PRATYUSH TIWARY

Millard and Lee Alexander Professorship in Chemical Physics

University of Maryland

Thursday, February 26th

10:30 AM – 11:30 AM

Steele 006

"AI for Chemistry: Bubble, Blockbuster, or Boomerang?"

Abstract: AI is now everywhere in chemistry, from structure prediction to molecule generation to automated synthesis. The excitement is real, but so is the unease about what is genuinely predictive and what is closer to impressive memorization. In this colloquium I will take a statistical physicist's perspective and use examples from my group's work to argue for cautious, but clear, enthusiasm for AI in chemistry and allied fields. I will show how we combine generative AI with statistical mechanics to learn Boltzmann weighted ensembles from limited training data, and then extrapolate across temperature, pressure, and other thermodynamic conditions reducing the need for explicit, expensive simulations or experiments. I will highlight the breadth of these methods through applications that include nucleation of crystal polymorphs under nanoconfinement, prediction of protein and RNA structural ensembles, and conformation selective drug discovery efforts aimed at Alzheimer's disease and hypertension. Time permitting, I will discuss briefly what I think are the biggest challenges facing chemistry research and education as we proceed with the perhaps inevitable adoption of AI.

Bio: Pratyush Tiwary is the Millard and Lee Alexander Professor at the University of Maryland, College Park, where he also directs the Center for Therapeutic Discovery at the Institute for Health Computing. His lab combines AI and statistical physics to solve problems of human health and energy relevance. Tiwary received his degrees from IIT-Varanasi and Caltech and completed postdoctoral work at ETH Zurich and Columbia University. He started as an Assistant Professor at Maryland in 2017, was promoted to tenured Associate Professor in 2022 and Full Professor in 2023. He is a member of the Scientific Advisory Board of Schrodinger and Associate Editor for Journal of Chemical Theory and Computation. He has been recognized through different awards, including student nominated Dean's Award for Excellence in Teaching, University of Maryland's Invention of the Year, and Sloan Research Fellowship in Chemistry.