Machine Learning and Chemistry: Progress so far and Challenges on the Way Forward

Organizers:

Pratyush Tiwary (University of Maryland)

Olexandr Isayev (University of North Carolina and Carnegie Mellon University)

Adrian Roitberg (University of Florida)

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CHEMISTRY &
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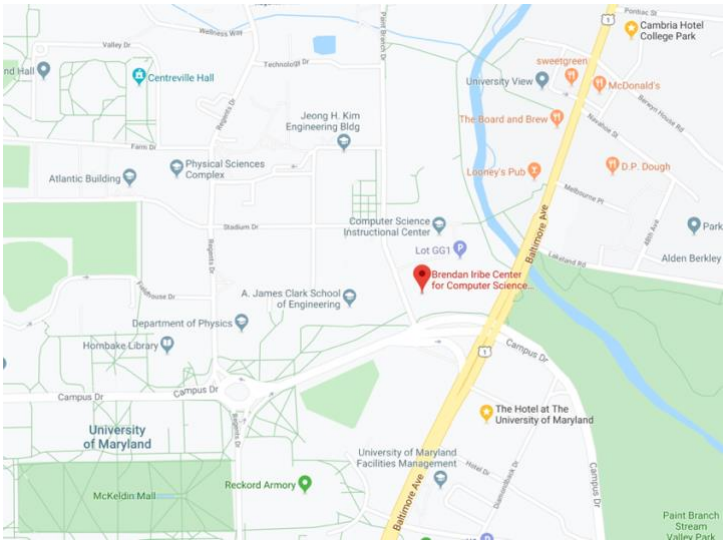
Locations:

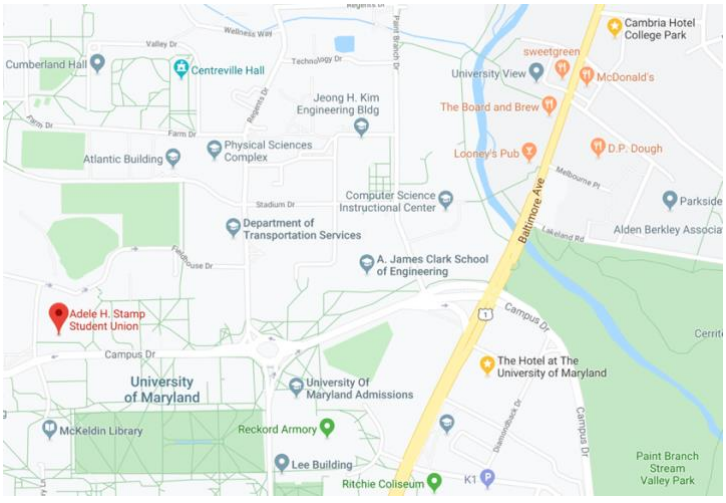
Saturday and Sunday:

Gannon auditorium, Brenan Iribe center for computer science, UMD



Monday:

Stamp Union grand ballroom lounge, UMD



WiFi: Eduroam across campus

Tutorial prerequisites: **Bring your laptop and have eduroam for internet. We will use PyTorch through google collab but you can (optional) also use your own local anacoda python**

Saturday 11/16

Gannon auditorium, Brenan Iribe center for computer science, UMD

Time	Activity/Speaker	Title
8:00 am-9:00 am	breakfast and registration for those attending tutorials	
9:00 am-10:00 am	tutorial	Intro to PyTorch
10:00 am-10:15 am	coffee	
10:15 am-12:15 pm	tutorial	Generative models and generation of molecular libraries with reinforcement learning
12:15 pm-1:45 pm	lunch (on your own)	
1:30 pm-1:55 pm	registration for those not attending tutorials	
1:55 pm-2:00 pm	opening remarks	
2:00 pm-2:30 pm	Tim Mueller	Fast and accurate interatomic potentials by symbolic regression
2:30 pm-3:00 pm	Olexandr Isayev	Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecule neural network
3:00 pm-3:30 om	Boris Kozinsky	Ex-machina computations of dynamics in complex materials using Bayesian force fields
3:30 pm-3:45 pm	coffee	
3:45 pm-4:15 pm	Adrian Roitberg	ANI and his associates. The way of the Force (and the Energy) through Machine Learning
4:15 pm-4:45 pm	Tom Miller	Quantum Machine Learning for Accurate and Low-Cost Computational Chemistry
4:45 pm-5:15 pm	Lucy Colwell	Data driven models that predict protein function from sequence
5:15 pm-5:45 pm	Pratyush Tiwary	Learning to learn, learning to forget
6:30 pm-8:30 pm	conference dinner (invitation only)	

Sunday 11/17

Gannon auditorium, Brenan Iribe center for computer science, UMD

Time	Activity/Speaker	Title
8:00 am-8:30 am	breakfast	
8:30 am-9:00 am	Michele Parrinello	Machine learning and molecular dynamics
9:00 am-9:30 am	Gerhard Hummer	Can machine learning make rare events more frequent?
9:30 am-10:00 am	Michele Ceriotti	Machine learning for atomic and molecular simulations
10:00 am-10:30 am	coffee	
10:30 am-11:00 am	Sapna Sarupria	Seeing the invisible to access the inaccessible – can machine learning help?
11:00 am-11:30 am	Brooke Husic	CGnet: Machine learning methods and modular software for coarse-grained molecular dynamics
11:30 am-12:00 pm	Robert Abel	The many possible roles of deep learning in drug discovery: separating reality from hype
12:00 pm-2:00 pm	lunch (on your own)	
2:00 pm-2:30 pm	John Chodera	Powering the next generation of research in machine learning in chemistry with OpenMM, the Open Force Field Initiative, and blind predictive challenges
2:30 pm-3:00 pm	Adrian Roitberg	Mprint Open Knowledge network. An NSF-funded community-wide approach to big data in chemistry
3:00 pm-3:30 pm	Shantenu Jha	DeepDriveMD: DL driven Adaptive Ensemble MD
3:30 pm-3:45 pm	coffee	
3:45 pm-4:15 pm	Johannes Hachmann	Making Machine Learning Work in Chemistry
4:15 pm-5:00 pm	Daniel G. A. Smith, Doaa Altarawy, and Matt Welborn	Computing, organizing, and sharing quantum chemistry data for machine learning with QCArchive
5:00 pm-5:30 pm	Discussion	
5:30 pm-6:30 pm	poster session	

Monday 11/18
Stamp Union grand ballroom lounge, UMD

Time	Activity/Speaker	Title
8:00 am-8:30 am	breakfast	
8:30 am-9:00 am	Florian Häse	Machine learning for accelerated experimentation and materials discovery with self-driving laboratories
9:00 am-9:30 am	Rafael Gomez-Bombarelli	Machine learning for atomistic design: from silicates to peptides
9:30 am-10:00 am	Paulette Clancy	Optimizing the use of Bayesian Optimization for Materials Discovery
10:00 am-10:30 am	coffee	
10:30 am-11:00 am	Evgeny Epifanovsky	Q-Chem 5.2: Facilitating Worldwide Scientific Breakthroughs
11:00 am-11:30 am	Robert Best	Exploring protein fitness landscapes
11:30 am-12:00 pm	Gaurav Chopra	Engineering Drug Discovery using Chemical Data Science
12:00 pm-2:00 pm	lunch (on your own)	
2:00 pm-2:30 pm	Amir Barati Farimani	Orbital Graph Convolution For Molecular Property Prediction
2:30 pm-3:00 pm	Connor Coley	Data-driven synthesis design for small organic molecules