Seminarium NOMATEN

Tuesday, 23 February, 13:00 – 15:00
https://gotomeet.me/ncbjmeetings/nomaten-seminar

Speaker:
Albert Bartok-Partay PhD, Assistant Professor, University of Warwick

Title:
Learning Atomic Interactions from Microscopic Observables

Abstract:

Designing new materials needs a detailed understanding of the structure and processes of matter on the atomistic scale, because all macroscopic properties ultimately depend on microscopic interactions. For such studies, quantum mechanical modelling combined with atomistic simulations has been proven to be predictive in addition to being able to explain experimental phenomena. However, larger length and timescales are not easily accessible due to the non-linear growth in computational resources required to numerically solve the quantum mechanical equations. We would like to enable fast simulations without a compromise in accuracy by using machine learning techniques to fit the quantum mechanical model. To realise this aim, we have developed the Gaussian Approximation Potentials framework, which uses microscopic data from quantum mechanical calculations on small systems to create fast, accurate and scalable models. Apart from data, the other main ingredient needed to fit Gaussian Processes are kernels. In my talk I will discuss kernels that are designed to compare atomic structures and show examples from molecular and condensed matter systems. These kernels are used to define a set of interatomic potentials or models, and a Bayesian approach determines which is the most likely, based on the data as evidence.

Bio:
Albert is an Assistant Professor at the University of Warwick. He earned his PhD degree in physics from the University of Cambridge in 2010, his research having been on developing interatomic potentials based on ab inito data using machine learning. He was a Junior Research Fellow at Magdalene College, Cambridge and later a Leverhulme Early Career Fellow. Before taking up his current position, he was a Research Scientist at the Science and Technology Facilities Council. His research focuses on developing theoretical and computational tools to understand atomistic processes.