Penn Engineering
University of Pennsylvania
Chemical and Biomolecular Engineering

Fall 2024 Seminar Series

YAMIL COLÓN

"Filling the Gaps of Machine Learning Workflows in the Molecular Sciences"

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3:30 PM
Wu & Chen Auditorium

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ABSTRACT

One of the main challenges in the molecular sciences is identifying promising candidates for a target application given the virtually limitless number of possibilities. Computer simulations and machine learning (ML) are integral tools to survey the vast molecular landscape and the thermodynamic conditions to evaluate their performance. Broadly, a typical pipeline for molecular characterization, design, and discovery with ML involves data curation and generation, featurization and/or descriptor development, and a model or algorithm for the final prediction. However, these tools are currently severely limited due to the lack of available data, because of the time and resource expense to generate it. In this seminar, I will discuss our research efforts focused on metal-organic frameworks (MOFs), which are nanoporous, crystalline materials composed of inorganic and organic components. I will begin by showcasing our use of large-scale, high-throughput computational screening techniques to generate gas adsorption data. Following this, I will illustrate how transfer learning and active learning can significantly reduce the data requirements of ML models, uncover insights into the material space, and enhance model capabilities when combined with thermodynamic information. Finally, I will present our recent work on utilizing sigma profiles—descriptions of molecular electrostatic surface charges—as chemical descriptors to efficiently navigate and optimize molecular landscapes.

BIO

Yamil J. Colón is an Assistant Professor in the Department of Chemical and Biomolecular Engineering at the University of Notre Dame from 2019. He holds a B.S. in Chemical Engineering (Univ. of Notre Dame, 2009) and a PhD in Chemical Engineering (Northwestern University, 2015). He was an invited participant at the Japan Frontiers of Engineering meeting, which is joint between the Japan Academy of Engineering and the US National Academy of Engineering. He has also been awarded the NSF CAREER Award in 2022. He is also a Faculty Fellow of the Institute for Latino Studies at Notre Dame. The Colón group leverages data science, statistical mechanics, molecular modeling, and machine learning tools to design and discover new materials for various applications including atmospheric water harvesting, gas separations, and quantum technologies.