


## Faculty Profile, IGNOU, New Delhi

	Name		Dr. VISHAL SINGH
	Designation		Assistant Professor
	Contact Address		Block-D, Raman Bhavan Academic Complex Discipline of Chemistry School of Sciences IGNOU, New Delhi-110068.
Vishal Singh Chemistry, SOS IGNOU, New Delhi	Contact No.	Office	
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EDUCATIONAL QUALIFICATIONS			
Degree	Year	Institute/University	
Bachelor B.Sc. (Hons.) Chemistry	2011	Banaras Hindu University, Varanasi (UP), India	
Masters (M.Sc.) Physical Chemistry	2013	Department of Chemistry, University of Delhi, Delhi, India	
Ph.D. Bio-Physical Chemistry “Stochastic Dynamics of Protein Misfolding and Aggregation”	2021	Theory and Simulation Lab, Department of Chemistry, University of Delhi, Delhi, India	
CAREER PROFILE			
<div><div><ul style="list-style-type: none"><li>Assistant Professor Discipline of Chemistry School of Sciences IGNOU, New Delhi</li><li>Post-Doctoral Fellow Delhi School of Public Health Institution of Eminence University of Delhi, Delhi</li></ul></div><div><div>July 2024 – Continuing to date</div><div>December 2021 - March 2024</div></div></div>			

AREA OF INTEREST/SPECIALIZATION			
<ul style="list-style-type: none"> <li>Theoretical and Computational Bio-Physical Chemistry</li> <li>Protein Misfolding, Aggregation and Neurodegenerative Diseases</li> <li>Mathematical Modelling of Complex Systems</li> <li>Barrier Crossing Dynamics and Rare Events</li> <li>Statistical Physics and Stochastic Processes</li> </ul>			
ROLE AND RESPONSIBILITIES AT IGNOU			
<ul style="list-style-type: none"> <li>Course Coordinator of the course MCH-013 (Mathematics for Chemists).</li> <li>Writing, editing and transformation of course units.</li> </ul>			
RESEARCH GUIDANCE			
Supervision of	Year of completion	Name	Ph. D. Topic
PUBLICATIONS			
<b>Papers in Refereed/Peer reviewed Journals</b> <p>(1) Publications in International/National Journals: : 11</p> <b>Books/Monographs (Authored/Edited)/ Book Chapter/ Lecture Notes</b> <p>(2) Book Chapter in International Journals: : 1</p> <b>A. Papers in Refereed/Peer reviewed Journals:</b> <ol style="list-style-type: none"> <li><b>Vishal Singh</b> and Parbati Biswas, Estimating the Mean First Passage Time of Protein Misfolding, <i>Physical Chemistry Chemical Physics</i>, <b>20</b>, 5692, 2018. DOI: <a href="https://doi.org/10.1039/C7CP06918A">10.1039/C7CP06918A</a></li> <li><b>Vishal Singh</b> and Parbati Biswas, A Generalized Langevin Equation Approach for Barrier Crossing Dynamics in Conformational Transitions of Proteins, <i>Journal of Statistical Mechanics: Theory and Experiment</i>, <b>2021</b>, 063502, 2021. DOI: <a href="https://doi.org/10.1088/1742-5468/ac08fd">10.1088/1742-5468/ac08fd</a></li> <li><b>Vishal Singh</b> and Parbati Biswas, Conformational transitions of Amyloid-<math>\beta</math> Protein: A Langevin and Generalized Langevin Dynamics Simulation Study, <i>ACS Omega</i>, <b>6</b>, 13611, 2021. DOI: <a href="https://doi.org/10.1021/acsomega.1c00516">10.1021/acsomega.1c00516</a></li> <li>Shivangi Sharma, <b>Vishal Singh</b> and P. Biswas, Effect of Ligand Binding on Riboswitch Folding: Theory and Simulation, <i>The Journal of Chemical Physics</i>, <b>154</b>, 185101, 2021. DOI: <a href="https://doi.org/10.1063/5.0047684">10.1063/5.0047684</a></li> </ol>			

5. **Vishal Singh** and Parbati Biswas, Predicting Protein Shelf Life from Mean First Passage Times, *Chemical Physics Letters*, **792**, 139426, 2022. DOI: [10.1016/j.cplett.2022.139426](https://doi.org/10.1016/j.cplett.2022.139426)
6. Shivangi Sharma<sup>†</sup>, **Vishal Singh**<sup>†</sup> and Parbati Biswas, Analysis of the Passage Times for Unfolding/Folding of Adenine Riboswitch Aptamer, *ACS Physical Chemistry Au*, **2**, 353, 2022. (<sup>†</sup>Equal Contribution to this article) DOI: [10.1021/acsphyschemau.1c00056](https://doi.org/10.1021/acsphyschemau.1c00056)
7. Hemant Kumar, Pramod Kumar, **Vishal Singh**, Shwetank Shashi Pandey and Balram Pani, Synthesis and Surface Modification of Biocompatible Mesoporous Silica Nanoparticles (MSNs) and its Biomedical Applications: A Review, *Research Journal of Chemistry and Environment*, **27**, 135, 2023. DOI: [10.25303/2702rjce1350146](https://doi.org/10.25303/2702rjce1350146)
8. Anjali Priya, Mohammed Dashti, Thangavel Alphonse Thanaraj, Mohammad Irshad, Virendra Singh, Ravi Tandon, Rekha Mehrotra, Alok Kumar Singh, Payal Mago, **Vishal Singh**, Md Zubair Malik, Ashwini Kumar Ray, Identification of Potential Regulatory Mechanisms and Therapeutic Targets for Lung Cancer, *Journal of Biomolecular Dynamics and Simulation*, **42**, 1, 2024. DOI: [10.1080/07391102.2024.2310208](https://doi.org/10.1080/07391102.2024.2310208)
9. Presenjit, Shubhra Chaturvedi, Divya, Ritika, **Vishal Singh**, K. Singh and AK Mishra, An *in silico* analysis of Schiff Base Derivatives to Identify Potential Inhibitors for Breast Cancer Multitargeted Proteins: Virtual Screening and Molecular Dynamics Simulation, *Current Medicinal Chemistry*, 2024 (Accepted). DOI: [10.2174/0109298673278191231226091716](https://doi.org/10.2174/0109298673278191231226091716)
10. Vishakha Chaudhary, Shubhra Chaturvedi, Anju Wadhwa, Presenjit, Divya Gautam, Deepika Sharma, Aastha Garg, **Vishal Singh**, Rupesh Kumar, A. K. Mishra, Homology Modeling, Molecular Docking and MD Simulations Study of 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline Derivatives as Sigma-2 Receptor Ligands, *Journal of Biomolecular Dynamics and Simulation*, 2024 (Accepted). DOI: Awaiting
11. Priya Dey<sup>†</sup>, **Vishal Singh**<sup>†\*</sup> and Hemant Kumar, Transport and Kinetic Property of the Butyric Acid in Water: A Simulation Study, *Chemical Physics Impact*, **9**, 100744, 2024. DOI: [10.1016/j.chphi.2024.100744](https://doi.org/10.1016/j.chphi.2024.100744)

## B. Books/Monographs (Authored/Edited)/ Book Chapter

1. **Vishal Singh**<sup>\*</sup> and Priya Dey, Theoretical Aspects of Protein Aggregation and Neurodegenerative Diseases, In **Neurological Problems in the Elderly**, IntechOpen, ISBN: 978-1-83769-958-2. DOI: [10.5772/intechopen.1006957](https://doi.org/10.5772/intechopen.1006957)

\* corresponding author; <sup>†</sup> equal contribution

## CONFERENCES/WORKSHOPS ORGANISED/PARTICIPATED/LECTURES

### A. CONFERENCES/SEMINARS/WORKSHOPS PARTICIPATED:

1. Participated in the BRNS School on “Computational Methodologies Across Length Scales” on 28<sup>th</sup> August-9<sup>th</sup> September 2017 at Bhabha Atomic Research Center, Mumbai, India.

2. Participated in the International Seminar on **“Effects of Pollution on Human Health”** jointly organized by Department of Chemistry, University of Delhi & Indian Academy of Biomedical Sciences (IABS) on 1<sup>st</sup> December 2017 at Seminar Hall, Department of Chemistry, University of Delhi, Delhi, India.
3. **“Estimating the Mean First Passage Time of Protein Misfolding”**, presented in 16th Theoretical Chemistry Symposium organized by BITS Pilani on 14<sup>th</sup> February 2019 at Pilani Campus, Rajasthan, India.
4. **“Estimating the Mean First Passage Time of Protein Misfolding and Aggregation”**, presented in 25th CRSI National Symposium in Chemistry (CRSI-2021) on 19<sup>th</sup>-21<sup>st</sup> July 2019 at IIT Kanpur, Uttar Pradesh, India.
5. Participated in the National Webinar on **“आज के संदर्भ में वैदिक गणित की प्रासंगिकता”** organized by Centre for Vedic Mathematical Studies Central University of Himachal Pradesh, Dharamshala, Himachal Pradesh, India on 3<sup>rd</sup> September 2021.
6. **“Dynamics of the Conformational Transitions of Proteins: Theoretical and Simulation Study”**, presented in Dynamics Days Delhi (DDD-XV) organized by Society for Dynamical Systems, Delhi on 27<sup>th</sup> November 2021.
7. **“Conformational transitions of Amyloid- $\beta$ : A Langevin and Generalized Langevin Dynamics Simulation Study”**, presented in 17th Theoretical Chemistry Symposium (TCS-2021) organized by IISER Kolkata, West Bengal, India on 11<sup>th</sup>-14<sup>th</sup> December 2021.
8. **“Stochastic Kinetics of Protein Misfolding and Aggregation”**, presented in International Symposium on Chemistry Wisdom by Her organized by Department of Chemistry, Deshbandhu College, University of Delhi, Delhi, India on 31<sup>st</sup> January 2022.
9. **“Dynamics of the Conformational Transitions of Amyloid- $\beta$ : A Simulation Study”**, presented in National Conference on Molecular Modelling and Simulations (NCMMS-2022) organized by Vellore Institute of Technology (VIT), Bhopal, Madhya Pradesh, India on 28<sup>th</sup> February-2<sup>nd</sup> March 2022.
10. **“Predicting Protein Shelf Lives From Mean First Passage Times”**, presented in Multi-Disciplinary National Conference on Recent Advances in Science & Technology for Sustainable Development (RASTSD-2022) organized by Department of Chemistry, DAV College on 5<sup>th</sup> March 2022 at DAV College, Bathinda, Punjab, India
11. **“A Generalized Langevin Equation Approach for Barrier Crossing Dynamics in Conformational Transitions of Proteins”** presented in 12th India-Japan Science and Technology Conclave: International Conference on Frontier Areas of Science and Technology (ICFAST-2022) organized by Indian JSPS Alumni Association (IJAA) and School of Physics, University of Hyderabad (UoH) on 9<sup>th</sup> September 2022 at University of Hyderabad, Hyderabad, India.
12. **“Dynamics of the Conformational Transition of Biomolecules: A Theoretical Perspective”** presented in 5th International Conference on Nutraceuticals and Chronic Diseases on Pharmaceuticals and Nutraceuticals for Cancer and other Chronic Diseases (INCD-2022) organized by Department of Zoology, University of Delhi on 9<sup>th</sup> October 2022 at Conference Center, University of Delhi, North Campus, Delhi, India.

13. **“Mathematical Model of the Neurodegenerative Diseases Progression”** presented in 2<sup>nd</sup> International Conference on Integrative Chemistry, Biology & Translational Medicine (ICBTM-2022) jointly organized by Hansraj College University of Delhi, Institute of Nuclear Medicine & Allied Sciences (DRDO-INMAS), Miranda House University of Delhi, and Mayo Clinic Florida USA on 7<sup>th</sup> December 2022 at Conference centre, University of Delhi, North Campus, Delhi, India.
14. **“Lifestyle and the Neurodegenerative Diseases”** presented in National Conference on Scientific Innovation for Human Wellbeing jointly organized by Department of Chemistry, University of Delhi, Delhi and The Indian Science Congress Association (IACS) Delhi Chapter on 17<sup>th</sup> March 2023 at Seminar Hall, Department of Chemistry, University of Delhi, Delhi-110007, India.
15. Participated in the **“11th Workshop on Bioinformatics and Drug Design: Artificial Intelligence (AI) and Machine Learning (ML) Based Methods (BIF-DD-2023)”** organized by Dr. B. R. Ambedkar Center for Biomedical Research (ACBR), University of Delhi on 18<sup>th</sup>-20<sup>th</sup> April 2023 at Seminar Hall, ACBR, University of Delhi, Delhi, India.

**B. Invited lectures / Resource Person/ Paper presentation in Seminars/ Conferences:**

1. Deliver a lecture on **“Protein Misfolding and Aggregation in Neurodegenerative Diseases: A Use of Computer”** in the 16<sup>th</sup> National Summit 2023 on Integrating Healthcare - The Way Forward organized by CSR Research Foundation on 1<sup>st</sup> July 2023 at Le Meridien, Janpath, New Delhi-110001, India.
2. Deliver a lecture on **“Importance of Computer in Research, Problems and Prospects”** in two days national conference on Sustainable Chemistry - A Step towards Steady Environment organized by Commission for Scientific and Technical Terminology (CSTT), Ministry of Education, Government of India on 23<sup>rd</sup> November 2024 at Ramjas College, University of Delhi, Delhi-110007, India.
3. Deliver a lecture on **“Concept of Mathematics and Computer in Chemistry”** in two days national conference on The Role of Language in Teaching Chemistry organized by Commission for Scientific and Technical Terminology (CSTT), Ministry of Education, Government of India on 23<sup>rd</sup> January 2025 at School of Sciences, Manav Rachna University, Faridabad-121004, Haryana, India.

**C. Refresher Courses/ Orientation Courses/FDP/FIP attended:**

1. Participated in 7<sup>th</sup> **“National Education Policy 2020 Orientation & Sensitization Programme”** under the UGC-Malaviya Mission Teacher Training Programme (MM\_TTP), MoE, GoI organized by Malaviya Mission Teacher Training Centre (MMTTC), Central University of South Bihar (CUSB) Gaya from 20<sup>th</sup>-29<sup>th</sup> August 2024 in online mode.
2. Participated in **“राजभाषा और यूनिकोड प्रशिक्षण कार्यक्रम”** organized by Staff Training and Research Institute of Distance Education (STRIDE), Indira Gandhi National Open University on 12<sup>th</sup> September 2024 at Staff Training and Research Institute of Distance Education (STRIDE), IGNOU, New Delhi-110068, India.

3. Participated in “**Induction cum Orientation Programme in Distance Education**” organized by Staff Training and Research Institute of Distance Education (STRIDE), IGNOU from 17<sup>th</sup>-24<sup>th</sup> September 2024 at Staff Training and Research Institute of Distance Education (STRIDE), IGNOU, New Delhi-110068, India.
4. Participated in “**24 Days Guru Dakshta- Faculty Induction Programme (Residential)**” under Malaviya Mission Teacher Training Programme (MMTTP) Organized by UGC-MMTTC from 4<sup>th</sup> to 30<sup>th</sup> November 2024 at Staff Training and Research Institute of Distance Education (STRIDE), IGNOU, New Delhi-110068, India.

### RESEARCH PROJECTS

Sponsoring Agency	Period	Amount of grant (in Lakhs)	Title of Project	Co-investigator(s) (if any)

### HONOURS/AWARDS/DISTINCTIONS


1. Junior Research Fellowship (JRF) awarded in Chemical Sciences by CSIR India (January 2016).
2. Senior Research Fellowship (SRF) awarded in Chemical Sciences by CSIR India (January 2018).
3. Maharishi Kanad Post-Doctoral Fellowship awarded by Institution of Eminence, University of Delhi, Delhi (December 2021).

### PROFESSIONAL ASSOCIATIONS

1. Life time member of Chemical Research Society of India (CRSI).

### OTHER ACTIVITIES

1. Serve as a coordinator in *AAHANG-18 A Annual Cultural Fest* in the D.S. Kothari Hostel, University of Delhi, Delhi for the session 2018-2019.
2. Serve as a member of anti-ragging committee in the D.S. Kothari Hostel, University of Delhi, Delhi for the session 2019-2021.
3. Participated in “Swachhata Hi Seva Campaign” held on 23<sup>rd</sup> and 24<sup>th</sup> September 2024 at Staff Training and Research Institute of Distance Education (STRIDE), IGNOU, New Delhi, India.

  
**VISHAL SINGH**