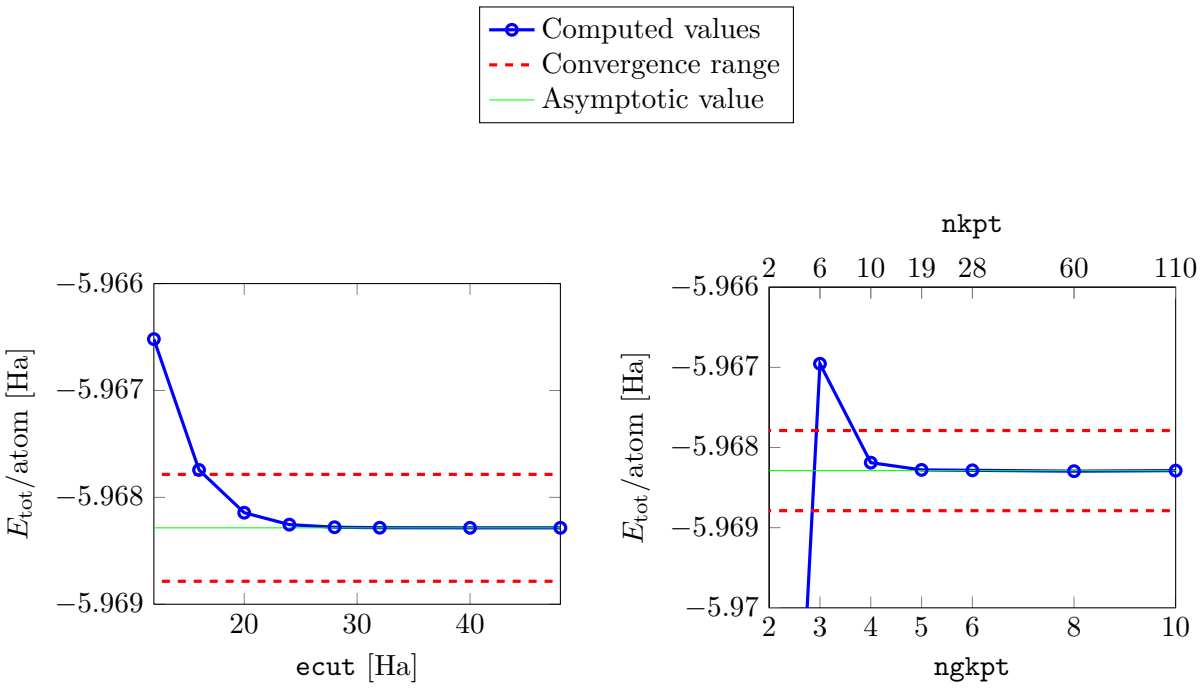
Appendix B

Convergence Studies

The graphs of the convergence studies of the total energy and the lattice parameter with respect to `ecut` and `ngkpt` are presented below. The convergence studies with respect to `ecut` were realised with a fixed `ngkpt` = 5x5x5 and the convergence studies with respect to `ngkpt` were realised with a fixed `ecut` = 28 Ha.

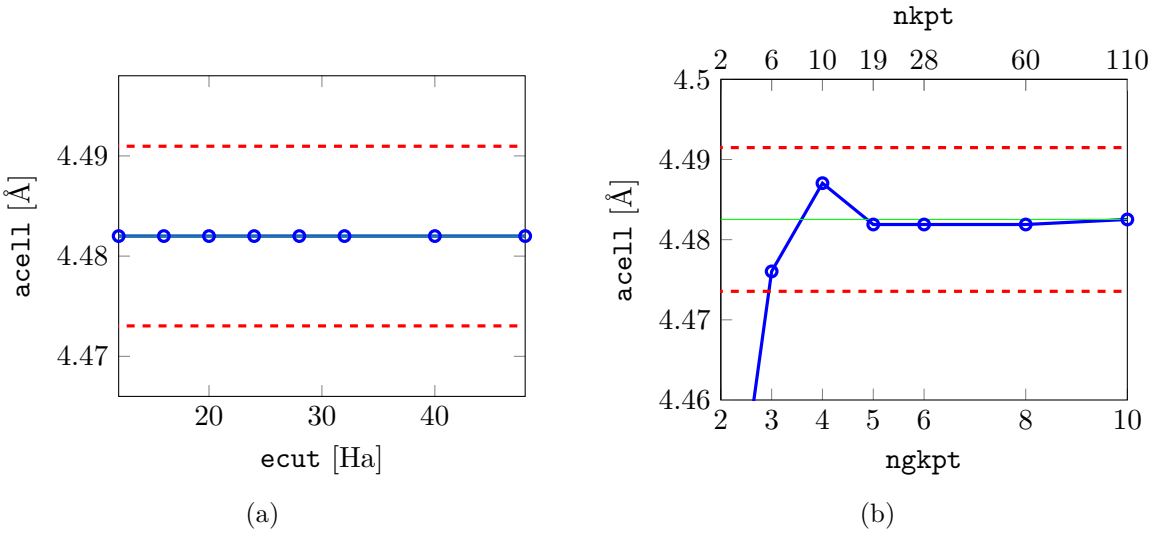
The tolerance criteria for the total energy per atom used in this work is maximum 0.05 mHa of difference with the asymptotic converged value. The convergence studies with respect to `ecut` and `ngkpt` are presented on the figure B.1. It can be seen that the total energy is converged for `ecut` = 20 Ha and `ngkpt` = 4x4x4 corresponding to 10 k-points in the IBZ.

The tolerance criteria for the lattice parameter used in this work is maximum 0.2 % of difference with the asymptotic converged value. The graphs of the convergence studies are presented on the figure B.2. It can be seen that `acell` is converged for every `ecut` and for a `ngkpt` = 3x3x3 corresponding to 6 k-points in the IBZ. The relaxation started with a lattice constant $a = 4.643$ Å found in the literature (Materials Project [21]) and ended with a relaxed lattice constant $a = 4.483$ Å.



(a) (b)

Figure B.1: Convergence study of the total energy per atom. (a) Convergence with respect `ecut` (`ngkpt`= 5). (b) Convergence with respect to the number of k-point (`ecut` = 28 Ha).



(a) (b)

Figure B.2: Convergence study of the lattice parameter a corresponding to the variable `acell` in ABINIT. (a) Convergence with respect `ecut` (`ngkpt`= 5). (b) Convergence with respect to the number of k-point (`ecut` = 28 Ha).