Physikalisches Institut
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg

IRTG-Seminar

Rodrigo A. Vargas-Hernández

University of British Columbia, Vancouver

“Machine learning for many-body quantum physics”

Solving the Schrödinger equation (SE) for many-body systems has been the main challenge for quantum physicists over the last century. In this talk, I will illustrate how with machine learning it may be possible to reduce the number of times the SE needs to obtain physical results. In the first part of my talk I will explain the application of kernel methods of machine learning for fitting potential energy surfaces (PES) of polyatomic molecules. In particular, I will illustrate the application of Bayesian optimization with Gaussian processes as an efficient method for sampling the configuration space of polyatomic molecules. In the second part of my talk I will discuss the possibility to extrapolate quantum observables with machine learning to discover phase transitions for condensed matter systems.

Tuesday, February 06, 2018, 6:00 p.m., HS II,
Physics high rise, Hermann-Herder-Str. 3

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