Data Science Colloquium

HiDA HELMHOLTZ Information & Data Science Academy

summer term 2021 ***Special Event: HIDA Lectures @ DASHH***
"Meet the Speaker" for Students After the Talk

We proudly announce the next joint Data Science Colloquium. This third event will take place ***online*** on **April 15th, 2021 at 2 pm** featuring

Prof. O. Anatole von Lilienfeld

Professor for Computational Materials Discovery

Faculty of Physics

Universität Wien, Austria

Quantum Machine Learning in Chemical Compound Space

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.

Subscription Link for Regular Updates and Zoom Links:
https://lists.desy.de/sympa/subscribe/datasciencecolloquium

DASHH Data Science in Hamburg HELMHOLTZ Graduate School for the Structure of Matter

TUHH Hamburg University of Technology

INSTITUTE OF MATHEMATICS

ahoi.digital

DESY.

Universität Hamburg DER FORSCHUNG | DER LEHRE | DER BILDUNG

CDCS CENTER FOR DATA AND COMPUTING IN NATURAL SCIENCES

DEPARTMENT OF INFORMATICS

CLUSTER OF EXCELLENCE QUANTUM UNIVERSE

CLUSTER OF EXCELLENCE CUI: ADVANCED IMAGING OF MATTER