

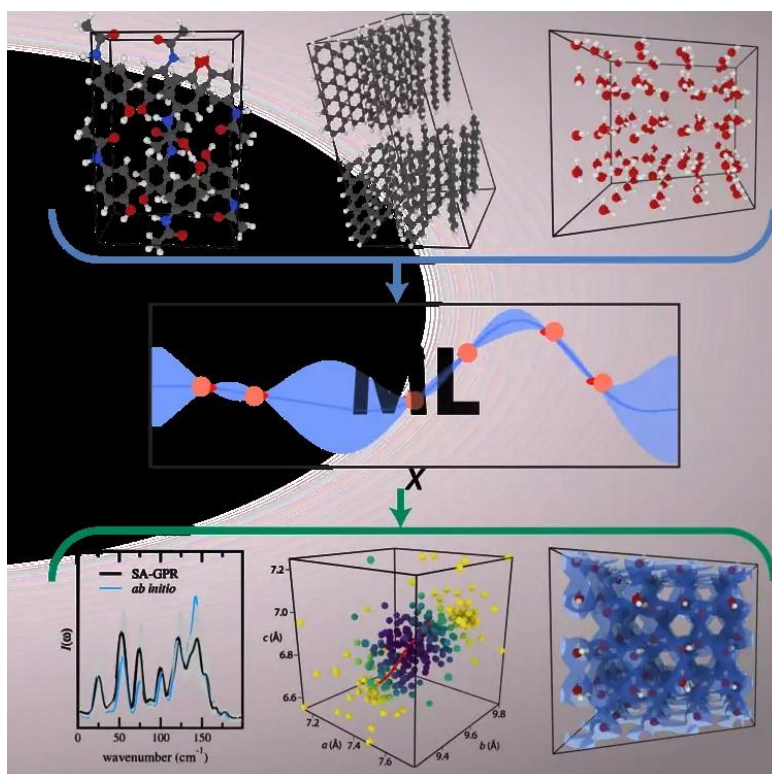
IMPRS UFAST Focus Course

Machine Learning Techniques in Atomistic Simulations

Mariana Rossi

Abstract:

In this course, an introductory overview of machine-learning methods applied to atomistic simulations will be given. We will cover the basics of supervised and unsupervised algorithms for property prediction and classification, based on kernel methods and on neural networks. Focus will be given on methods geared towards speeding up theoretical quantum chemistry methods and dealing with larger amounts of data. The course will consist of lectures and hands-on sessions that showcase some of the algorithms. Knowledge of basic python programming is necessary.



CFEL, Seminar room O2.104

16th – 19th Sept 2024

09:30 h – 12:30 h

Register on Geventis I-UF FC6