Title: Machine learning with kernel methods in high dimensional spaces

Abstract:
Machine learning (ML) has been acquiring increasing importance in various areas of science and technology. Applications in physics and chemistry range from modeling the topology of energy landscapes to structure-property relations to resolving accuracy and CPU cost bottlenecks of computational methods such as DFT (density functional theory). Kernel methods such as kernel ridge regression (KRR) and Gaussian process regression (GRP) are among the most widely used methods. These methods are attractive as they combine advantages of the high expressive power of non-linear methods with some of the advantages of linear regressions. In many applications, ML is done in sufficiently high-dimensional feature spaces that effects arise that are specific to high-dimensional settings and that may negate any advantages of nonlinear kernels. I will show how this arises in applications ranging from potential energy function construction to renewable energy system management. I will also show how these issues can be palliated by the use of additive kernels. I will also introduce an additive kernel based approach which is equivalent to a neural network with optimized neuron activation function and combines advantages of GPR and NN while significantly containing their disadvantages such as overfitting.