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Einladung zum Vortrag

"Quantum machine learning and perturbation theory for accelerated exploration of chemical compound space"

Otto Anatole von Lilienfeld

Chemistry Departement, University of Basel

Termin: **Donnerstag, 10. Oktober 2019, 13:30 Uhr,** **Lehrvortrag 10:00 Uhr**

Ort: **Victor-Franz-Hess-Hörsaal, Währinger Straße 17, 1. Stock (Hoftrakt), Raum 112**

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 and alchemical perturbation based approaches for interpolating quantum mechanical observables throughout chemical compound space. Numerical results indicate remarkable performance in terms of efficiency, accuracy, scalability and transferability.

Im Rahmen des Vortrages findet eine Lehrprobe zum Thema „The quantum harmonic oscillator" statt.