# PHYSIKALISCHES KOLLOQUIUM

WINTERSEMESTER 2023/24

Montag, 11.12.2023, 12 Uhr c.t.

MACHINE LEARNING CONVENTIONAL SUPERCONDUCTORS

Miguel Marques, Ruhr Universität Bochum

We perform a large scale study of conventional superconducting materials using a machine-learning accelerated high-throughput workflow. We start by creating a comprehensive dataset of around 7000 electron-phonon calculations performed with reasonable convergence parameters. This dataset is then used to train a robust machine learning model capable of predicting the electron-phonon and superconducting properties based on structural, compositional, and electronic ground-state properties. Using this machine, we evaluate the transition temperature (Tc) of approximately 200000 metallic compounds, all of which on the convex hull of thermodynamic stability (or close to it) to maximize the probability of synthesizability. Compounds predicted to have Tc values exceeding 5 K are further validated using density-functional perturbation theory.

Rh Pd Ir Pt
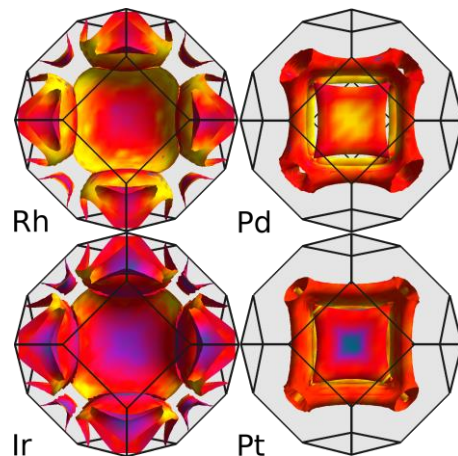
As a result, we identify 541 compounds with Tc values surpassing 10 K, encompassing a variety of crystal structures and chemical compositions. We also identified a series of (thermodynamically unstable) hydride compounds that superconduct at temperatures reaching more than 80 K at ambient pressure.

Die Einführung erfolgt durch Ilya Eremin

Die Fakultät lädt alle Interessierten herzlich ein. Die Veranstaltung findet im Hörsaal HZO 20 statt.

Physik und Astronomie
from matter to materials