Kurzzusammenfassung

Abstract

This thesis examines Quantum ESPRESSO, a suite of computer code for electronic-structure calculations and materials modeling in terms of its scalability on multiple processors on the PHYSnet compute cluster. A series of benchmarks is carried out to test different combination of compilers as well as parallelization parameters offered by Quantum ESPRESSO itself. These benchmarks show that using a set of compilers and auxiliary code in Intel oneAPI offered by Intel significantly improves scaling and that the parallelization parameters offered by Quantum ESPRESSO let calculations scale beyond a single node when used right. Results from these benchmarks were then used to carry out phonon calculations on TaS_2 in charge density wave phase, the results of which could possibly explain a gap feature near the Fermi niveau observed in a 2019 Scanning Tunneling Spectroscopy (STS) experiment on this material.