



## Dr Ashok Kumar

Assistant Professor

Department of Physical Sciences

Central University of Punjab, Bathinda, India 151001

e-mail: [ashok.1777@yahoo.com](mailto:ashok.1777@yahoo.com); [ashokphy@cup.edu.in](mailto:ashokphy@cup.edu.in)

Phone: 0164-2864218 (O); +91 9418581622 (M)

### Education

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Ph. D – 2013: Himachal Pradesh University Shimla

M. Sc – 2008: Himachal Pradesh University Shimla

### Academic Employment

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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

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

### Awards/Scholarships/Grants

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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

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Invited Talks

1. “Elements of Density Functional Theory” in National Workshop on Transport Phenomenon in Low Dimensional Systems and First Principles Simulation of Condensed Matter Systems (2016) at Post-graduate Department of Physics, DAV College Jalandhar, Punjab.
2. “MoS<sub>2</sub>: 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.
3. “Ultrathin Metallic Nanowires on Monolayer MoS<sub>2</sub>” 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

## Research Guidance

Ph. D – 01 (ongoing)

M.Phil. – 02

M. Sc. – 05

## Courses Taught

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

Ph. D Level: Condensed Matter Physics

## Publications

Publications in SCI Journals (h-index: 15; i-10 index: 18; Citations: > 800; CIF: ~90) Google Scholar Link: <a href="https://scholar.google.co.in/citations?user=i59k6UcAAAAJ&amp;hl=en">https://scholar.google.co.in/citations?user=i59k6UcAAAAJ&amp;hl=en</a>		Impact Factor (2016/17)
<b>Year-2018</b>		
1. “Stability and Carrier Transport Properties of Phosphorene-based Polymorphic Nanoribbons” Sumandeep Kaur, <b>Ashok Kumar</b> , Sunita Srivastava, Ravindra Pandey and K. Tankeshwar, <i>Nanotechnology</i> <b>29</b> 155701 (2018).		3.44
2. “Alloyed Monolayers of Cu, Ag, Au and Pt in Hexagonal Phase: A Comprehensive First Principles Study” Pooja Kapoor, Arun Kumar, Munish Sharma, Jagdish Kumar, <b>Ashok Kumar</b> , P. K. Ahluwalia, <i>Materials Science &amp; Engineering B</i> <b>228</b> 84-90 (2018).		2.55
<b>Year-2017</b>		
3. “Stability and Electronic Properties of Hybrid SnO Bilayers: SnO/Graphene and SnO/BN” Qing Guo, Gaoxue Wang, <b>Ashok Kumar</b> , Ravindra Pandey <i>Nanotechnology</i> <b>28</b> 475708 (2017).		3.44
4. “Tunnelling Characteristics of Stone-Wales Defects in Monolayers of Sn and Group-V Elements” Pooja Jamdagni, <b>Ashok Kumar</b> , Anil Thakur, Ravindra Pandey, P. K. Ahluwalia <i>Journal of Physics: Condensed Matter</i> <b>29</b> 395501 (2017).		2.65
5. “van der Waals Heterostructures based on Allotropes of Phosphorene and MoSe <sub>2</sub> ” Sumandeep Kaur, <b>Ashok Kumar</b> , Sunita Srivastava, K. Tankeshwar <i>Physical Chemistry Chemical Physics</i> <b>19</b> 22023-22032 (2017).		4.12
6. “Size Dependent Tunnel Diode Effects in Gold Tipped CdSe Nanodumbbells” Deepashri Saraf, <b>Ashok Kumar</b> , Dilip Kanhere, Anjali Kashirsagar <i>Journal of Chemical Physics</i> <b>146</b> 054703 (2017)		2.96
7. “Ultra-narrow Blue Phosphorene Nanoribbons for Tunable Optoelectronics” Ram Swaroop, P. K. Ahluwalia, K. Tankeshwar, <b>Ashok Kumar</b> <i>RSC Advances</i> <b>7</b> 2992 (2017)		3.11

8. "Electronic Properties and STM Images of Vacancy Clusters and Chains in Functionalized Silicene and Germanene" Pooja Jamdagni, <b>Ashok Kumar</b> , Anil Thakur, Munish Sharma, P. K. Ahluwalia <i>Physica E</i> <b>85</b> 65-73 (2017)	2.22
9. "Electronic, Mechanical and Dielectric Properties of Two-Dimensional Atomic Layers of Noble Metals" Pooja Kapoor, Jagdish Kumar, Arun Kumar, <b>Ashok Kumar</b> , P. K. Ahluwalia, <i>Journal of Electronic Materials</i> <b>46</b> 651 (2017)	1.58
<b>Year-2016</b>	
10. "2D-HfS <sub>2</sub> as an Efficient Photocatalyst for Water Splitting" Deobrat Singh, Sanjeev Kumar Gupta, Yogesh Kumar Sonvane, <b>Ashok Kumar</b> , Rajeev Ahuja, <i>Catalysis Science &amp; Technology</i> <b>6</b> 6605 (2016)	5.77
11. "Tunable Electronic and Dielectric Properties of $\beta$ -phosphorene Nanoflakes for Optoelectronic Applications" Pradeep Bhatia, Ram Swaroop <b>Ashok Kumar</b> <i>RSC Advances</i> <b>6</b> 101835 (2016)	3.11
12. "Electronic Structure Engineering of Various Structural Phases of Phosphorene" Sumandeep Kaur, <b>Ashok Kumar</b> , Sunita Srivastava, K. Tankeshwar, <i>Physical Chemistry Chemical Physics</i> <b>18</b> 18312 (2016).	4.12
13. "Optical Fingerprints and Electronic Transport Properties of DNA Bases Adsorbed on Monolayer MoS <sub>2</sub> " Munish Sharma, <b>Ashok Kumar</b> , P. K. Ahluwalia, <i>RSC Advances</i> <b>6</b> 60223 (2016)	3.11
<b>Year-2015</b>	
14. "Pressure and Electric Field Induced Metallization in Phase Engineered ZrX <sub>2</sub> (X = S, Se, Te) Bilayers" <b>Ashok Kumar</b> , Haiying He, Ravindra Pandey, P. K. Ahluwalia, K. Tankeshwar <i>Physical Chemistry Chemical Physics</i> <b>17</b> 19215 (2015)	4.12
15. "Electronic, Dielectric and Mechanical Properties of MoS <sub>2</sub> /SiC Hybrid Bilayer: A First Principle Study" Munish Sharma, Pooja Jamdagni, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> <b>71</b> 49 (2015)	2.22
16. "Stability and Electronic Properties of SiGe-based 2D Layered Structures" Pooja Jamdagni, <b>Ashok Kumar</b> , Anil Thakur, Ravindra Pandey, P. K. Ahluwalia <i>Materials Research Express</i> <b>2</b> 016301 (2015)	1.07
<b>Year-2014</b>	
17. "Electronic Stability and Transport Properties of Atomic wires Anchored on the MoS <sub>2</sub> Monolayer" <b>Ashok Kumar</b> , Douglas Banyai, P. K. Ahluwalia, Ravindra Pandey Shashi P. Karna <i>Physical Chemistry Chemical Physics</i> <b>16</b> 20157 (2014)	4.12
18. "Electronic and Optical Properties of Silicene under Uni-axial and Bi-axial Mechanical Strains: A First Principle Study" Brij Mohan, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> <b>61</b> 40 (2014)	2.22
19. "Strain and Electric Field Induced Electronic Properties of Two-Dimensional Hybrid Bilayers of Transition-metal Dichalcogenides" Munish Sharma, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Journal of Applied Physics</i> <b>116</b> 063711 (2014)	2.07
20. "Topology Dependent Electronic and Dielectric Properties of Free Standing Alloyed Ultrathin Nanowires of Noble Metals" Arun Kumar, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> <b>62</b> 136 (2014)	2.22
21. "Strain Engineering of Dirac Cones in Graphyne" Gaoxue Wang, Mingsu Si, <b>Ashok Kumar</b> , Ravindra Pandey <i>Applied Physics Letters</i> <b>104</b> 213107 (2014)	3.41
22. "Electronic and Dielectric Properties of Silicene Functionalized with Monomers, Dimers and Trimers of B, C and N Atoms" Brij Mohan, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>RSC Advances</i> <b>4</b> 31700 (2014)	3.11
23. "Electronic Transport and Dielectric Properties of Low-Dimensional Structures of Layered Transition Metal Dichalcogenides" <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Journal of Alloys and Compounds</i> <b>587</b> 459 (2014)	3.13
<b>Year-2013</b>	
24. "A First Principle Calculation of Electronic and Dielectric Properties of Electrically Gated Mono and Bilayer Silicene" Brij Mohan, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> <b>53</b> 233 (2013)	2.22
25. "Effect of Quantum Confinement on Electronic and Dielectric Properties of NbX <sub>2</sub> (X= S, Se,Te)" <b>Ashok Kumar</b> , P. K. Ahluwalia, <i>Journal of Alloys and Compounds</i> <b>550</b> 283 (2013)	3.13
26. "Mechanical Strain Dependent Electronic and Dielectric Properties of Two-Dimensional Honeycomb Structure of MoX <sub>2</sub> (X=S,Se,Te)" <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica B: Condensed Matter</i> <b>419</b> 66 (2013)	1.39
27. Semiconductor to Metal Transition in Bilayer Transition Metal Dichalcogenides MX <sub>2</sub> (M=Mo,W;	

X=S,Se,Te) <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Modeling and Simulation in Materials Science and Engineering</i> <b>21</b> 065015 (2013)	1.89
<b>Year-2012</b>	
28. “Ab-initio Study of Structural, Electronic and Dielectric Properties of Free Standing Nanowires of Noble Metals” Arun Kumar, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> <b>46</b> 259 (2012)	2.22
29. “First Principle Study of Interband Transitions and Electron Energy Loss in Mono and Bilayer Graphene: Effect of External Electric Field” Brij Mohan, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica E: Low-dimensional Systems and Nanostructures</i> <b>44</b> 1670 (2012)	2.22
30. “Tunable Dielectric Response of Transition Metal Dichalcogenides MX <sub>2</sub> (M = Mo, W; X= S, Se,Te)” <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica B: Condensed Matter</i> <b>407</b> 4627 (2012)	1.39
31. “A First Principle Comparative Study of Electronic and Optical Properties of 1H-MoS <sub>2</sub> and 2H-MoS <sub>2</sub> ” <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Materials Chemistry and Physics</i> <b>135</b> 755 (2012)	2.08
32. “Electronic Structure of Transition Metal Dichalcogenides Monolayers 1H-MX <sub>2</sub> (M=Mo,W; X=S,Se,Te) from Ab-initio Theory: New Direct Band Gap Semiconductors” <b>Ashok Kumar</b> , P. K. Ahluwalia <i>European Physical Journal B</i> <b>85</b> 186 (2012)	1.46
<b>Year-2011</b>	
33. “Ab-initio Study of Platinum Induced Reconstructions on Ge(001)-(1×2) Surface” <b>Ashok Kumar</b> , P. K. Ahluwalia <i>Physica B: Condensed Matter</i> <b>406</b> 4691 (2011)	1.39
<b>Publications as Book Chapters</b>	
1. “Tunable Electronic and Dielectric Properties of Molybdenum Disulfide” <b>Ashok Kumar</b> , P. K. Ahluwalia <b>Vol. 21</b> of the series Lecture Notes in Nanoscale Science and Technology, pp 53-76 Publisher: Springer International Publishing Switzerland ISBN: 978-3-319-02849-1 (2014)	
<b>Publications in Conference Proceedings</b>	
1. “Electronic Properties of Phosphorene/MoSe <sub>2</sub> Vertical Heterostructure” Sumandeep Kaur, <b>Ashok Kumar</b> , Sunita Srivastava, K. Tankeshwar, <i>AIP Conference Proceedings</i> <b>1832</b> 050049 (2017).	
2. “Electronic Properties of Ultrathin 1D and 2D Alloyed Nanostructures of Stanene” Geeta Sachdeva, Chandra Kumar, K. Tankeshwar, <b>Ashok Kumar</b> , <i>AIP Conference Proceedings</i> <b>1832</b> 090049 (2017).	
3. “First Principles Study of Electronic and Thermoelectric Performance of Li Intercalated MoSe <sub>2</sub> Nanotube” Munish Sharma, <b>Ashok Kumar</b> , Ravindra Pandey, P. K. Ahluwalia <i>AIP Conference Proceedings</i> <b>1832</b> 140036 (2017).	
4. “Energetics and electronic properties of Pt wires of different topologies on monolayer MoSe <sub>2</sub> ” Pooja Jamdagni, <b>Ashok Kumar</b> , Anil Thakur, Ravindra Pandey, P. K. Ahluwalia <i>AIP Conference Proceeding</i> <b>1731</b> 090028 (2016).	
5. “Electronic properties of phosphorene/graphene heterostructures effect of external electric field” Sumandeep Kaur, <b>Ashok Kumar</b> , Sunita Srivastava, K. Tankeshwar <i>AIP Conference Proceeding</i> <b>1731</b> 050012 (2016).	
6. “Stability, structural and electronic properties of benzene molecule adsorbed on free standing Au layer” Neha Katoch, Pooja Kapoor, Munish Sharma, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>AIP Conference Proceeding</i> <b>1731</b> 090039 (2016).	
7. “Topological insulator behavior of WS <sub>2</sub> monolayer with square-octagon ring structure” <b>Ashok Kumar</b> , Ravindra Pandey, P. K. Ahluwalia, K. Tankeshwar <i>AIP Conference Proceeding</i> <b>1731</b> 140049 (2016).	
8. “Interactions of gas molecules with monolayer MoSe <sub>2</sub> : A first principle study” Munish Sharma, Pooja Jamdagni, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>AIP Conference Proceeding</i> <b>1731</b> 140045 (2016)	
9. “Structural, electronic and magnetic properties of Au-based monolayer derivatives in honeycomb structure” Pooja Kapoor, Munish Sharma, <b>Ashok Kumar</b> , P. K. Ahluwalia <i>AIP Conference Proceeding</i> <b>1731</b> 050080 (2016)	
10. “Shape-dependent electronic properties of blue phosphorene nano-flakes” Pradeep Bhatia, Ram Swaroop <b>Ashok Kumar</b> <i>AIP Conference Proceeding</i> <b>1728</b> 020598 (2016)	
11. “Electronic properties and mechanical strength of β-phosphorene nano-ribbons” Ram Swaroop, Pradeep Bhatia, <b>Ashok Kumar</b> <i>AIP Conference Proceeding</i> <b>1728</b> 020600 (2016)	
12. “Electronic and Mechanical Properties of Hybrid Graphene/h-BN Nanoribbons” Pooja Jamdagni, <b>Ashok Kumar</b> , Munish sharma, Anil Thakur, P K Ahluwalia <i>AIP Conference Proceeding</i> <b>1665</b> 090023 (2015)	
13. “Electronic and Dielectric Properties of Vacancy Clusters as Quantum Dot in Silicene” Brij Mohan, Munish sharma, <b>Ashok Kumar</b> , P K Ahluwalia <i>AIP Conference Proceeding</i> <b>1665</b> 090041 (2015)	
14. “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)
15. “Stability and Electronic Properties of SiC Nanowire Adsorbed on MoS<sub>2</sub> Monolayer” Munish Sharma, Pooja Jamdagni, **Ashok Kumar**, P K Ahluwalia *AIP Conference Proceeding* **1665** 140023 (2015)
  16. “Semiconductor-to-metal Phase Transition in Monolayer ZrS<sub>2</sub>: GGA+U Study” **Ashok Kumar** Haiying He Ravindra Pandey P. K. Ahluwalia K. Tankeshwar *AIP Conference Proceeding* **1665** 090016 (2015)
  17. “Electronic and Dielectric Properties of MoS<sub>2</sub>-MoX<sub>2</sub> Heterostructures” Munish Sharma Pooja Jamdagni, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1661** 080028 (2015)
  18. “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)
  19. “First principle study of manganese doped cadmium sulphide sheet” Sanjeev Kumar, **Ashok Kumar**, P. K. Ahluwalia *AIP Conference Proceeding* **1591** 1732 (2014)
  20. “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)
  21. “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)
  22. “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)
  23. “Mechanically strained tuning of the electronic and dielectric properties of monolayer honeycomb structure of tungsten disulphide (WS<sub>2</sub>)” **Ashok Kumar**, Brij Mohan, Arun Kumar, P. K. Ahluwalia *AIP Conference Proceeding* **1512** 1242 (2013)
  24. “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)
  25. “Electronic structure and optical conductivity of two dimensional (2D) MoS<sub>2</sub>: Pseudopotential DFT versus full potential calculations” **Ashok Kumar**, Jagdish Kumar, P. K. Ahluwalia *AIP Conference Proceeding* **1447** 1269 (2012)
  26. “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)
  27. “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)
  28. “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.