



Department of Chemistry & Biochemistry Seminar

Friday, March 26th 2021

1:30pm – 2:45pm

Zoom ID: 960 452 0800

Password: Cellular



Engineering Immunology using Chemistry and Data Science

Speaker: *Dr. Guarav Chopra, Purdue University*

Abstract: Chemical and biological function depends on the interplay between the system and its surrounding where the outcome depends on the context of the problem, typically identified by its environment. How do you represent the context for system and surroundings at different scales ranging from atoms to cells? How do you develop molecules with specific properties ranging from controlling reactivity to developing immunomodulators as drug leads? How to teach computers to do this by combining physical modeling, principles of data science, autonomous measurements and instrumentation? How to target immune cell function in different environments using chemical biology and bioanalytical chemistry? I will give an overview of my research program in Chemical and Cellular Immunology with selected examples to address the above questions including descriptions of chemical tools and interpretable machine learning models with prospective experimental validation in situ, in vitro and in vivo.

Biography: Gaurav Chopra is a tenure-track Assistant Professor in Department of Chemistry at Purdue University since 2016 and the Director of Merck-Purdue Center for Measurement Science - a Merck sponsored center funding projects across Purdue University. Chopra is a core member of the Purdue Center for Cancer Research, Purdue Institute for Drug Discovery, Integrative Data Science, Purdue Institute for Integrative Neuroscience and Purdue Institute of Inflammation, Immunology and Infectious Disease. Chopra did his PhD with Michael Levitt (2013 Nobel Laureate in Chemistry) in computational mathematics, chemistry and biology at Stanford School of Engineering and School of Medicine and then was a JDRF fellow in experimental immunology with Jeffrey Bluestone at the University of California – San Francisco School of Medicine. He directs a hybrid experimental/computational group in Chemical and Cellular Immunology. Chopra's research program is focused on developing methods to understand immune cells dysfunction in chronic inflammation and disease by identifying and then targeting “brakes” of the immune system for cancer and neurodegeneration. His laboratory brings AI/machine learning, chemical reactivity, physical modeling, mass spectrometry and experimental immunology together in a chemically guided experimental research program. Chopra is the winner of two NIH ASPIRE Challenge awards, Showalter Research Trust Award, Jim and Diann Robbers Research Award for New Investigators and Purdue University Award in Teaching for Tomorrow and College of Science Award for Undergraduate Advising. Chopra has consulted for several companies, including Merck & Co, Deciduous Therapeutics. Chopra's research is externally funded by the Department of Defense (DoD) including Congressionally Directed Medical Research Programs (CDMRP), National Institutes of Health (NIH), National Science Foundation (NSF), Merck & Company, The Geneva Foundation, Agilent Technologies, Indiana Biosciences Research Institute (IBRI), Indiana CTSI and the Center for Bioanalytical Metrology. Chopra has mentored 4 postdoctoral fellows, 13 graduate students and 30 undergraduates from chemistry, computer science, and biochemistry. He is passionate about outreach, teaching and discovery. To this end, his lab has created a virtual reality based molecular interaction game, MINT and have conducted several outreach events for K-12 and university students to enhance their love for science.