

# Curriculum Vitae

## **Dr. Shivani Gupta**

**Ph.D. in Physics**

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**Google Scholar:** <https://scholar.google.com/citations?user=N0gK68kAAAAJ&hl=en>



## CAREER PROFILE

### **Objective:**

To carry out research and development activities as an active member of team towards the accomplishment of the organization goals, to achieve success in my career and prove to be an asset to the organization and the society.

### **Strength:**

Leadership skill, Hardworking, Teamwork, Flexibility and Adaptability, Optimistic Attitude

### **Research Interests and Specialization:**

**Specialization:** Electronic structure analysis of ionic conducting polymers by using a computational program SIESTA.

**Area of Interest:** Computational Chemistry, Density Functional Theory, Polymeric electrolytic materials for different electrochemical devices viz solid-state battery, super capacitors.

### **Educational Qualifications:**

**Ph.D. in Physics** (July 2018- June 2022)

**Thesis Title:** Density-Functional Theory Studies of Interaction of Alkali Metal Salts and Plasticizers with Polyethylene Oxide PEO

Department of Physics and Material Science

Madan Mohan Malaviya University of Technology, Gorakhpur-273010, India

**M.Sc. in Physics** (2015- 2017)

Department of Physics

Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur-273001, India

Division/Class: 1<sup>st</sup> (68.5 %)

**B.Sc. with Physics, Mathematics and Chemistry** (2012- 2015)

M. G. P. G. College, Gorakhpur

Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur-273001, India  
Division/Class: 1<sup>st</sup> (66 %)

**10+2** with *Physics, Chemistry, Mathematics, English and Hindi* (2010- 2012)

C.B.S.E Board

G.N National Public School, Gorakhnath, Gorakhpur-273001, India

Division/Class: 1<sup>st</sup> (76 %)

**10-th** standard with *Science, Mathematics, Social Science, Arts, English and Hindi* (2010)

C.B.S.E Board

G.N National Public School, Gorakhnath, Gorakhpur-273001, India

Division/Class: 1<sup>st</sup> (83.6%)

### **Teaching Experience:**

**Research cum Teaching Fellow** in Department of Physics and Material Science, Madan Mohan Malaviya University of Technology, Gorakhpur, U.P. since 27 July 2018 to 21 June 2022.

### **Technical Expertise:**

- **Modeling packages:** Gaussian (03, 09, & 16), ORCA 4.0.1.2, Gauss view, SIESTA and related post processing plotting and visualization tools such as Jmol, GNU plot, Avogadro, Xcrysden, Molden, Xmgrace.
- **Characterizations of materials:** UV-visible, Fourier-transform infrared (FT-IR) spectroscopy, Scanning electron microscopy (SEM), Differential scanning calorimetry (DSC).
- **Tools:** Microsoft Office, Chem Draw, Origin, MATLAB.
- **Languages:** LaTeX markup
- **Operating system:** Linux (CentOS 6.4) and Windows

### **Achievement and Award:**

1. **Research cum Teaching Fellowship** in Madan Mohan Malaviya University of Technology from 25<sup>th</sup> July 2018 to 21<sup>st</sup> June 2022.
2. **Young Scientist Award** in 21st National Conference on Solid State Nuclear Track Detectors and Their Applications (SSNTDs-21), jointly organized by Department of Physics, Ramjas College and Department of Physics & Astrophysics, University of Delhi in Collaboration with Nuclear Track Society of India (NTSI) during 29-31 January 2021.
3. **Best Paper Presentation for Paper titled “Electronic and optical properties of pure and doped PEO-PVP solid polymer electrolyte: Insight from DFT study”** in 21st National Conference on Solid State Nuclear Track Detectors and Their Applications (SSNTDs-21), jointly organized by Department of Physics, Ramjas College and Department of Physics & Astrophysics, University of Delhi in Collaboration with Nuclear Track Society of India (NTSI) during 29-31 January 2021.

4. **Placed among top 10% in National Graduate Physics examination 2012-2013** organised by Indian Association of Physics Teachers.
5. **Cleared National Level Science Talent Search examination (NSTSE-2012)** conducted nationwide on 4<sup>th</sup> Dec 2011 by Unified Council.

### **ACADEMIC & RESEARCH CONTRIBUTION SUMMARY:**

#### **Total book, book chapter, research paper publications:**

1. International SCI Journal Paper Publication	<b>:5</b>
2. International SCImago Journal Paper publication	<b>:2</b>
3. Conference Paper	<b>:3</b>
4. National Other indexed Journal	<b>:1</b>
5. Book Chapters	<b>:3</b>

#### **Indexing, citations**

Google Scholar Citations	<b>: 11</b>
h- Index Citations	<b>: 2</b>

#### **List of significant publication:**

##### **A. International Journals (SCI)**

[1] First-principle study on ionic pair dissociation in PEO-PVP-NaClO<sub>4</sub> blend for solid polymer electrolyte

**Shivani Gupta**, Abhishek Kumar Gupta, B. K. Pandey

*Polymer. Bulletin* (2021): p.1-20

**ISSN: 0170-0839 [Impact Factor: 2.87]**

[2] Influence of polyethylene glycol plasticizer on the structural and electronic properties of PEO-NaI complex: a density functional study

**Shivani Gupta**, Abhishek Kumar Gupta, B. K. Pandey, Mohan L. Verma,

*Journal of Molecular Modeling* (2021), Vol. 27: p.1-11

**ISSN: 0948-5023 [Impact Factor: 2.17]**

[3] Insight into structural, electronic, and chemical bonding properties of PEO-PEG-LiI polymer electrolyte: A first-principles investigation

**Shivani Gupta**, Abhishek Kumar Gupta, B. K. Pandey

*Computational and theoretical chemistry* (2022), Vol. 1211: p. 113667

**ISSN: 2210-271X [Impact Factor: 2.29]**

[4] One-Pot Highly Efficient Synthesis of N-Enrich Graphene Quantum Dots as a Photocatalytic Platform for NAD<sup>+</sup>/NADP<sup>+</sup> Reduction

**Shivani Gupta**, R. K. Yadav, A. K. Gupta, B. Yadav, A. Singh, and B. K. Pandey

*Photochemistry and Photobiology* (2021), Vol. 97: p. 1498-1506

**ISSN:1751-1097 [Impact Factor: 3.52]**

[5] Electronic, Vibrational, and Structural Study of Polysaccharide Agar-Agar Biopolymer. Ankita Pandey, Abhishek Kumar Gupta, **Shivani Gupta**, Sarvesh Kumar Gupta, and Rajesh Kumar Yadav  
*Nano Hybrids and Composites*, Trans Tech Publications Ltd (2021), Vol. 33: p.35-46.  
ISSN: 2297-3400

### **B. International Journals (SCI Mago / Conference proceedings)**

[6] Poly (vinylidene fluoride-co-hexafluoropropylene): An Emerging Host Material for Ion Conducting Gel Polymer Electrolyte-Cum-Separator Membrane  
**Shivani Gupta**, Sarvesh Kumar Gupta, B. K. Pandey, and Abhishek Kumar Gupta  
*Advanced Science, Engineering and Medicine* (2020), Vol.12: p 50-59.  
ISSN: 2164-6627

[7] Ionogels: Present Opportunities, and Challenges for Future in Energy Storage Applications.  
Sarvesh Kumar Gupta, **Shivani Gupta**, Abhishek Kumar Gupta  
*Advanced Science, Engineering and Medicine* (2020), Vol.12: p 11-26.  
ISSN: 2164-6627

[8] Computational studies of PEO<sub>3</sub>-NaClO<sub>4</sub> based solid polymer electrolyte for Na-ion batteries  
**Shivani Gupta**, Vinay Shukla, Sarvesh Kumar Gupta, B. K. Pandey, and Abhishek Kumar Gupta  
In *AIP Conference Proceedings* (2020), Vol. 2220, No. 1, p. 130065, AIP Publishing LLC.

[9] Structural and electronic properties of PVDF derived polymer: Ab initio study  
Sarvesh Kumar Gupta, Jyoti Singh, **Shivani Gupta**, Abhishek Kumar Gupta  
In *AIP Conference Proceedings* (2020), Vol. 2220, No. 1, p. 130058, AIP Publishing LLC, 2020.

[10] Studies on the interaction of Na<sup>+</sup> ion with binary mixture of carbonate-ester solvents: A density functional theory approach  
Sakshi Tiwari, Abhishek Kumar Gupta, **Shivani Gupta**, Sarvesh Kumar Gupta, Sujeet Kumar Chaurasia.  
*Journal of Physics: Conference Series* (2021), Vol. 1849, no. 1, p. 012024. IOP Publishing.

### **C. National Journal**

[11] Computational Studies on PVDF-HFP/Li-salt Composite Electrolyte for Lithium-ion Batteries  
Jyoti Singh, Abhishek Kumar Gupta, **Shivani Gupta**, Sarvesh Kumar Gupta, Ramesh Kumar Arya, Amarjeet Yadav  
*Journal of Nanoscience, Nanoengineering & Application* (2021), Vol. 11, no.3: p.18-25.  
ISSN: 2321-5194

### **D. Book Chapters**

[12] Investigation on ionic conductivity and Raman spectroscopic studies of ionic liquid immobilized PEO based polymer electrolytes

Sujeet Kumar Chaurasia, Abhishek Kumar Gupta, Sarvesh Kumar Gupta, **Shivani Gupta**, Pramod Kumar, Manish Pratap Singh  
*Advances in Functional Materials, Springer Nature* (2022): p. 41-49.  
**ISBN: 978-981-16-5970-6.**

[13] Hybrid Mechanism of Supercapacitor and Battery for Building High Performance of Electric Vehicles  
Divya Prabha, Abhishek Kumar Gupta, **Shivani Gupta**, Sarvesh Kumar Gupta, Jyoti Singh, Rajesh Kumar Yadav  
*Advances in Functional Materials, Springer Nature* (2022): p.187-195.

[14] Recent advancements in the design of electrode materials for rechargeable batteries  
**Shivani Gupta**, Abhishek Kumar Gupta, Sarvesh Kumar Gupta, Mohan L Verma  
*Advanced Materials and Nano Systems* (2022): p.53-66 (Accepted)  
Sciences (ICE2M), 2019 (**Accepted**)

### **CONFERENCES AND WORKSHOP ATTENDED:**

#### **Conference:**

- **2021 Oral Presentation on paper titled: “Computational Studies on PVDF-HFP/Li-Salt Composite Electrolyte for Lithium-ion Batteries” in International Conference on Modern Approaches in Engineering, Science and Management (MAESM-2021)** organized by Bansal Institute of Engineering and Technology, Lucknow (UP) India, (April 16-17, 2021).
- **2021 Oral Presentation on “Insight into structural, electronic, and chemical bonding properties of PEO-PEG-LiI polymer electrolyte: A first-principles investigation” in 14th National Conference on Solid State Ionic (NCSSI-14)** organised by Department of Physics & Astrophysics, University of Delhi, Delhi (December 16-18, 2021)
- **2020 Oral Presentation on “First Principle Study of electronic and chemical bonding properties of PEG based electrolyte” In National Conference on Environment and Energy Materials (NCEEM-2020)** organised by Dept of Environmental Science, Sharda University (27-28 June 2020)
- **2019 Poster Presentation in National conference on “Smart Materials Devices and Sustainable Technologies (SMDST-2019)”**, MMMUT, Gorakhpur, (15<sup>th</sup> to 16<sup>th</sup> March 2019).
- **2019 Poster presentation on “Computational Studies of PEO<sub>3</sub>-NaClO<sub>4</sub> Based Solid Polymer Electrolyte for Na-ion Batteries”** at International Conference on Condensed Matter & Applied Physics (**ICC-2019**), Govt. Engineering College, Bikaner (14<sup>th</sup> – 15<sup>th</sup> Oct. 2019)

- **2019 Oral Presentation in “International Conference on Electro-active Polymers” (ICEP-2019)**, organized by Department of Physics and Astrophysics Delhi University, New Delhi (4<sup>th</sup>-8<sup>th</sup>Feb, 2019)
- **2018 Poster Presentation in “Research Scholar Day”** organised by MMMUT, Gorakhpur (17 dec 2018)
- **2018 Poster Presentation in “National Symposium on Advanced Material Science”** organised by Dept. of Physics, DDU Gorakhpur University, (7-8<sup>th</sup> Dec, 2018)
- **2016 Participated in “National Conference on Functional Materials”**, organised by Dept.of Physics, Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur (10<sup>th</sup>-12<sup>th</sup> March, 2016)

#### **Workshops/Short-term Course/FDP:**

- **2020 Participated TEQIP-III sponsored 3-day online workshop on “Experimental Methods in Analytical Electrochemistry and Advanced Chemical Engineering”** conducted during organized by Department of Chemical Engineering, Ujjain Engineering College. Ujjain (November 23 - 25, 2020).
- **2020 Attended one-week TEQIP-III sponsored short-term course on the topic “Basic Principles of DFT Calculations and Molecular Dynamics Simulations”** from organized by the department of Chemical Engineering, Malaviya National Institute of Technology, Jaipur, Rajasthan (23 to 27 November 2020).
- **2020 Participated & completed successfully AICTE Training And Learning (ATAL) Academy Online FDP on "Novel Materials"** at Shri Shankaracharya Technical Campus-Shri Shankaracharya Group of Institutions ( 2-6 Nov,2020)
- **2020 Participated in two days National Webinar on “Computational Simulation: A Powerful Tool for Advance Scientific Research” (CSPTASR-2020)** organized by Madan Mohan Malviya Post Graduate College, Bhatpar Rani, Deoria (India)-274702 during 18<sup>th</sup> & 19<sup>th</sup> October 2020.)
- **2020 Completed successfully AICTE Training And Learning (ATAL) Academy Online FDP on "Energy Storage"** from at Bharathiar University (5-9 Oct,2020)
- **2020 Attended and successfully completed the one-week Online Faculty Development Programme on “Recent Advances in Material Science and Research Ethics”** organized by Physics and Material Science Department, Madan Mohan Malaviya University of Technology Gorakhpur-273010, India (21-25 Sept 2020)

- **2020 One-week online FDP, “Recent Advances in Material Science and Research Ethics (RAMSRE-2020)”**, organized by Physics & Material Science Department, M.M.M. University of Technology, Gorakhpur.
- **2020 Completed Online course on “How to Write Successful Research Paper”** by Udemy (23<sup>rd</sup> July 2020)
- **2020 Attended Webinar on “Challenges in Recycling of Li-ion Batteries”** by RSC (6<sup>th</sup> July 2020)
- **2020 Participated in one day webinar on “VIRTUAL LAB”** Conducted by F.E.T, M.J.P., Rohilkhand University, Bareilly (6 June,2020)
- **2020 One-week training workshop on “Density Functional Theory and Its Application Using GAUSSIAN software”** jointly organised by Dept. of Chemistry, NIT Uttarakhand, MNIT Jaipur and SLIET Longowal at MNIT Jaipur (24<sup>th</sup> – 28<sup>th</sup> Feb,2020)
- **2020 Participated in TEQIP III sponsored One Week Short Term Course on “Nascent Research Methodology: Challenges and Various Analytical Tools & Techniques”** held from 24<sup>th</sup> -29<sup>th</sup> June 2020, Organized by Department of Humanities and Management Science, in collaboration With Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat and Madan Mohan Malaviya University of Technology Gorakhpur, Uttar Pradesh, India.
- **2019 One-week Workshop on “Material Modeling for Device Application”**, held at Shri Shankracharya Technical Campus –SSGI, Bhilai (18<sup>th</sup>-23<sup>rd</sup> Feb,2019)
- **2019 5 Days workshop on “LaTeX and its application”**, organized by Department of Computer Science and Engineering by M.M.M university of technology, Gorakhpur,11-15 March 2019.
- **2019 Short term course on “Research Methods and Data Analysis Using SPSS and AMOS”** organised by MMMUT (27<sup>th</sup>-31<sup>st</sup> Jan 2020)
- **2019 International Workshop on “Energy Management in Smart Sustainable Cities”**, conducted by Electrical Engineering College, M.M.M. University of Technology, Gorakhpur. (November 30<sup>th</sup> – December 1<sup>st</sup>, 2019)

- **2019 E and ICT workshop on MATLAB organized by IIT Kanpur** (Feb 28 to 11 March,2019)
- **2018 Short -Term Course on Research Methodology and Statistics (STCRMS-2018)**, sponsored by TEQIP-III and organized by Department of Applied science M.M.M. University of Technology, Gorakhpur. (October 24th – 30th, 2018)
- **2017 Hands on Training Cum Workshop on “Soft Skill for Scientist and Engineers”** (SCSSE-17) organised by Dept. of Applied Science, Madan Mohan Malaviya University of Technology, Gorakhpur, (17<sup>th</sup>-19<sup>th</sup> March 2017)
- **2014 Completed 3 credit course on “Personal Computing and Digital Lifestyle”** by NIIT (2 Dec 2014).