I Motivation

For a realistic description of matter, methods derived from first principle (so called ab-initio methods) are needed. Phenomena explainable from ab initio methods span from thermodynamics properties of matter to superconductivity. The former deals with the description of quasi-particles emerging from the quantization of vibrational modes and the latter still lacks a theory explaining all kinds of known superconductivity.

One such ab-initio method is Density Functional Theory (DFT), the foundations of which were laid in 1964 by Hohenberg and Kohn [1], and in 1965 by Kohn and Sham [2]. Since 1990, methods within the density functional formalism have been very successful across a number of disciplines in physics, chemistry and biology, with over 160 000 publications on the topic between 1990 and 2015 [3]. The appeal of DFT methods lies in the fact that the complexity of calculations is reduced in such a way that objects such as the full wave function cannot be computed, total energies are very reliably produced, which in turn enables calculations of lattice dynamics, thermodynamical properties of matter or chemical reactions. These calculations are computationally cheap in comparison to methods working with full wave functions, so that simple systems can be simulated on a home computer today. In software suites such as Quantum ESPRESSO [4, 5] DFT methods are easily available today.

Going beyond simple calculations of a few atoms and towards current research questions makes parallel calculations over multiple nodes on compute cluster with hundreds or thousands of CPUs the only feasible possibility. An important step therefore is to guarantee that the process of scaling the work across multiple processors is done in an effective manner to utilize available computing resources as efficiently as possible.

Thus, the task of this thesis was two-fold: First, examining the way Quantum ESPRESSO calculations are best parallelized on the PHYSnet cluster and then using this knowledge to run calculations for a system of current interest and relate to recent experimental data of this system [6].

The examined system is TaS_2, a Transition Metal Dichalcogenide (TMDC). As bulk structures, TMDCs have been first described in 1923 by Dickinson and Pauling [7], in 1969 Wilson et al. characterized over 60 TMDCs. The more recently discovered monolayers of TMDCs [8] have brought a new focus on these materials, as they are among the candidates for materials enabling controllable electronic quantum phases [9]. TaS_2 in particular is notable as a superconducting material, both in the bulk and the monolayer case. Furthermore, both bulk and monolayer TaS_2 form a charge density wave (a periodic modulation of the electronic charge density of a solid) at low temperatures [6]. This particular phase of monolayer TaS_2 is an active area of research and will be examined in this thesis.

The structure of this thesis is as follows: first, all relevant theory needed to understand the calculations made with Quantum ESPRESSO will be outlined in **??**. Following that, details regarding the computational work done, such as the concrete metrics evaluating performance as well as a description of the parallelization parameters offered by QUANTUM ESPRESSO will be presented in ??. In ??, a overview over the examined systems is given. ?? examines scalability of the `PWscf` module, which enables electronic structure calculations, the same is done in ?? for the `PHonon` module, which is used for calculation of phonon and phonon related properties. The results from these chapters are then used to run an optimized phonon calculation on TaS_2 in the charge density wave phase. This optimized phonon calculation is then the foundation for a possible explanation of experimental data on TaS_2 in ??.