DEPARTMENT OF PHYSICS AND ASTRONOMY

COLLOQUIUM ***IN-PERSON EVENT***

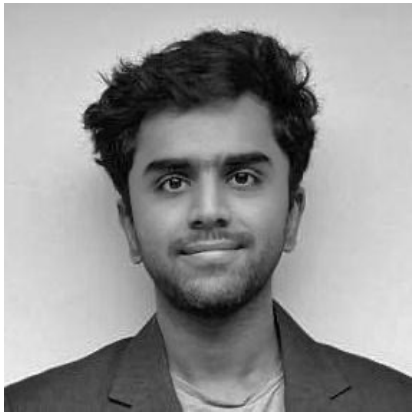
Electron density prediction using a hierarchy of atomic descriptors: A tale of two machine learning paradigms

Gopal Iyer

Department of Chemistry

Brown University

Ab initio electronic structure methods are often caught in a tug-of-war between predictive accuracy and computational efficiency, undermining their applicability to complex/large-scale chemical systems. While density functional theory (DFT) is considered a relatively efficient ab initio method compared to quantum Monte Carlo and other many-body electronic structure theories, it remains practically infeasible at the large length scales of interest in many molecular and mesoscale simulation studies. Central to DFT is the accurate prediction of the ground-state electron density distribution of molecules and materials. In this talk, I will discuss recent work conducted in collaboration with the Lawrence Livermore National Laboratory on the use of simple regression models, combined with the construction of novel atomic environment descriptors, to directly predict the electron density from atomic configurations using small training datasets. I will also discuss the use of symbolic regression to identify non-intuitive descriptors that improve the expressivity of the electron density prediction models, highlighting the potential of machine learning methods to accelerate, or even bypass completely, the expensive solution of the Kohn–Sham equations in DFT.



Thursday, August 31, at 3:55 PM

IN-PERSON EVENT

Local Contact: Prof. Y. Abate, yohannes.abate@uga.edu