I Examined systems

I.1 Silicon

Silicon is the fundamental material in integrated circuits and as such is one of the pillars of the digital revolution. Analogue to the Stone, Bronze or Iron Age, this age of civilization can thus be called the Silicon Age [1]. Consequently, silicon is a well studied material from an experimental and theoretical standpoint with established properties. This combined with the fact that with only 8 electrons per unit cell DFT calculations on silicon are not particularly expensive makes it an ideal system for an introduction to DFT calculation as well as a good benchmarking system. Consequently, all benchmarks in this thesis were run on silicon first and with the information gained from that benchmarks on a more expensive system were run.

crystal structure?

I.1.1 Computational parameters

The calculations in ch. **??** were made with a plane wave cutoff of

made on a 40x40x40 k point grid,

All calculations use a PBE (Perdew-Burke-Ernzerhof [2]) XC-functional with a norm-conserving PP generated using Vanderbilt's method [3].

I.2 TaS_2

TaS_2 belongs to the class of Transition Metal Dichalcogenide (TMDC)'s, the most common stoichiometry of which is MX_2, where M is a transition-metal and X is a chalcogen atom. TMDC's were known and studied as a bulk material since more than five decades [4],

the discovery of freestanding monolayers [5]

Both bulk and monolayer TaS_2 show superconductivity, with the dimensionality reduction enhancing the critical temperature from 0.5 K to 2.2 K [6].

I.2.1 Charge-density waves

I.2.2 Computational parameters

The calculations use a PBE XC-functional with a norm-conserving PP generated by Hartwigsen et al. [7].