भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

Applied Physics & Machine Learning Seminar Series, IIT Hyderabad

Online webinar on **Sept 22, 2020 at 3 :00 PM**

Date : 22-09-2020
Time : 3:00 PM (IST)
Topic : Seminar at IITH
Speaker : **Dr. Rocío Mercado**
Affiliation : AstraZeneca
Title : **Molecular Design Using Graph Neural Networks**
Link : https://meet.google.com/wmu-ompq-ygs

Abstract

The process of designing novel, drug-like molecules can be viewed as one of generating graphs which optimize all the features of the desirable molecules. Our group has recently introduced GraphINVENT, a platform developed for graph-based molecular design using GNNs.(1,2) GraphINVENT uses a tiered deep neural network architecture to probabilistically generate new molecules a single bond at a time. All models implemented in GraphINVENT can quickly learn to build molecules resembling the training set molecules without any explicit programming of chemical rules, showing how GNN-based models are promising tools for molecular discovery. In this talk, I will provide an introduction to the field of AI-driven drug discovery, focusing on how deep learning methods such as GNNs can be applied to complex drug design tasks.

Short Bio

Dr. Rocío Mercado joined the Molecular AI group at AstraZeneca in October 2018. Her work focuses on using deep learning methods for graph-based molecular design. Before AstraZeneca, she was a PhD student in Professor Berend Smit's molecular simulation group at UC Berkeley and EPFL. She received my PhD in Chemistry from UC Berkeley in July 2018, and BS in Chemistry from Caltech in June 2013.