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**FAKULTÄT FÜR MATHEMATIK**
Dekan Univ.-Prof. Dr. Radu Ioan Boţ

Einladung zur öffentlichen Defensio

## Leon GERARD

Thema der Dissertation

# Solving the electronic Schrödinger equation using Deep Neural Networks and Transfer Learning

Abstract:
The thesis comprises a series of publications in the emerging field of deep learning-based Variational Monte Carlo (DL-VMC), which offers a highly accurate ab-initio method for computing electronic properties of molecules by solving the Schrödinger equation. The time-independent, non-relativistic Schrödinger equation is an eigenvalue equation, whereas the thesis places particular emphasis on the smallest eigenvalue and its corresponding eigenfunction. In DL-VMC, in an unsupervised manner, a neural network is optimized to represent the solution of the Schrödinger equation, also called the wave function. The method has recently demonstrated superior accuracy compared to other computational methodologies, albeit at a substantial computational cost due to the large number of trainable parameters in the neural network and the need for Monte Carlo integration to obtain a precise estimate of the eigenvalue.
The following thesis contributes to the recent improvements to enhance the method's efficiency by introducing a novel technique for effectively learning wave functions for various molecules and their geometrical conformations in parallel. For the first time, we are able to optimize a single wave function model on a diverse range of molecules and transfer this pretrained neural network to previously unencountered molecules, yielding competitive results with only a few fine-tuning steps. Furthermore, this work aims to improve the understanding of specific design choices involved in constructing neural network-based wave functions.

**Prüfungssenat**

Univ.-Prof. Mag. Dr. Andreas Cap
(Vorsitz, Universität Wien)

Univ.-Prof. Dr. Philipp Grohs
(Universität Wien)

Prof. Dr. Reinhold Schneider
(TU Berlin)

Prof. Dr. Risi Kondor
(University of Chicago)

**Zeit und Ort**

Donnerstag, 23. Mai 2024, 15:30 Uhr

Online:

> https://univienna.zoom.us/j/68409697007?pwd=NEZiajBXcEtSL2JzOGVCT3lLMzBWUT09
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> Meeting ID: 684 0969 7007
>
> Kenncode: 776439