# **BIO-DATA**

| Name<br>Designation    | :<br>: | Dr. Babita Rani<br>Assistant Professor  |
|------------------------|--------|---|
| Official Address       | :      | Department of Physics,<br>Punjabi University, Patiala-147002<br>Mobile: 94641-05001<br>E-mail : dr.babita@pbi.ac.in |
| Area of Specialization | :      | Theoretical Computational Physics (Nanomaterials)   |

#### Academic Qualifications:

- 1. Ph.D. (2016) in Physics from Department of Physics, Panjab University, Chandigarh.
- 2. UGC-CSIR, NET (2007) qualified in Physical Sciences.
- 3. M.Sc. Physics (2007) from Department of Physics, Punjabi University, Patiala.
- 4. B.Sc. (C.A.) (2004) from Panjab University, Chandigarh.

## **Teaching Experience:**

| 2012-till date: | Assistant Professor, Physics Department, Punjabi University, Patiala. |
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| 2009-2012:      | Assistant Professor, Physics Department, Punjabi University, Patiala. |
| 2007-2009:      | Lecturer (Adhoc), Physics Department, Punjabi University, Patiala.    |

## Membership of Professional Bodies/Organisations:

- 1. Life Member, Indian Society of Radiation Physics
- 2. Life Member, Punjab Academy of Sciences

## Medals/Awards/ Honours received:

- 1. First position holder throughout the academic career.
- 2. M.Sc. with University Gold Medal.

# List of Publications in National/ International Journals:

1. Interaction of Nitrogen Molecule with Graphene, Babita Rani, V. K. Jindal and Keya Dharamvir, AIP Conf. Proc. 1512, 300, 2013; doi: 10.1063/1.4791030.

2. Interaction of Two Nitrogen Molecules with Graphene, Babita Rani, V. K. Jindal and Keya Dharamvir, AIP Conf. Proc., 1536, 363, 2013; doi: 10.1063/1.4810251.

3. Adsorption Configurations of Two Nitrogen Atoms on Graphene, Babita Rani, V. K. Jindal and Keya Dharamvir, AIP Conf. Proc., 1591, 450, 2014; doi: 10.1063/1.4872635.

4. A First Principle Study of Adsorption of Two Proximate Nitrogen Atoms on Graphene, Babita Rani and Keya Dharamvir, Int. J. Quantum Chem., 1619, 114, 2014; doi: 10.1002/qua.24741.

5. Adsorption of Two Sodium Atoms on Graphene -- A First Principles Study, Gagandeep Kaur, Babita Rani, Shuchi Gupta and Keya Dharamvir, AIP Conf. Proc., 1675, 020003, 2015; doi: 10.1063/1.4929161.

6. Energetics of a Li Atom Adsorbed on B/N Doped Graphene with Monovacancy, Babita Rani, V. K. Jindal and Keya Dharamvir, J. Solid State Chem., 240, 67, 2016; doi: 10.1016/j.jssc.2016.05.014.

7. A DFT study of pure and lithium doped gold clusters, Babita Rani, AIP Conf. Proc., 1953, 030164, 2018; doi: 10.1063/1.5032499.

8. Geometries, electronic and magnetic properties of  $Au_n$  and  $Au_{n-1}Li$  (n=2-6) clusters using density functional theory, Amanjot Kaur, Babita Rani, AIP Conf. Proc., 2142, 110010, 2019; doi: 10.1063/1.5122470.

9. Atomistic insights into lithium adsorption and migration on phosphorus-doped graphene, Babita Rani, Vladimir Bubanja, Vijay K. Jindal, Int. J. Quantum Chem., 121, 14, 2021; doi: 10.1002/qua.26659.

10. Density functional theory study of the enhancement of quantum capacitance of graphene by phosphorous doping, Babita Rani, Vladimir Bubanja, Vijay K. Jindal, Int. J. Quantum Chem., 123, 6, 2023; doi: 10.1002/qua.27052.

11. Adsorption of Li/Na atom on pristine and boron doped armchair graphene nanoribbons: A DFT study, Nancy, Babita Rani, Materials Today: Proceedings, doi: 10.1016/j.matpr.2023.03.783. (in press)

12. Enhanced quantum capacitance of  $MX_4$  (M = Fe, Co, Ni, Cu, and Zn; X = N, P) moieties embedded graphene: a DFT study, Babita Rani, Vladimir Bubanja, Vijay K. Jindal, J. Phys.: Condens. Matter, 35, 415503, 2023; doi: 10.1088/1361-648X/ace578.

## List of Book Chapters:

1. A chapter "Graphene Nanoribbons and Graphene", Nancy, Babita Rani, in a book titled as Current and Future Developments in Nanomaterials and Carbon Nanotubes: Synthesis and Applications of Semiconductor Nanostructures, Vol. 4, p. 278-300, 2023. ISBN (Online): 978-981-5080-11-7.

#### Presentations in National/ International Conferences/ Symposia:

1. 23<sup>rd</sup> AGM-MRSI Functional Materials for sustainable Energy and Advanced Technologies at Thapar University, Patiala during Feb 13-15, 2012.

2. International Conference on Emerging Trends in Physics for Environmental Monitoring & Management (ETPEMM-12) at Punjabi University, Patiala during Dec 17-19, 2012.

**3.** International Conference on Recent Trends in Applied Physics & Material Science (RAM-2013) at Government College of Engineering & Technology, Bikaner during Feb 01-02, 2013.

4. National Symposium on Emerging Trends in Physics for Ionizing Radiations, Aerosols and Material Science (ETPRAM-13) at Punjabi University, Patiala during Dec 13-14, 2013.

5. 58<sup>th</sup> DAE Solid State Physics Symposium at Thapar University, Patiala during Dec 17-21, 2013.

6. 4<sup>th</sup> National Conference on Advanced Materials and Radiation Physics (AMRP-15) at SLIET, Longowal during Mar 13-14, 2015.

7. 2<sup>nd</sup> International Conference on Condensed Matter and Applied Physics (ICC-2017) at Govt. Engg. College, Bikaner during Nov 24-25, 2017.

8. National Seminar on Emerging Research Trends in Experimental Physics (ERTEP-2019) at Guru Nanak College for girls, Sri Muktsar Sahib on Feb 22, 2019

9. International Symposium on Semiconductor Materials and Devices (ISSMD-2020) at Dr. B. R. Ambedkar N.I.T., Jalandhar during Oct 31-Nov 2, 2020.

10. International Conference on Energy and Advanced Materials (ICEAM-2021) at Jaypee Institute of Information Technology, Noida during Oct 21-23, 2021.

11. 6<sup>th</sup> National Conference on Current Advances in Physical Sciences (CAPS-2023) at Khalsa College, Amritsar on Feb 8, 2023.

12. 8<sup>th</sup> National Conference on Science & Technology for Nation Development : Opportunities & Global Challenges (NCSTND-2023) at Arya P.G. College, Panipat on Feb 28, 2023.

13. One Day National Seminar on Condensed Matter Physics and Materials (CMPM-2023) at Punjabi University, Patiala on May 8, 2023.

## Workshops/Programmes/Courses Attended:

1. Visited IUAC, New Delhi from 02-09-2012 to 09-09-2012 for high performance computing.

2. Seminar cum Workshop on First Principle and other Simulation Methods in Condensed Matter Physics at Department of Physics, Himachal Pradesh University, Shimla from 22-03-2010 to 29-03-2010.

3. UGC sponsored 24th Orientation Programme at UGC-HRDC, Punjabi University, Patiala from 08-04-2015 to 05-05-2015.

4. UGC sponsored Refresher Course in Physical Sciences at UGC-HRDC, Punjabi University, Patiala from 20-06-2016 to 09-07-2016.

5. UGC sponsored Short term course on Research Methodology at UGC-HRDC, Punjabi University, Patiala from 24-09-2018 to 29-09-2018.

6. UGC sponsored 61<sup>st</sup> online short term course on e-content development at UGC-HRDC, Gujarat University, Patiala 25-06-2020 to 01-07-2020.

7. Completed MOOC course "Mechanics: Motion, Forces, Energy and Gravity, from particles to Planets" authorized by UNSW, Sydney through Coursera on 22.08.2021.

8. UGC sponsored Refresher course in Information Communication Technology (ICT) at UGC-HRDC, Punjabi University, Patiala from 13.09.2021 to 25.09.2021.

9. UGC-Approved Short-Term Professional Development Programme on Implementation of NEP-2020 for University and College Teachers from 18.11.2022 to 26.11.2022.

## No. of Ph.D./M.Sc. Students guided/under guidance:

Completed: 03, Ongoing: 02

## List of Papers/ Courses taught at P.G. and U.G. Level:

1. Classical Mechanics- PG

- 2. Quantum Mechanics- PG
- 3. Mathematical Methods of Physics- PG
- 4. Introduction to Nanotechnology- PG

#### **Technical Proficiency:**

Working knowledge of DFT based softwares like VASP, different visualization tools/softwares like Xmakemol, Xcrysden, Origin, and VMD, well versed in Linux based OS (Ubuntu), DOS, and Windows and Fortran programming language.

--sd--Dr. Babita Rani