Machine Learning in Molecular Sciences

Machine learning (ML) and data-driven computational approaches have recently emerged as promising new tools to tackle complex optimization and computational problems. This workshop offers exciting new developments in applying such approaches to address challenging theoretical and computational issues in molecular sciences. Experts in quantum calculations, dynamics, molecular reactions, and materials design will share unique ideas and challenges.

Friday 21 September 2018
Science Center (Room 4102)

9:00 - 9:30 AM Bagels and Coffee

9:30 - 10:40 AM Data-enabled chemistry and material science: Using machine learning to make density functionals
Kieron Burke, UC Irvine

11:00 - 12:10 PM More efficient and accurate DFT-based dynamics via machine learning
Marivi Fernandez-Serra, Stony Brook University

12:10 - 1:30 PM Lunch

1:30 - 2:40 PM Deep potential molecular dynamics
Weinan E, Princeton University

3:00 - 4:10 PM Data-driven approaches for materials synthesis: Discovering reactions and uncovering mechanisms
Joshua Schrier, Fordham University

4:40 - 5:40 PM Machine learning for molecular property predictions and rational design in chemistry
Johannes Hackmann, Buffalo University

Sponsored by the Initiative for the Theoretical Sciences, and by the CUNY doctoral programs in Chemistry and Physics. Please send an email to sjang@qc.cuny.edu for any question.

The Graduate Center is located at 365 Fifth Avenue, between 34th and 35th Streets, in Manhattan.