# IWR Colloquium
# Winter Semester 2019 / 2020

**January 22, 2020 • 16:15**
**Mathematikon, Conference Room / 5th Floor**
**Im Neuenheimer Feld 205, 69120 Heidelberg**

**Speaker:**
Prof. Anatole von Lilienfeld
University of Basel

**Title:**
"Quantum Machine Learning"

**Abstract:**
Many of the most relevant observables of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to computational materials design mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of material candidates is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical compound space, i.e. all the compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms exploit implicit redundancies and correlations. I will discuss recently developed statistical learning based approaches for interpolating quantum mechanical observables throughout chemical compound space. Numerical results indicate remarkable performance in terms of efficiency, accuracy, scalability and transferability.

**Website Prof. von Lilienfeld:**
https://chemie.unibas.ch/de/personen-207/anatole-von-lilienfeld/

**Website IWR-Colloquium:**
www.iwr.uni-heidelberg.de/iwr-colloquium