Jarvist Frost:

Lecture:

In material science we have one central theorem: that material properties result from the electronic structure of the atoms that make up the material. Everything, from atomic forces to (bulk) yield properties of metals, from band gaps (the colour of materials) to emergent properties such as thermal and electrical conductivity, arises from solving the Schrodinger equation of motion for the electrons. However, the fundamental computational limits of quantum mechanics means that we face an enormous chasm of length and time scales between what is computable, and what is needed for rational design of materials.

From a machine learning perspective - this is a fantastic position to be in! We have an enormous set of well validated computational methods developed to calculate properties, and this data can be generated entirely 'synthetically' (within the computer), and on-the-fly (enabling active learning).

In this lecture I will present pedagogical background to how both the machine learning and the electronic structure methods work, and then showcase some of the latest developments in machine learning developed for material science, including graph based regression models, diffusion based generative models, and extremely powerful equivariant models for molecular dynamics.

Tutorial:
In this tutorial we will focus on modelling potential energy surfaces, starting with basic Gaussian Processes which we will code up ourselves, and then progressing to fitting one of the latest equivariant machine learning force-fields (MLFFs), the Message-passing-neural-network Atomic Cluster Expansion.