

Nitin Kumar Singh (Curriculum Vitae)

CONTACT INFORMATION

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G-Scholar: Nitin Kumar Singh

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RESEARCH INTERESTS

Molecular Simulations, Computational Chemistry/Biology, Drug Discovery, Drug Delivery, Machine Learning, Enzyme engineering.

EDUCATION

Michigan State University East Lansing, United States 2024 - Present

Postdoctoral Researcher.

- Advisor: Dr Josh Vermaas

Indian Institute of Technology Gandhinagar, India 2019 - 2024

PhD, Chemical Engineering.

- Dissertation Topic: "Investigating the role of charged residues in protein structural dynamics and adsorption."
- Advisor: Dr Mithun Radhakrishna

Visvesvaraya National Institute of Technology, Nagpur, India 2017 - 2019

M. Tech., Chemical Engineering

- Dissertation Topic: "Molecular dynamics simulations of peptide nanotubes and their application in drug entrapment."
- Advisor: Dr Piyush P. Wanjari

Dr. APJ Abdul Kalam Technical University, Lucknow, India 2013 - 2017

B. Tech., Biotechnology

- Dissertation Topic: "Production of Xylanase enzyme using agro-industrial waste by solid substrate fermentation and its process optimization."
- Advisor: Dr Santosh Kumar Mishra

INTERNSHIPS AND INDUSTRIAL TRAINING

- Visiting Graduate Student: Understanding the interplay of helical stability and membrane interactions of charged peptides. Dr. Paulo C. T. Souza, École Normale Supérieure de Lyon and CNRS (August 2023- December 2023)
- Summer Internship : Hindustan Coca-Cola Beverages Private Limited, Varanasi, Uttar Pradesh, India. (July-2016)
- Summer Internship : Cytogene Research and Development, Lucknow, Uttar Pradesh, India. (June-2015)

TECHNICAL SKILLS

- Molecular Simulation and Computational Chemistry Software Packages: GROMACS, AMBER, NAMD, LAMMPS, Gaussian, GAMESS, Packmol, AutoDock Vina, Open Babel, HADDOCK.
- AI-Based Structural Biology Tools: AlphaFold, RosettaFold.

	<ul style="list-style-type: none"> • High-Performance Computing: Experience in using Linux-based clusters (SLURM and PBS). • Programming Skills: Bash scripting, Batch scripting, Python, FORTRAN, Tcl scripting, HTML, PHP, MATLAB, Scikit-learn, TensorFlow, RDKit. • Visualization and Plotting Softwares: VMD, UCSF Chimera, PYMOL, Avogadro, gnuplot, Grace, Matplotlib, Microsoft Excel, Graphpad-prism, Originlab. • Biotechnology Lab Operations: Gel Electrophoresis, Polymerase Chain Reaction, Spectroscopy and Spectrophotometry, Cell Culture.
TEACHING	<ul style="list-style-type: none"> • Independent Tutor: Molecular Simulations (Theory and Application): Sem II, 2023-2024, Indian Institute of Technology Gandhinagar.
CERTIFICATIONS	<ul style="list-style-type: none"> • Machine Learning Specialization (Stanford University & DeepLearning.AI Coursera) • Hands-on Introduction to Linux Commands and Shell Scripting (Coursera) • Introduction to Networking and Storage (Coursera) • Project Management Principles and Practices Specialization (University of California, Irvine) • Certification in Scientific Writing (Indian Institute of Technology Gandhinagar)
PUBLICATIONS	<ul style="list-style-type: none"> • Nitin Kumar Singh, Manish Agarwal, and Mithun Radhakrishna. “Statistical analysis of the unique characteristics of secondary structures in proteins” Computational Biology and Chemistry(2024):108237. • Nitin Kumar Singh, Pratyasha Bhardwaj, and Mithun Radhakrishna. “Hydrophobicity - A single parameter for accurate prediction of disordered regions in proteins” Journal of Chemical Information and Modeling,63,16(2023):5375–5383. • Nitin Kumar Singh, Kartik Pushpavanam, and Mithun Radhakrishna. “Tuning Electrostatic Interactions to Control Orientation of GFP Protein Adsorption on Silica Surface” ACS Appl. Bio Mater. 7.2 (2023): 596-608. • Nitin Kumar Singh, Manish Agarwal, and Mithun Radhakrishna. “Understanding the helical stability of charged peptides” Proteins: Structure, Function, and Bioinformatics 91.2 (2023): 268-276. • Kumar, Avishek, Nitin Kumar Singh, Deepshikha Ghosh, and Mithun Radhakrishna. “Understanding the role of hydrophobic patches in protein disaggregation.” Physical Chemistry Chemical Physics 23, no. 22 (2021): 12620-12629. • Medesety, Padmesh, Hrushikesh M. Gade, Nitin Kumar Singh, and Piyush P. Wanjari. “Highly selective carbon capture by novel graphene-carbon nanotube hybrids.” Molecular Simulation 47, no. 16 (2021): 1326-1334.
CONFERENCE PRESENTATIONS	<ul style="list-style-type: none"> • International Conference on Drug Discovery 2022 (2022), ‘Evaluating the uniqueness of α-helical structures in proteins’, Nitin Kumar Singh, Manish Agarwal, Mithun Radhakrishna • The American Physical Society Meeting March 2022 (2022), ‘Understanding helical stability of charged peptides’, Nitin Kumar Singh, Manish Agarwal, Mithun Radhakrishna • 5th International Conference on Physics and Biological System (2021), ‘Understanding helical stability of charged peptides’, Nitin Kumar Singh, Manish Agarwal, Mithun Radhakrishna • 2020 Workshop on Free Energy Methods in Drug Design (2021), ‘Understanding helical stability of charged peptides’, Nitin Kumar Singh, Manish Agarwal, Mithun Radhakrishna

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- National Conference on Intra and inter-disciplinary blends of Chemical Engineering CHEMIX'19 (2019), 'Peptide self-assembly and its applications in drug delivery', Nitin Kumar Singh and Piyush Wanjari
- School of Biosciences, IMSUC, Ghaziabad (2016), 'Xylanase production using Solid Substrate fermentation', Nitin Kumar Singh and Santosh Kumar Mishra

WORKSHOPS

- CHARMM-GUI CECAM School, (2021), Université Paul Sabatier, Toulouse, France.
- Basic Principles of DFT Calculations and Molecular Dynamics Simulations, (2020), Malaviya National Institute of Technology, Jaipur, Rajasthan, India.
- Fundamentals of Molecular Simulations (2020), Indian Institute of Technology Kanpur, Kanpur, India.

AWARDS AND RECOGNITION

- Graduate Aptitude Test in Engineering (GATE) 2017- All India Rank 730
- 2nd position: Logo Quiz, Gems Society, DBT, IMSEC

CO-CURRICULAR ACTIVITIES

- General Secretary- Gems Society, Department of Biotechnology, IMS Engineering College. (2014-2015)
- Volunteer at Rotary Club Ghaziabad. (2015 and 2017)
- Represented IMSEC at 'Swedish Embassy Quiz'. (2015)

ACADEMIC REFEREES

1. Dr Mithun Radhakrishna (PhD dissertation advisor)
Associate Professor,
Discipline of Chemical Engineering,
Indian Institute of Technology Gandhinagar, Gujarat, India.
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2. Dr Manish Agarwal
Administrator, HPC Facility,
Indian Institute of Technology Delhi, India.
Email: zmanish@cc.iitd.ac.in
Phone: +919891566246
3. Dr. Paulo C. T. de Souza
Researcher,
LBMC/CBP,
École Normale Supérieure de Lyon and CNRS.
Email: paulo.telles_de_souza@ens-lyon.fr
4. Dr Piyush P. Wanjari (M. Tech. dissertation advisor)
Assistant Professor,
Department of Chemical Engineering,
Visvesvaraya National Institute of Technology, Nagpur, Maharashtra, India.
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