, **Ashok Kumar**, P K Ahluwalia *AIP Conference Proceedings* **2115** 030377 (2019).
4. "Strain Controlled Electronic and Transport Properties of Si-C Atomic Wire", Rajesh Thakur, **Ashok Kumar**, P K Ahluwalia, Raman Sharma, *AIP Conference Proceedings* **2115** 030374 (2019).
5. "Tuning of Schottky Barriers in Borophene/MoS₂ Van der Waals Heterostructure by External Electric Field", Neha Katoch, Rajesh Thakur, **Ashok Kumar**, P K Ahluwalia, Jagdish Kumar, *AIP Conference Proceedings* **2115** 030362 (2019).
6. "Stability and Tunable Electronic Structure of Planar Phosphorus Nanotubes", Shilpa Singh, Sumandeep Kaur, Sanjeev K Gupta, **Ashok Kumar**, Sunita Srivastava, *AIP Conference Proceedings* **2115** 030383 (2019). (Also received Best Poster Award in DAESSPS-2018).
7. "Adsorption of Nucleobases on Different Allotropes of Phosphorene", Mukesh Jakhar, **Ashok Kumar**, Sunita Srivastava, Prakash Parida, K. Tankeshwar, *AIP Conference Proceedings* **2115** 030361 (2019).
8. "Energetics and Electronic Structure of Novel Hybrid Dumbbell Monolayers", Sumandeep Kaur, Jaspreet Singh, **Ashok Kumar**, Sunita Srivastava, K. Tankeshwar, *AIP Conference Proceedings* **2115** 030382 (2019).
9. "Electronic Properties of ZnPSe₃-MoS₂ van der Waals Heterostructure", Munish Sharma, **Ashok Kumar** and P. K. Ahluwalia, *AIP Conference Proceedings* **1942** 120019 (2018). (Also received Best Poster Award in DAESSPS-2017).
10. "Electronic Structure and Simulated STM Images of Non-honeycomb Phosphorene Allotropes", Sumandeep Kaur, **Ashok Kumar**, Sunita Srivastava, K. Tankeshwar, *AIP Conference Proceedings* **1942** 080020 (2018).
11. "Armchair and Zigzag Nanoribbons of Gold and Silver: A DFT Study", Pooja Kapoor, Munish Sharma, **Ashok Kumar** and P. K. Ahluwalia, *AIP Conference Proceedings* **1942** 050050 (2018).
12. "Electronic and Transport Properties of 1D Aluminium at Atomic Scale" Prabal Dev Bhuyan, Sanjeev K. Gupta, Yogesh Sonvane and **Ashok Kumar**, *AIP Conference Proceedings* **1942** 110026 (2018).
13. "Electronic Properties of Phosphorene/MoSe₂ Vertical Heterostructure" Sumandeep Kaur, **Ashok Kumar**, Sunita Srivastava, K. Tankeshwar, *AIP Conference Proceedings* **1832** 050049 (2017).
14. "Electronic Properties of Ultrathin 1D and 2D Alloyed Nanostructures of Stanene" Geeta Sachdeva, Chandra Kumar, K. Tankeshwar, **Ashok Kumar**, *AIP Conference Proceedings* **1832** 090049 (2017).
15. "First Principles Study of Electronic and Thermoelectric Performance of Li Intercalated MoSe₂ Nanotube" Munish Sharma, **Ashok Kumar**, Ravindra Pandey, P. K. Ahluwalia *AIP Conference Proceedings* **1832** 140036 (2017).
16. "Energetics and electronic properties of Pt wires of different topologies on monolayer MoSe₂" Pooja Jamdagni, **Ashok Kumar**, Anil Thakur, Ravindra Pandey, P. K. Ahluwalia *AIP Conference Proceeding* **1731** 090028 (2016).
17. "Electronic properties of phosphorene-graphene heterostructures effect of external electric field" Sumandeep Kaur, **Ashok Kumar**, Sunita Srivastava, K. Tankeshwar *AIP Conference Proceeding* **1731** 050012 (2016).
18. "Stability, structural and electronic properties of benzene molecule adsorbed on free standing Au layer" Neha Katoch, Pooja Kapoor, Munish Sharma, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1731** 090039 (2016).
19. "Topological insulator behavior of WS₂ monolayer with square-octagon ring structure" **Ashok Kumar**, Ravindra Pandey, P. K. Ahluwalia, K. Tankeshwar *AIP Conference Proceeding* **1731** 140049 (2016).
20. "Interactions of gas molecules with monolayer MoSe₂: A first principle study" Munish Sharma, Pooja Jamdagni, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1731** 140045 (2016)
21. "Structural, electronic and magnetic properties of Au-based monolayer derivatives in honeycomb structure" Pooja Kapoor, Munish Sharma, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1731** 050080 (2016)
22. "Shape-dependent electronic properties of blue phosphorene nano-flakes" Pradeep Bhatia, Ram Swaroop **Ashok Kumar** *AIP Conference Proceeding* **1728** 020598 (2016)
23. "Electronic properties and mechanical strength of β -phosphorene nano-ribbons" Ram Swaroop, Pradeep Bhatia, **Ashok Kumar** *AIP Conference Proceeding* **1728** 020600 (2016)
24. "Electronic and Mechanical Properties of Hybrid Graphene/h-BN Nanoribbons" Pooja Jamdagni, **Ashok Kumar**, Munish sharma, Anil Thakur, P K Ahluwalia *AIP Conference Proceeding* **1665** 090023 (2015)
25. "Electronic and Dielectric Properties of Vacancy Clusters as Quantum Dot in Silicene" Brij Mohan, Munish sharma, **Ashok Kumar**, P K Ahluwalia *AIP Conference Proceeding* **1665** 090041 (2015)

26. "Shape and Edge Dependent Electronic and Magnetic Properties of Silicene Nanoflakes" Brij Mohan, Pooja Jamdagni, **Ashok Kumar**, P K Ahluwalia *AIP Conference Proceeding* **1665** 140041 (2015)
27. "Stability and Electronic Properties of SiC Nanowire Adsorbed on MoS₂ Monolayer" Munish Sharma, Pooja Jamdagni, **Ashok Kumar**, P K Ahluwalia *AIP Conference Proceeding* **1665** 140023 (2015)
28. "Semiconductor-to-metal Phase Transition in Monolayer ZrS₂: GGA+U Study" **Ashok Kumar** Haiying He Ravindra Pandey P. K. Ahluwalia K. Tankeshwar *AIP Conference Proceeding* **1665** 090016 (2015)
29. "Electronic and Dielectric Properties of MoS₂-MoX₂ Heterostructures" Munish Sharma Pooja Jamdagni, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1661** 080028 (2015)
30. "Electronic, Mechanical and Dielectric Properties of Silicene under Tensile Strain" Pooja Jamdagni, **Ashok Kumar**, Munish Sharma, Anil Thakur, P. K. Ahluwalia *AIP Conference Proceeding* **1661** 080007 (2015)
31. "First principle study of manganese doped cadmium sulphide sheet" Sanjeev Kumar, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1591** 1732 (2014)
32. "Structural and electronic properties of free standing one-sided and two-sided hydrogenated silicene: A first principle study" Brij Mohan, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1591** 1714 (2014)
33. "Band gap engineering in nano structured graphane by applying elastic strain" Naveen Kumar, J. D. Sharma, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1512** 192 (2013)
34. "Electronic structure and electron energy loss spectra of armchair and zigzag edged buckled silicene nanoribbons" Brij Mohan, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1512** 378 (2013)
35. "Mechanically strained tuning of the electronic and dielectric properties of monolayer honeycomb structure of tungsten disulphide (WS₂)" **Ashok Kumar**, Brij Mohan, Arun Kumar, P. K. Ahluwalia *AIP Conference Proceeding* **1512** 1242 (2013)
36. "Electronic and optical properties of free standing Pt nanowires using localized basis sets" Arun Kumar, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1447** 831 (2012)
37. "Electronic structure and optical conductivity of two dimensional (2D) MoS₂: Pseudopotential DFT versus full potential calculations" **Ashok Kumar**, Jagdish Kumar, P. K. Ahluwalia *AIP Conference Proceeding* **1447** 1269 (2012)
38. "Ab-initio Study of Structural and Electronic Properties of Homo and Hetro Platinum Dimers on Ge (001)-(2×1) Surface" **Ashok Kumar**, Brij Mohan, P. K. Ahluwalia *AIP Conference Proceeding* **1393** 195 (2011)
39. "Dimer Induced Reconstruction and Metallicity of Ge (001) Surface: Ab-initio SIESTA Study" **Ashok Kumar**, Jagdish Kumar, P. K. Ahluwalia *AIP Conference Proceeding* **1349** 629 (2011)
40. "Surface relaxation and electronic states of Pt (111) surface with varying slab thickness" **Ashok Kumar**, Shanta Mullik, P. K. Ahluwalia *AIP Conference Proceeding* **1349** 693 (2011)

Participation in Schools/Workshops/Orientation Programmes

1. "Orientation Programme-27" Nov 20-Dec 16, 2017, Human Recourse Development Centre GJUS&T, Hisar, Haryana, India.
2. "International Workshop on Materials Modeling and Simulations (IWMMS)" June 24-28, 2013, Sri Shankaryacharya Group of Institute, Bhilai, Chattisgarh, India.
3. "School and Workshop on Electronic Structure Calculations" May 29-June 4, 2013, The Lake Resort, Naukuchiatl (Nainital), Uttarakhand (Organized by Inter University Accelerator Center (IUAC) New Delhi), India.
4. "International Summer School on New Trends in Computational Approaches for Many Body Systems" May 28-June 08, 2012, University de Sherbrooke, Sherbrooke, Quebec, Canada.
5. "National Workshop on Advanced Characterization and Simulation Techniques (ACST-2012)" March 12-17, 2012, Kurukshetra University, Kurukshetra, Haryana, India.
6. "Seminar cum Workshop on First Principle and Other Simulation Methods in Condensed Matter Physics" March 22-29, 2010, Himachal Pradesh University, Shimla, H.P., India.