universität wien
Vienna Doctoral School in Physics

ESI Erwin Schrödinger International Institute for Mathematics and Physics

Machine Learning for Materials Hard and Soft

ESI-DCAFM-TACO-VDSP Summer School 2022
11–22 July 2022
ESI, University of Vienna

David Pfau (DeepMind, London)
Deep Learning and Ab-initio Electronic Structure

Abstract:
Advances in deep neural networks in recent years have made them an attractive tool for ab-initio electronic structure calculations. In the first part of the talk, we will discuss advances in the theory of equivariant neural networks, which have found applications in graph neural networks, machine learning of molecular force fields, and *ab-initio* electronic structure. In the second part of the talk, we will discuss methods for second-order optimization of neural networks. While many of these advances have struggled to gain traction in mainstream machine learning, they are particularly well suited for variational quantum Monte Carlo calculations, and closely related to methods like stochastic reconfiguration. Lastly, we will discuss ways that these ideas have been applied to variational QMC calculations in recent years, including Neural Network Quantum States, the Fermionic Neural Network, and PauliNet.

FWF Der Wissenschaftsfonds.
DOCTORAL COLLEGE
TACO
TU WIEN TECHNISCHE UNIVERSITÄT WIEN Vienna University of Technology