Artificial Intelligence and Machine Learning for Molecular Design

The optimal design of compounds through manipulating properties at the molecular level is often the key to considerable scientific advances and improved process systems performance. In spite of century-long efforts in chemical synthesis and the large set of synthesized molecules (~10^7), the so-called chemical space is still an unexplored galaxy with an estimated number of small organic molecules populating the space of more than 10^{60}.

This project focuses on Computer-Aided Molecular Design (CAMD) using machine learning techniques, such as variational autoencoders, generative adversarial networks, self-supervised learning, and reinforcement learning.

Maximum students: 5