

# nanoSeminar Series 2021

Institute for Materials Science

**Prof. Dr. Anatole von Lilienfeld**

Department of Physics, University of Vienna

**“Quantum Machine Learning”**

Thursday, July 15<sup>th</sup> 2021  
13:00 – 14:00

Normal: Seminar Room 115, Hallwachsstr. 3 (HAL)  
Pandemic version: <https://tinyurl.com/nanoSeminar-GA>

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 compound space, i.e. all the possible combinations of compositional and structural degrees of freedom. Consequently, efficient exploration algorithms exploit implicit redundancies and correlations. I will discuss recently developed statistical learning based approaches for interpolating quantum mechanical observables throughout compound space. Numerical results indicate promising performance in terms of efficiency, accuracy, scalability and transferability.

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As of 2020, Anatole von Lilienfeld joined the Faculty of Physics at the University of Vienna as a professor of Computational Materials Discovery. Before, he was an associate professor of Physical Chemistry at the Department of Chemistry of the University of Basel. In 2016, he was an associate professor at the Free University of Brussels after having spent two years as a Swiss National Science Foundation professor at the University of Basel prior to which he worked for Argonne and Sandia National Laboratories. From 2007 to 2010 he was a distinguished Harry S. Truman Fellow at Sandia National Laboratories, after postdoctoral work with Mark Tuckerman at New York University and at the University of California Los Angeles. In 2005, he was awarded a PhD in computational chemistry, under the supervision of Ursula Rothlisberger at EPF Lausanne .