### **BIO-DATA**

1.	Name	:Dr. Isha Mudahar
2.	Designation	:Assistant Professor
3.	Department	:Physics
4.	Date of Birth	:23-09-1983
5.	Address for Correspondence	: 466, Urban Estate, Phase-I Patiala-
		147002
6.	Mobile	:8146992328
7.	E-mail	:dr.ishamudahar@gmail.com,
		isha@pbi.ac.in
8.	Areas of Specialisation	Material Science : Nanoscience

#### 9. Academic Qualifications:

Sr. no.	Degree Held	Year	Board/Univ./ Inst.	% of marks	Div./ Rank	Subjects Taken
1	10 <sup>th</sup>	1999	C.B.S.E., New Delhi	86.8	1 <sup>st</sup>	English, Science, Maths, Social science, Sanskrit, Punjabi
2	12 <sup>th</sup>	2001	P.S.E.B., Mohali	76.6	1 <sup>st</sup>	English, Physics, Chemistry, Maths, Punjabi
3	B.Sc.	2004	Punjabi University, Patiala	75.0	1 <sup>st</sup>	English, Physics, Chemistry, Maths, Punjabi
4	M.Sc. (Physics)	2006	Punjabi University, Patiala	78.8	1 <sup>st</sup>	Quantum, Statistical, electronics, Mathematical, condensed matter, radiation, classical, nuclear, electrodynamics, computational methods and simulation
5	PhD	2011	Punjab University, Chandigarh	-	-	Nanoscience –theoretical simulation methods.

### 10. Membership of Professional Bodies/Organisations

- i) Life time membership holder of High Energy Material Society of India
- ii) Life time membership holder of Indian Physics Association
- iii) Lifetime membership of Indian Society for Radiation Physics
- iv) Lifetime membership of Punjab Academy of Sciences.

#### 9. Medals/Awards/Honours/Received

- i) College Color holder for getting 3<sup>rd</sup> Position in Punjabi University Merit List for session 2003-04.
- ii) 2<sup>nd</sup> Position in M.M. Modi College Merit List for session 2003-04.
- iii) 1<sup>st</sup> Position in B.Sc. (2004) in the subject of Mathematics and English.
- iv) Best oral presentation in Chandigarh Science Congress 2011.

#### 10. Scholarships:

i) Award of Research Fellowship under "Meritorious Students Scheme funded by University Grants Commission (UGC)" from December 2007 –July 2010.

#### **11. Details of Experience:**

S. No.	Name of the Inst./Employer	Position Held	Duratio n	Major Job Responsibilities and Nature of Experience
1.	University College of Engineering, Punjabi University, Patiala	Lecturer	1 year	Teaching and Research
2.	Khalsa College Patiala	Assistant Professor	6 months	Teaching and Research
3.	Department of Basic and Applied Sciences, Faculty of Engineering, Punjabi University Patiala	Assistant Professor	Dec. 2011 – March 2022	Teaching and Research
4.	Department of Physics	Assistant Professor	April 2022-till date	Teaching and Research

#### 12. Published Work (Please specify numbers only):

a. **Research Papers** i) National =1

ii) International = 22

#### **In International Journals**

- Structural, Electronic, and Vibrational Properties of C<sub>60-n</sub>N<sub>n</sub> (n=1-12) Hitesh Sharma, Isha Garg, Keya Dharamvir, and V. K. Jindal *J. Phys. Chem. A* 113, (2009), 9002.
- Polynitrogen Clusters Encapsulated in C<sub>60</sub>: A Density Functional Study Hitesh Sharma, Isha Garg, Keya Dharamvir, and V. K. Jindal *J. Phys. Chem. C* 114, (2010), 9153.
- 3) Ab-initio study of structural and electronic properties of  $Al_nN$  (n = 1-22) clusters Hitesh Sharma, Isha Garg, Keya Dharamvir and V. K. Jindal

- J. Comput. and Theoret. Nanosc., 7, (2010), 2297 (11).
- 4) Ab initio study of Al<sub>n</sub> (1-13) clusters encapsulated inside Single Walled Carbon Nanotubes Isha Garg, Hitesh Sharma, Keya Dharamvir, V.K. Jindal and D.G. Kanhere J. Phys. Chem. C 114, (2010), 18762.
- Substitutional Patterns of Boron-doped Heterofullerenes Isha Garg, Hitesh Sharma, Keya Dharamvir, and V. K. Jindal J. Comput. and Theoret. Nanosc., 8, (2011), 642.
- 6) Transition metal induced magnetism in smaller fullerenes ( $C_n$  for  $n \le 36$ ) Isha Garg, Hitesh Sharma, Neha Kapila, Keya Dharamvir and V.K. Jindal *Nanoscale*, **3**, (2011), 217.
- 7) Boron and Nitrogen doped heterofullerenes Isha Garg, Hitesh Sharma, Keya Dharamvir, and V. K. Jindal International Journal of Nanoscience 10, (2011), 15.
- 8) Magnetism in endohedral metallofullerenes: A spin polarized density functional study Hitesh Sharma, Isha Garg, Keya Dharamvir and V.K. Jindal *Proceedings of ICANN-09 American Inst. of Physics*, **1276**, (2010), 432.
- 9) First principle investigation into structural growth and magnetic properties in Ge<sub>n</sub>Cr clusters for n=1-13

Neha Kapila, **Isha Garg**, V.K. Jindal, Hitesh Sharma, *J. Magnetism and magnetic materials*, **324**, (2012), 2885.

- 10) Effect of Nitrogen as co-dopant in carbon and boron doped ZnO clusters. NehaKapila, Gaurav Sharma, Isha Mudahar, Hitesh Sharma
   J. Magnetism and magnetic materials, 405 (2015), 187.
- 11) Interaction between fullerene halves C<sub>n</sub> (n ≤ 40) and single wall carbon nanotube Amrish Sharma, Sandeep Kaur, and Isha Mudahar\*
  AIP Conference Proceedings 1728, 020221 (2016)
- 12) DFT study of small fullerene dimer complexes  $C_{20}$ - $N_m@C_n$  (m = 1-6 and n = 24, 28, 32, 36 and 40)

Sandeep Kaur, Amrish Sharma, and Isha Mudahar\* AIP Conference Proceedings **1728**, 020656 (2016)

13) Substitutional Doping of Asymmetrical Small Fullerene Dimers Sandeep Kaur, Hitesh Sharma, Isha Mudahar\*

Advanced Science Letters, American Scientific Publishers, 24 (2018) 888.

14) A First Principle study of  $C_{20}$  and  $C_{40}$  Carbon Nanobud

Amrish Sharma, Hitesh Sharma, and **Isha Mudahar**\* Advanced Science Letters, American Scientific Publishers, **24**(2018), 790.

- 15) Structural and magnetic properties of small symmetrical and asymmetrical sized fullerene dimers Sandeep Kaur, Amrish Sharma, Hitesh Sharma and Isha Mudahar\*
   Mater. Res. Express (IOP), 5 (2018) 016105.
- 16) Electronic and Magnetic Properties of Small Fullerene Carbon Nanobuds: A DFT Study Amrish Sharma, Sandeep Kaur, Hitesh Sharma, Isha Mudahar\* Mater. Res. Express (IOP), 5 (2018) 065032.
- **17)** Graphene nanoribbons under axial compressive and point tensile stresses Sandeep Kaur, Hitesh Sharma, V.K. Jindal, Vladimir Bubanja, Isha Mudahar\* *Physica E: Low-dimensional Systems and Nanostructures* **111** (2019) 1–12.

#### 18) Substitutional doping of symmetrical small fullerene dimers

Sandeep Kaur, Amrish Sharma, Hitesh Sharma, Shobhna Dhiman and Isha Mudahar\* International Journal Of Quantum Chemistry, Int J Quantum Chem. (2019) 119:e.26019

#### 19) Lattice thermal conductivity of pure and doped (B, N) Graphene

Sarita Mann, **Isha Mudahar**, Hitesh Sharma, V K Jindal, Girija S Dubey, Godfrey Gumbs and Vassilios Fessatidis.

Mater. Res. Express 7 (2020) 095003.

#### 20) Ab initio study of nitrogen and boron doped C<sub>60</sub> dimers Sandeep Kaur, Hitesh Sharma, V.K. Jindal, Vladimir Bubanja and Isha Mudahar *Molecular Physics* 120, e2100294 (2022).

**21)** Carbon nanotubes with periodic vacancy defects to phenine nanotubes: A DFT study Amrish Sharma, Hitesh Sharma and Isha Mudahar *Computational and Theoretical Chemistry* **1211**, 113692, (2022).

# 22) Understanding the interaction between Fullerene and Graphene Nanoribbons using Density Functional Theory

Sandeep Kaur, Hitesh Sharma and Isha Mudahar *ECS Transactions* **102**, 19863, (2022).

### 23) Understanding Stability of FeTiVNi and CoFeVNi High Entropy Alloys Using Density Functional Theory

Payal, Hitesh Sharma and Isha Mudahar *ECS Transactions* **107**, 20005, (2022).

24) Hybrid Biowaste Materials for Supercapacitors, Energy from Waste: Production and Storage Prashant Dubey, Ashwinder Kaur, Vishal Shrivastav, Isha Mudahar, Sunita Mishra, Shashank Sundriyal *CRC, Taylor & Francis Group, (eBook ISBN: 9781003178354)* (2022).

### 25) Effect of Sm2O3 on the physical, structural and optical properties of 40 SiO2-40 B2O3-10 V2O5-(10-x) Fe2O3 glasses

Jaspreet Kaur, P Kaur, **Isha Mudahar**, Kulvir Singh *Ceramics International* **49** (**9**), 13610 (2023).

## 26) Role of Sm2O3 on surface to bulk crystallization and thermal properties of Fe2O3-V2O5-B2O3-SiO2 glasses

Jaspreet Kaur, NK Mattu, Isha Mudahar, Kulvir Singh Journal of Non-Crystalline Solids 610, 122304 (2023)

## 27) Waste Paper-Derived Porous Carbon Incorporated with Mesoporous ZIF-8 Crystals for Symmetrical Supercapacitors

Ashwinder Kaur, Vishal Shrivastav, Prashant Dubey, Akash Deep, **Isha Mudahar**, Shashank Sundriyal, and Sunita Mishra

Energy Fuels 37, 11376 (2023)

#### 28) Surface and Diffusion Characteristics of Nanoporous UiO-66/Pineapple Peel-Derived Carbon Composites for Solid-State Supercapacitors

Ashwinder Kaur, Vishal Shrivastav, Prashant Dubey, **Isha Mudahar**, Shashank Sundriyal, and Sunita Mishra

ACS Applied Nano Materials, (2023), doi/10.1021/acsanm.3c01897

**29) Theoretical investigation of substitutionally doped symmetrical finite phenine nanotubes** Amrish Sharma, Hitesh Sharma and **Isha Mudahar** *Physica Scripta* **98**,075802 (2023)

#### In National Journals

#### 1) Electronic and magnetic properties of Ge<sub>n</sub>Cr for n=1-13

Neha Kapila, **Isha Garg**, Hitesh Sharma, Keya Dharamvir and V.K. Jindal *Proceedings of DAE Solid State Physics Symp. (India)*, **54**, (2009), 1039.

#### b. Conference/Seminar Presentation: National- 13 and International -5

#### **National Conferences**

- 1) Poster presentation in 1st Chandigarh Science Congress, Panjab University, Chandigarh (2007).
- 2) National Seminar on Theoretical and Experimental Techniques in Nanoscience Nanotechnology, Panjab University, Chandigarh (2007).
- 3) Poster presentation in 2nd Chandigarh Science Congress, Panjab University, Chandigarh (2008).
- 4) Diamond Jubilee National Seminar "Advances in Physics", Panjab University, Chandigarh (2008).
- 5) Workshop on Emerging technologies in Nano-Science, Punjabi University, Patiala (2008).
- 6) Technology Workshop on Optimizing Performance of Parallel Programs on Emerging Multi-Core Processors GPUs, IIT-Madras (2009).
- 7) Seminar cum workshop on First principle and other simulation methods in condensed matter theory, Himachal Pradesh University, Shimla (2010).

- 8) Workshop on High Performance Computing, Inter University Accelerator Centre, New Delhi (2010).
- 9) Oral presentation in 4th Chandigarh Science Congress, Panjab University, Chandigarh (2010).
- 10) Oral Presentation in 5<sup>th</sup> Chandigarh Science Congress, Panjab University Chandigarh (2011).
- 11) Attended and presented at National Symposium on Radiation Physics and Nanomaterials held on Feb 04-05, 2011 at Punjabi University Patiala.
- 12) Attended and presented paper at Punjab Science Congress held at Guru Nanak Dev University, Amritsar on 11-12 Feb 2012
- 13) Attended and delivered a talk at Workshop on High Performance computing , Inter University Accelerator Centre, New Delhi on 11-13<sup>th</sup> March, 2014
- Attended One Day National Seminar on Condensed Matter Physics and Materials, Department of Physics, 2023

#### **International Conferences**

- 15) Oral presentation in International Conference on Advances in Nanotechnology, MATS University, Raipur (2008).
- 16) Poster presentation in International Conference on Advanced nanomaterials and nanotechnology, IIT Guwahati (2009).
- 17) Poster Presentation in International Conference on Advances in Condensed and Nano Materials, Panjab University Chandigarh (2011).
- Presented paper at International Conference on Nanomaterials and Nanotechnology, University of Delhi, India from 18-21 Dec (2011).
- Poster presentation at Punjab Science Congress, "Review on High entropy Alloys", SLIET Longowal from 7-9 the Feb. (2020).
- 20) Oral Presentation at Punjab Science Congress," A DFT Study on Interaction of Pure and Doped Fullerene with Graphene Nanoribbons ",Shri Guru Teg Bahadur Khalsa College, Sri Anandpur Sahib, Rupnagar, Punjab from 7-9 the Feb. (2022).
- Poster presentation at 7<sup>th</sup> National Conference on Innovations in Science, Engineering and Technology, "A review on 2D Nanomaterials" at Arya Post Graduate College, Panipat Feb.19 (2022).

#### c. Books

i) Original : Endohedral and Hetero-Doped Fullerenes and Carbon Nanotubes (LAP LAMBERT Academic Publishing GmbH & Co. KG, Germany)

#### 13. R & D Projects

#### 1) Awarded Young Scientist SERB DST Project entitled "Interaction between carbon nanostructures", Govt. of India.

#### 13. Invited Talks/Articles

- i) Talk on some concepts of Statistical mechanics was delivered in Baba Farid College, Deon, Bathinda.
- ii) Talk on the basics of nanotechnology was given at Dev Samaj College, Ferozepur.
- iii) Talk on Heterofullerenes and Endo-doped fullerenes was given at IUAC, New Delhi.
- iv) Talk on Applications of Nanotechnology & its influence on environment at Government College for Women Shahzadpur (Ambala) Haryana, January 2020

#### Name of the Student Title of Thesis Year of Completion S. No. 1. Sandeep Kaur Study of interaction 2021 between pure and doped nanostructures VIVA pending 2. Amrish Sharma Structural and **Electronic properties** of Hybrid Carbon Nanostructures 3. **Jaspreet Kaur** Registered 4. Paval Registered 5. Ashwinder Kaur Registered 6. Jyoti Registered 7. Neha Sharma Registered 8. **Hardeep Singh** Registered

#### 14. Ph.D. Students guided/under guidance (Details) :

15.

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

S. No.	Paper	Class
1.	Applied Physics-I	U.G
2.	Applied Physics-II	U.G
3.	Classical Mechanics	P.G
4.	Mechanics	U.G
5.	Thermal Physics	U.G
6.	Quantum Mechanics	P.G

### 16. Technical Proficiency

• Worked with many softwares like SIESTA, VASP, Quantum Espresso and Material Studio based on DFT to study various properties of nanostructures. Also many visualization softwares like XCRSYDEN, XMAKEMOL, WESTA and RASMOL to visualize and study various structural parameters of nanostructures have been used. Knowledge of Operating Systems- Linux and Windows along with Latex/Mik Tex/Origin6.0.