Rakshit Kumar Jain

4th Year Ph.D. Candidate
rkjain2@ncsu.edu
Personal Webpage

EDUCATION

CHEMICAL AND BIOMOLECULAR ENGINEERING | NORTH CAROLINA STATE UNIVERSITY
August 2018 – Present | Ph.D. in Chemical Engineering
Current Overall Grade: 4/4 | Estimated Graduation: April 2023

CHEMICAL ENGINEERING | INDIAN INSTITUTE OF TECHNOLOGY ROORKEE, INDIA
August 2014 – May 2018 | B.Tech. in Chemical Engineering
Overall Grade: 8.91/10

PUBLICATIONS

Effect of dispersion forces on the behavior of thermosensitive nanogels: A coarse-grained simulation study, Luis Perez-Mas, Alberto Martin-Molina, Rakshit Kumar Jain, Manuel Quesada-Perez
Journal of Molecular Liquids, 288, 2019

CONFERENCES

2021 AIChE Annual Meeting
November 7-19, 2021 | Boston, Massachusetts, USA

MolSim 2021
January 4-15, 2021 | Van't Hoff Institute of Molecular Sciences, University of Amsterdam, Netherlands

2020 APS and ICTP-SAIFR Young Physicists Forum on Biological Physics: from Molecular to Macroscopic Scale (Bio2020)
March 9-15, 2020 | ICTP-SAIFR, Sao Paulo, Brazil

INTERNSHIPS

Effect of dispersive forces between nanogels and ions of the Hofmeister series
Department of Applied Physics, University of Granada, Spain
May-July 2017 | Supervisor: Dr. Alberto Martin-Molina
We studied poly-NIPAM, a polymer mesh important due to its specific thermal responses. Electrostatic, hydrophilic and hydrophobic were the major forces with the excluded volume interactions included using Lennard-Jones potential and dispersion forces. Parameters like ion distribution, the charge enclosed within the nanogel etc. were calculated with the view to perform a comparative study in the presence and absence of dispersion forces.

RESEARCH PROJECTS

Development of a Discontinuous Molecular Dynamics (DMD) forcefield for Peptoids
Chemical and Biomolecular Engineering, North Carolina State University, USA
January 2019 - Present | Supervisors: Dr. Erik E. Santiso, Dr. Carol Hall
Peptoids are a recently discovered class of peptidomimetics (1980s) but there is a lack of computational methods to analyze them because of large energetic barriers between various minima states. We are using relative entropy bottom up coarse graining and SAFT-γ SW top down coarse graining using the atomistic forcefield NTOID developed in our lab. This method is expected to overcome the cis-trans peptoid barrier and allow long-time simulations.

UNDERGRADUATE THESIS | Kinetic Monte Carlo Simulations of Drug-Eluting Nanogels
Chemical Engineering, Indian Institute of Technology, Roorkee, India
August 2016 - May 2018 | Supervisor: Dr. Prateek K. Jha
We theorize a new model to explain the loading and release behavior of nanogels using pressure as the driving force. We verify the model using kinetic Monte Carlo (kMC) simulations, a method to simulate non-equilibrium systems using C++ libraries like GSL, BOOST and Tina's Random Number Generator (TRNG).

Flow Induced Erosion of Controlled Release Formulations

Chemical Engineering, Indian Institute of Technology, Roorkee, India

August 2017 - May 2018 | Supervisor: Dr. Prateek K. Jha

Here, we are trying to model the behavior of carrier polymers and controlled release mechanisms under the consideration of surface erosion due to a moving fluid, developing an improved model over the pre-existing ones, subsequently verifying the same with the help of dissolution experiments.

SOFTWARE SKILLS

PROGRAMMING LANGUAGES

C • C++ • Python • Bash Scripting

SOFTWARE PACKAGES

NAMD • Gaussian13 • VMD • LIGGGHTS • OpenFOAM • Aspen PLUS • ANSYS Fluent • MATLAB • LATEX

TEACHING EXPERIENCE

CHE-711 : Chemical Engineering Process Modeling, Fall 2019-2021
CHE-311 : Transport Phenomena 1, Spring 2019

RELEVANT COURSES UNDERTAKEN

CHE 713 : Thermodynamics
CHE 775 : Multiscale Modeling of Matter
CHE 596-025 : Special Topics "Introduction to Molecular Simulations"
PY 721 : Statistical Physics
CHE 711 : Chemical Engineering Process Modeling

ADDITIONAL CERTIFICATES UNDERTAKEN

TEACHING AND COMMUNICATION CERTIFICATE , Summer 2021-Present | 50/100 credit hours
WRITING CERTIFICATE , Summer 2021-Present | 35/100 credit hours

ACADEMIC AWARDS

Best Poster, MolSim 2021
First Prize, Prototype, IIChE IIT Roorkee Chapter, 2015
First Prize, Think Ecstasy, ASHRAE IIT Roorkee Chapter, 2015
Scholar, Kishore Vaigyanik Protsahan Yojana (K.V.P.Y.), 2013

POSITIONS OF RESPONSIBILITY

TREASURER, CHEMICAL AND BIOMOLECULAR ENGINEERING GRADUATE STUDENT ASSOCIATION , North Carolina State University, 2021-2022
SECRETARY, INDIAN INSTITUTE OF CHEMICAL ENGINEERS , IIT Roorkee, 2016-2017

COMMUNITY SERVICE

SPECIAL INTEREST GROUP , Indian Institute of Technology Roorkee, 2015-2018

We initiated a discussion forum to bolster research atmosphere in the home department, conducting regular meetings to discuss various topics via presentations, as well as take up industrial and theoretical problems, providing viable solutions to industries.

STUDENT MENTORSHIP PROGRAM , Indian Institute of Technology Roorkee, 2015-2018

Initiated the program in the department in the year 2015, with the view of easing the transition between home and college life for the first year students. I was also one of the first mentors to join for the year. After the formation of the college-wide system in the year 2016, was selected to be one of the 100 mentors each year, from a pool of about 1000 students.