GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Fachbereich Physik
Institut für Theoretische Physik

CONDENSED MATTER THEORY SEMINAR

Subject: **From physics to machine-learning and back**

Speaker: **Dr. Edgar A. Engel, EPFL, Lausanne, CH**

Date & time: **Friday, July 5th, 2019 at 3:15 p.m.**

Venue: **Seminar room 1.114**

Abstract: Over recent years machine-learning (ML) approaches have prominently found their place in the physical and biological sciences — whether it is as surrogate models promising chemically-accurate properties predictions at the atomic scale (while sidestepping much of the computational cost of first-principles methods), or as a means of performing data-driven classifications and extracting important physical insight into the behaviour of complex systems and the structure-property relations of materials.

Against the backdrop of the proliferation of different descriptions of atomistic systems in ML (and learning strategies), I will argue that exploiting fundamental physics and chemistry in the description of atomistic systems facilitates effective ML for chemistry and materials. To this purpose I will outline how the smooth overlap of atomic positions (SOAP) representation arises from a description of atomic structures based on atom densities. This physically motivated descriptor has been widely used to regress different scalar properties, and has more recently been extended to machine-learn also more complex properties such as tensors and the charge density.
Furthermore, I will present an example of how ML can be beneficial for more complex tasks, namely the identification of stabilisable phases among databases of (computationally) locally-stable atomic structures, by means of a generalized convex hull construction.