

Education

Virginia Polytechnic Institute and State University

PhD. in Chemical Engineering, GPA: 3.7/4.0

– Advisor: Dr. Sanket Deshmukh

Blacksburg, VA

2021–Present

Stevens Institute of Technology

B.E. in Chemical Engineering, Minor in Computer Science, GPA: 3.7/4.0

Hoboken, NJ

2015–2019

Publications

- Singh, S. K.; King, K.; Gannet, C.; Chuong, C.; Joshi, S. Y.; **Plate, C. J.**; Farzeen, P.; Webb, E.; Kumar K. L.; Weger-Lucarelli, J.; Lowell, A. N.; Brown, A. M.; Deshmukh, S. A; “Data driven computational design and experimental validation of drugs for SARS-CoV-2” *Journal of Physical Chemistry Letters* 2023

Awards

NSF Fellowship - IRES : ASSURE

Forschungszentrum Jülich - Computational Biomedicine INM-9

Jülich, Germany

2023-2024

- **Program** : International Research Experience for graduate Students (IRES) Algorithms and Software for Supercomputers with emerging architectures (ASSURE)
- **Research Team** : Mercedes Alfonso-Prieto, Christoph Falkhe, **Paolo Carloni**
- **Project** : Metadynamics simulations to investigate substrate release from the D-galactonate transporter
- **Proposal** : Submitted computational hours proposal, awarded 8 million core-hours on FZJ Jureca (accepted April 2024, valid through April 2025)

Presentations

- “MD Knockout: A Smart Approach to Molecular Dynamics for High Throughput Virtual Screening in Drug Design”, *ChEGSA Symposium*, Virginia Tech, May 2024 - **Oral - Winner of Session**
- “Integrated Computational and Experimental Approach for Identifying Drugs Targeting Hepatitis E Virus”, *PPP DA Symposium*, Virginia Tech, May 2024 - **Poster**
- “MetaDynamics to investigate the binding mechanism of non-nucleoside inhibitor of picornavirus 3Dpol in the RNA template channel”, *American Chemical Society*, New Orleans, April 2024 - **Poster**
- “Improving high-throughput structure-based virtual screening with MM/GBSA free energy and MD knockout”, *ACS*, New Orleans, April 2024 - **Poster**
- “Fully automated drug design pipeline for the development of small molecule protein inhibitors”, *American Chemical Society*, Indianapolis, April 2023 - **Oral**

- “Fully automated drug design pipeline for the development of carbohydrate-based protein inhibitors”, *GlycoMIP Annual Conference*, University of Georgia, March 2023 - **Poster**
- “A Two-Step Computational Drug Design Framework using a Hybrid Evolutionary Algorithm”, *Cancer Research Alliance Retreat*, Virginia Tech Roanoke Campus, March 2022- **Poster**
- “A Two-Step Computational Drug Design Framework using a Hybrid Evolutionary Algorithm”, *ChEGSA Annual Research Symposium*, Virginia Tech, March 2022 - **Oral**
- “A Two-Step Computational Drug Design Framework using a Hybrid Evolutionary Algorithm”, *VTCCD Spring 2022 Poster Session*, Virginia Tech, April 2022 - **Poster**

Primary Projects

- **MD Knockout** - A framework/codebase for accelerated molecular dynamics in high throughput virtual screening applications, deployed on Virginia Tech’s ARC
- **HEV Drug Design** - High throughput virtual screening, MD Knockout, and metadynamics to discover/design antiviral compounds targeting highly conserved regions of the RNA-dependent RNA polymerase
- **D-galactonate Transporter** - Metadynamics simulations to determine protonation states in the D-galactonate transport mechanism

Affiliated Projects

- **Hyper-Soluble Glycans** - Genetic algorithm for designing hyper-soluble carbohydrate materials
- **GyloData Website** - Web server for polysaccharide generation and preparation for molecular dynamics
- **Polymeric Lubricants** - Genetic algorithm for designing polymeric lubricant materials
- **Peptide-mimetics** - Genetic algorithm for designing peptide-mimetic polymers binding truncated green fluorescent protein

Research Skills

- **Programming Languages** *Expert:* Python, Shell | *Coursework:* Java, C++
- **Computational Tools:** Rdkit, MDAnalysis, GROMACS, PLUMED, AlphaFold, BioPython, AutoDock Vina, PLANTS, LeDock, rDock, PyMOL, VMD
- **Methods/Models:** Molecular Dynamics, Metadynamics, MM/GBSA, Docking, Optimization Algorithms, Machine Learning (coursework only)
- **Biological Systems:** Hepatitis E Virus - RNA Dependent RNA Polymerase, Cystine Protease | Hepatitis C Virus - RNA Dependent RNA Polymerase, Picornavirus - RNA Dependent RNA Polymerase, COVID 19 - Main Protease | Dengue Virus - Main Protease

Coursework

- CHE 5044 : Engineering Mathematics A
- CHE 5094 : Advanced Chemical Engineering Kinetics A

- CHE 5125 : Transport Phenomena B
- CHE 5144 : Advanced Thermodynamics B
- CHEM 5424 : Advanced Polysaccharide Chemistry B+
- MSE 5394 : Advanced Molecular Dynamics Simulation A
- CS 5824 : Advanced Machine Learning A-
- CHE 5414 : Explainable Artificial Intelligence Domain Insights A
- BIOL 5884 : Molecular Biology of the Cell A
- PHYS 3355 : Intermediate Mechanics A-

Early Experience

Stony Brook University

Research Assistant - Department of Marine and Atmospheric Sciences

Stony Brook, NY

2020

- Analyzed marsh peat and lake sediment for heavy metal contaminants
- Designed and executed an atomic absorption spectroscopy procedure

Brookhaven National Laboratory

Sustainable Energy Technologies Department Intern

Upton, NY

Summer 2018, 2019

- Investigated the flue gas contaminants of wood burning stoves and helped to develop cleaner, more efficient wood stove systems
- Programmed a data acquisition system for the judging of 12 teams from 4 countries in the Alliance for Green Heat's 2018 Wood Stove Design Challenge
- Incorporated mass and energy balance equations into the program for the calculation of flue gas emissions, burn rate, and efficiency
- Quantified, recorded, and displayed detailed flue-gas emissions data during uncharted transient regions of the wood burning process
- Selected to deliver an oral presentation to the staff at Brookhaven regarding the research

Teaching Experience

Dave's Pod Learning

High School Classroom Instructor : Physics, Chemistry, Math, and Computer Science

Huntington, NY

2019 - 2021

The Tutoring Center

Head Instructor : K-12 Math

Commack, NY

2019 - 2021

Stevens Institute of Technology

Hosted review sessions in Organic Chemistry, Chemical Thermodynamics, Mass Transfer

Hoboken, NJ

2015 - 2019

Mathnasium

K-12 Mathematics Tutor

Hoboken, NJ

2015 - 2019