

Appendix D

Convergence studies

This chapter contains the different graphs linked to the convergence studies explained in Section 5.1. Figs. D.1, D.2 and D.3 show the convergence of the total energy per atom in the LaCrO_3 unit cell as a function of the cut-off energies and the number of k points. Figs. D.4, D.5 and D.6 represent the convergence of the three unit cell parameters of this material. Figs. D.7, D.8, D.9, D.10, D.11 and D.12 depict the same convergence study for the SrCrO_3 crystal.

These figures show that for LaCrO_3 as well as for SrCrO_3 , $E_{\text{cut}} = 30$ Ha, $E_{\text{cut}}^{\text{PAW}} = 50$ Ha and $\text{ngkpt} = 6 \times 6 \times 6$ are the parameters needed in order to reach a sufficient convergence. Actually, it can be seen that $E_{\text{cut}}^{\text{PAW}}$ does not play an important role : the convergence study with respect to this parameter is usually not important. It has still been realized and plotted for the sake of completeness.

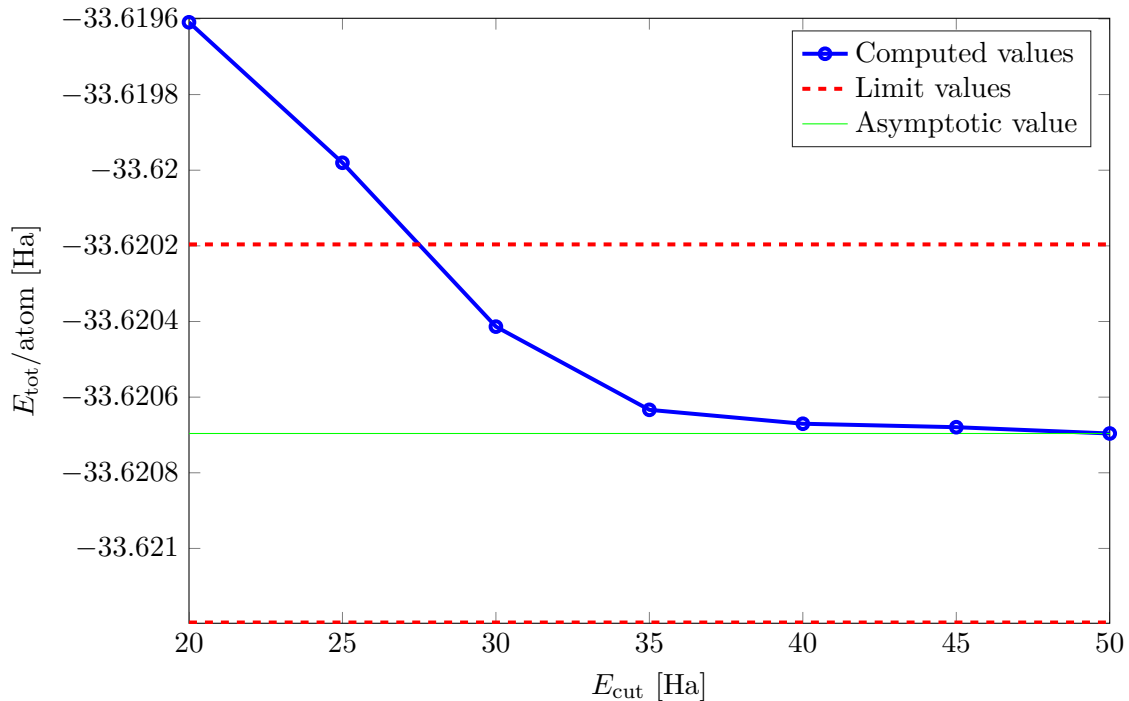


Figure D.1: Convergence study of the energy per atom of LaCrO_3 as a function of E_{cut} .

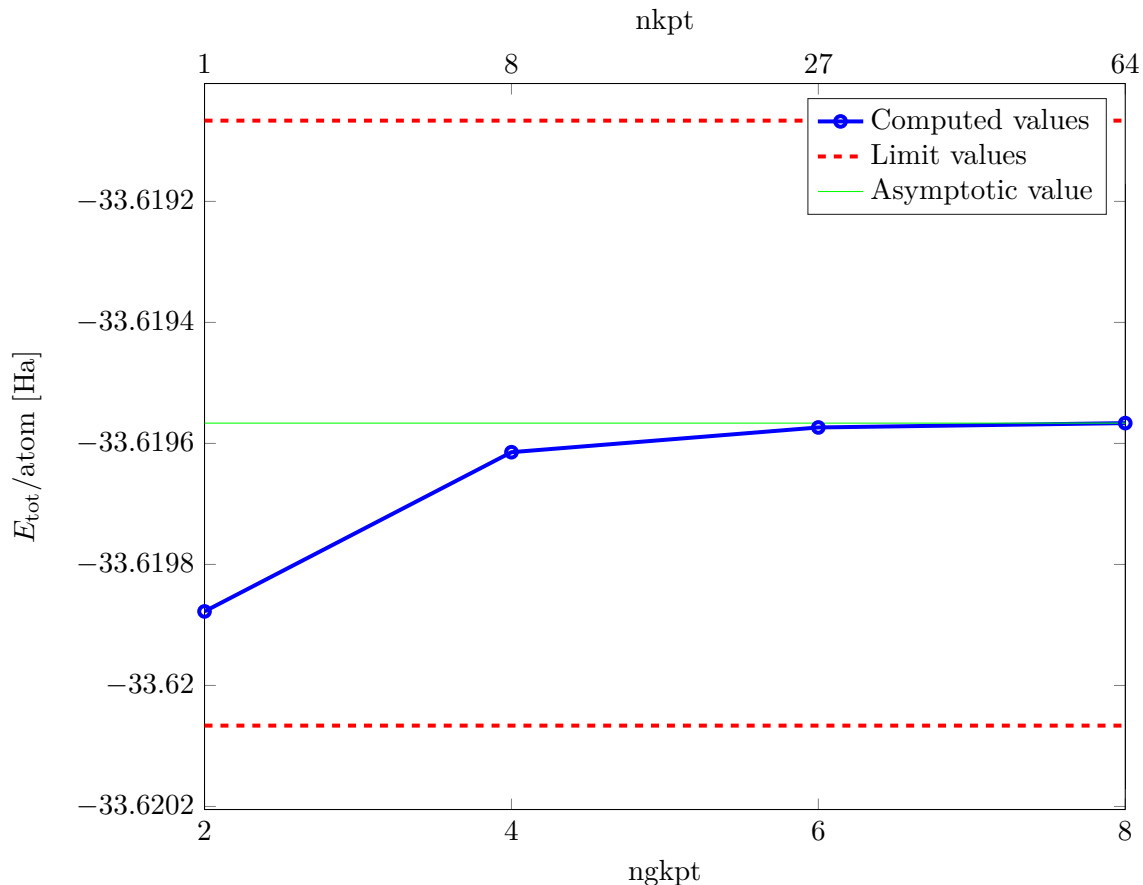


Figure D.2: Convergence study of the energy per atom of LaCrO_3 as a function of the number of k points.

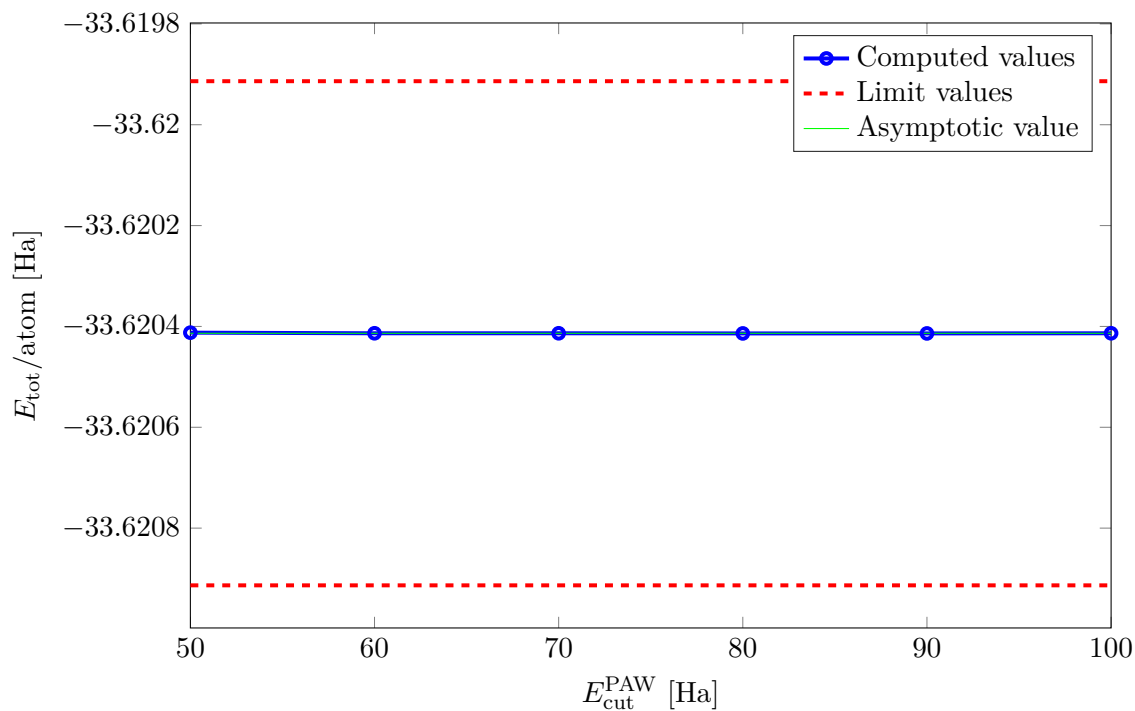


Figure D.3: Convergence study of the energy per atom of LaCrO_3 as a function of $E_{\text{cut}}^{\text{PAW}}$.

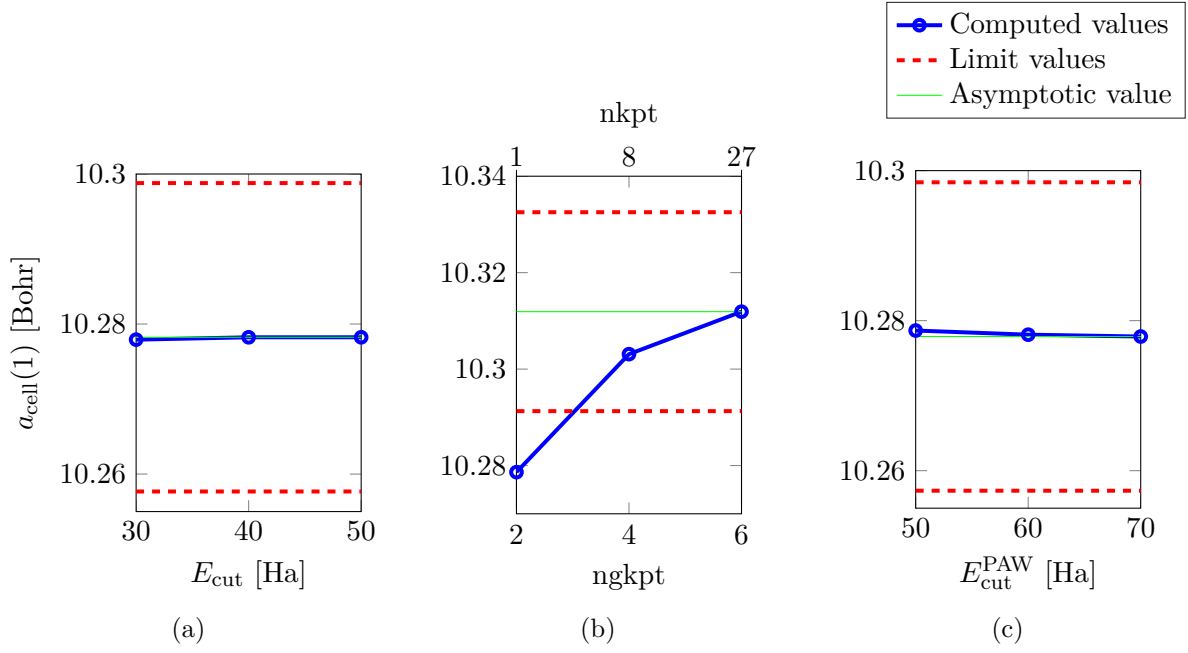


Figure D.4: Convergence study of $a_{\text{cell}}(1)$ of LaCrO_3 as a function of (a) E_{cut} , (b) the number of k points and (c) $E_{\text{cut}}^{\text{PAW}}$.

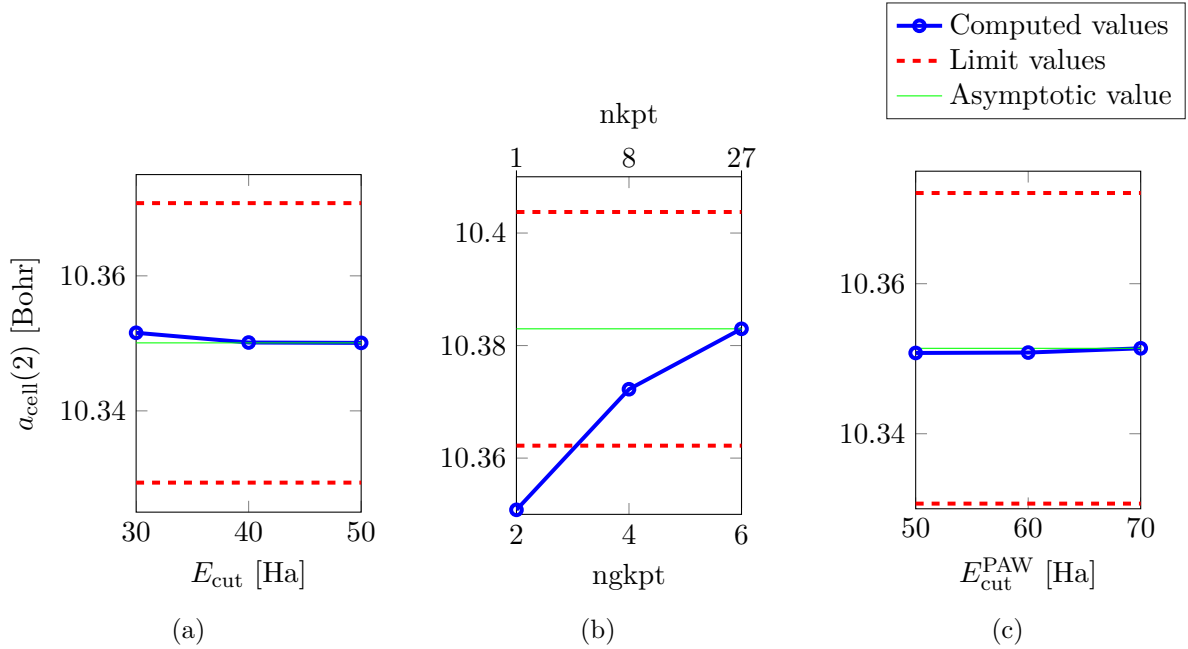


Figure D.5: Convergence study of $a_{\text{cell}}(2)$ of LaCrO_3 as a function of (a) E_{cut} , (b) the number of k points and (c) $E_{\text{cut}}^{\text{PAW}}$.

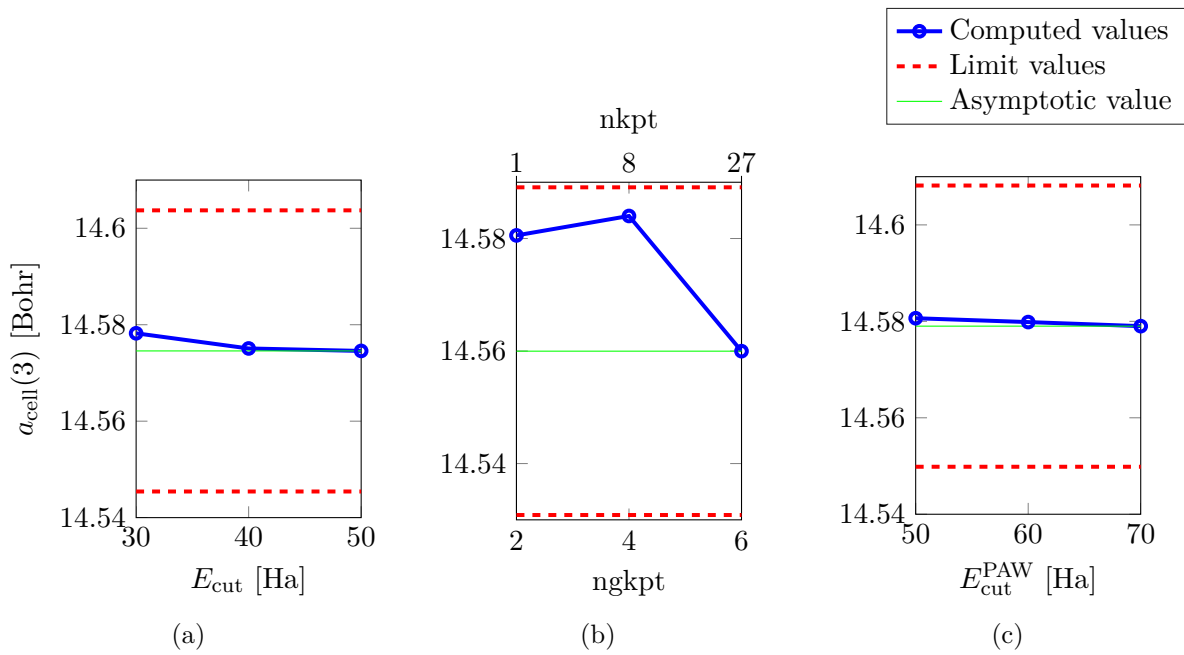


Figure D.6: Convergence study of $a_{\text{cell}}(3)$ of LaCrO_3 as a function of (a) E_{cut} , (b) the number of k points and (c) $E_{\text{cut}}^{\text{PAW}}$.

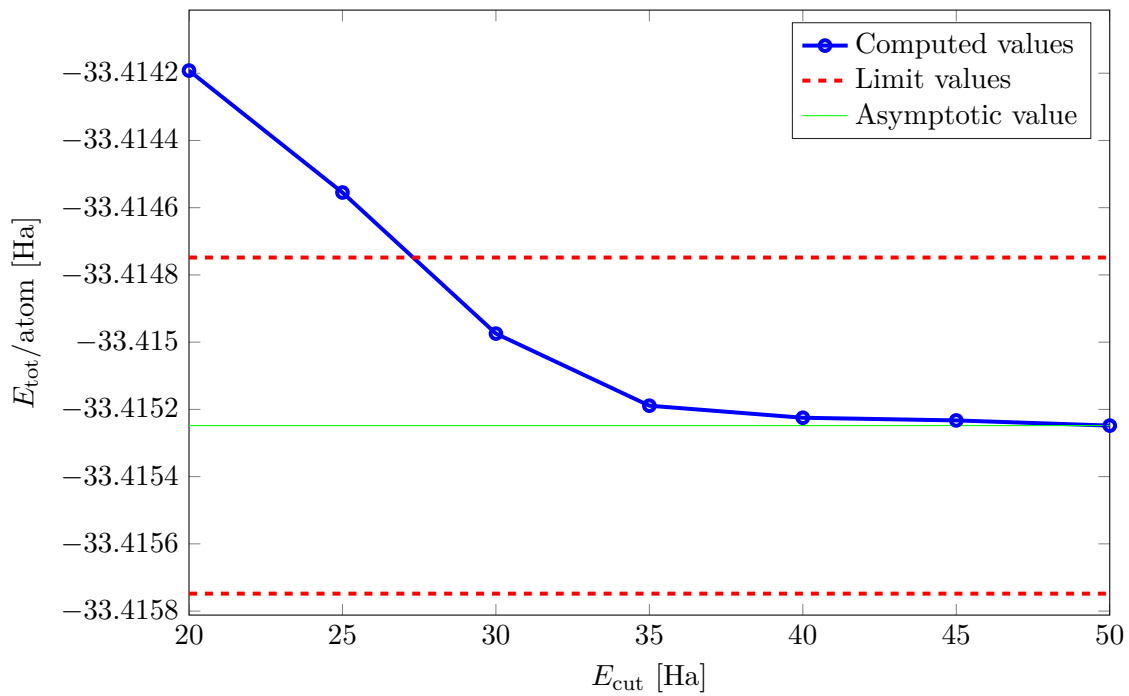


Figure D.7: Convergence study of the energy per atom of SrCrO_3 as a function of E_{cut} .

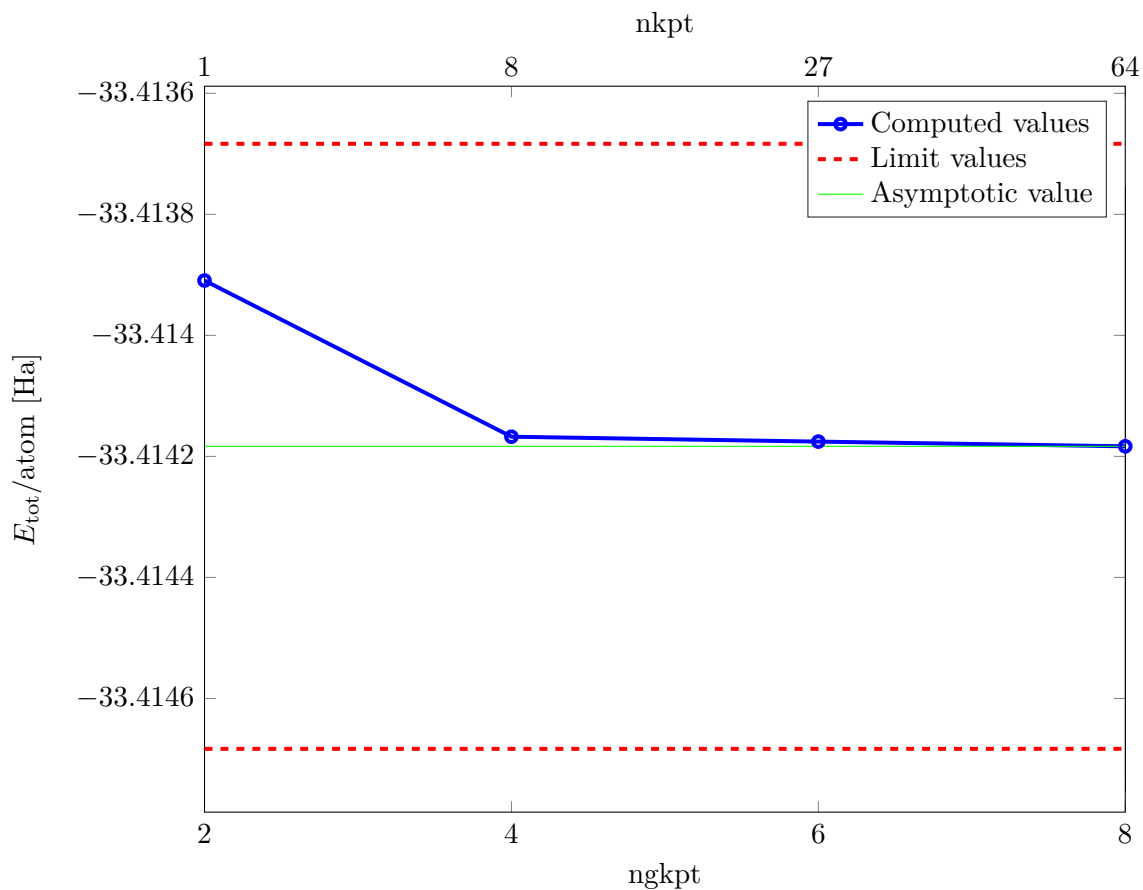


Figure D.8: Convergence study of the energy per atom of SrCrO_3 as a function of the number of k points.

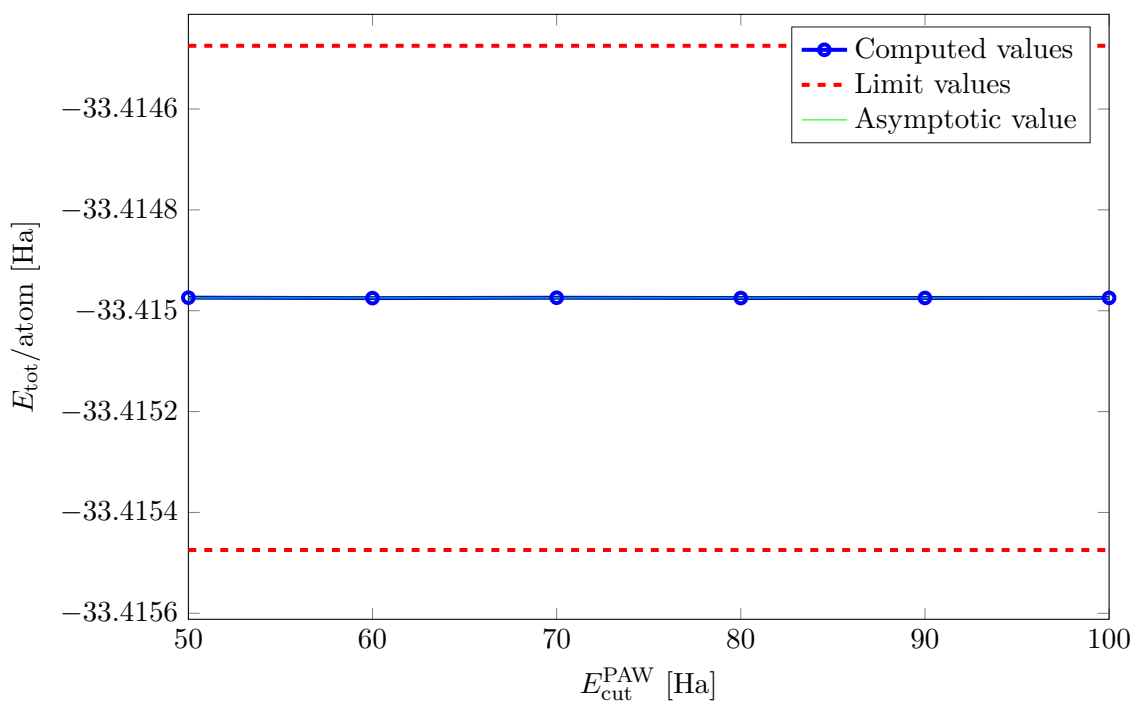


Figure D.9: Convergence study of the energy per atom of SrCrO_3 as a function of $E_{\text{cut}}^{\text{PAW}}$.

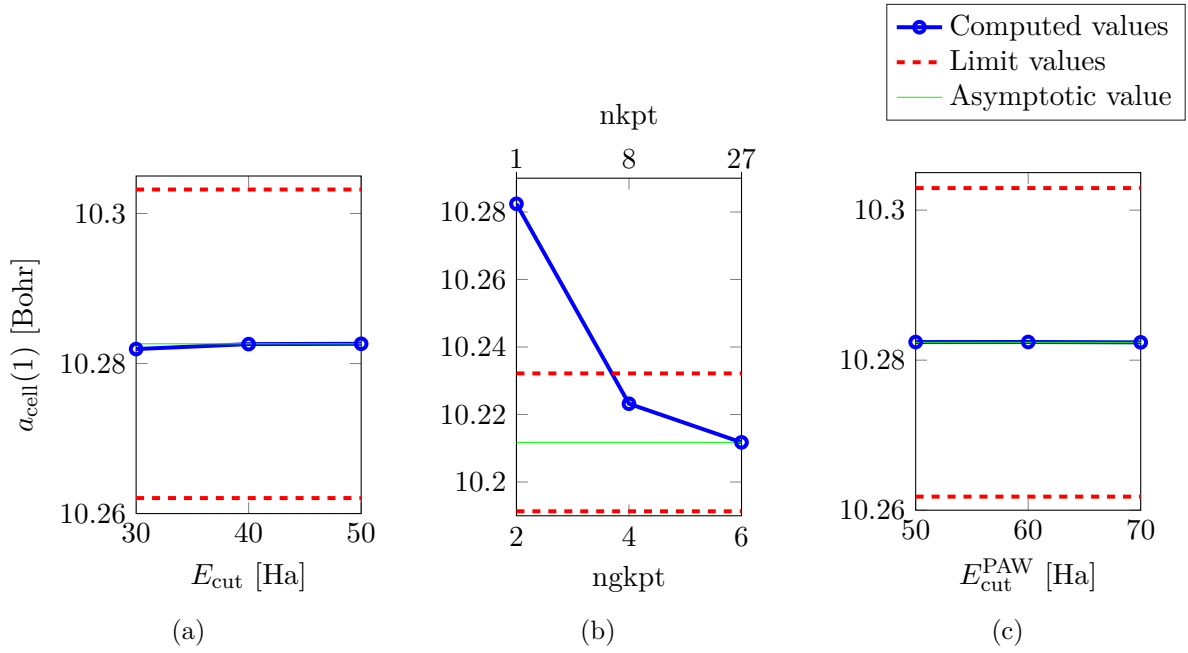


Figure D.10: Convergence study of $a_{\text{cell}}(1)$ of SrCrO_3 as a function of (a) E_{cut} , (b) the number of k points and (c) $E_{\text{cut}}^{\text{PAW}}$.

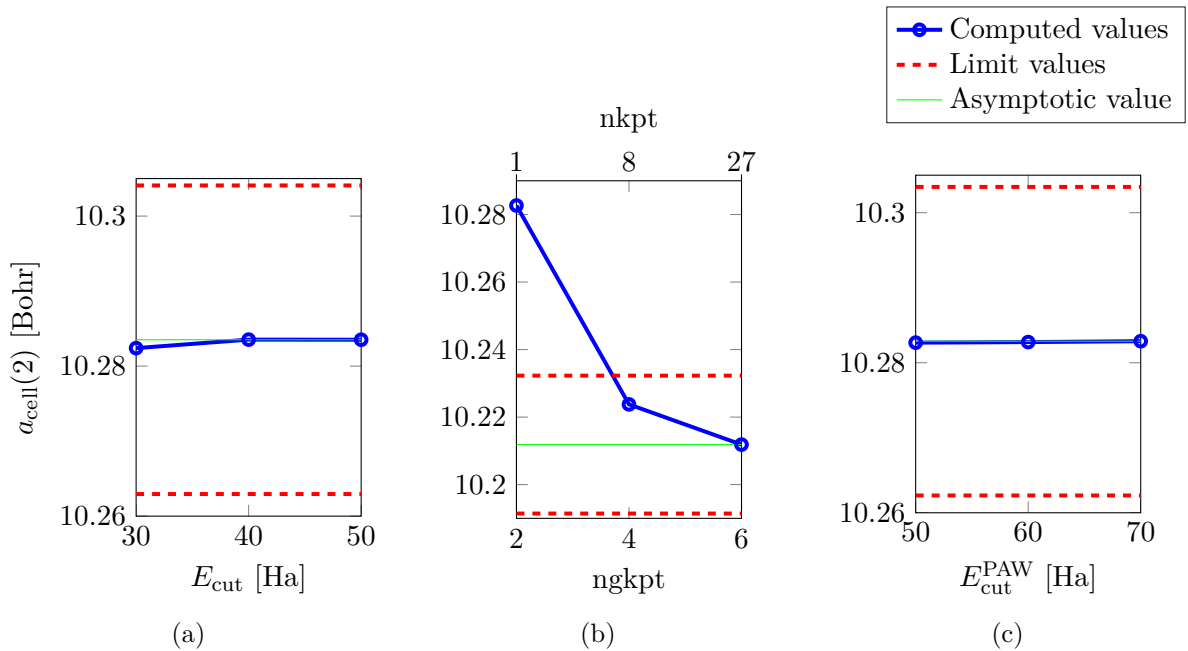


Figure D.11: Convergence study of $a_{\text{cell}}(2)$ of SrCrO_3 as a function of (a) E_{cut} , (b) the number of k points and (c) $E_{\text{cut}}^{\text{PAW}}$.

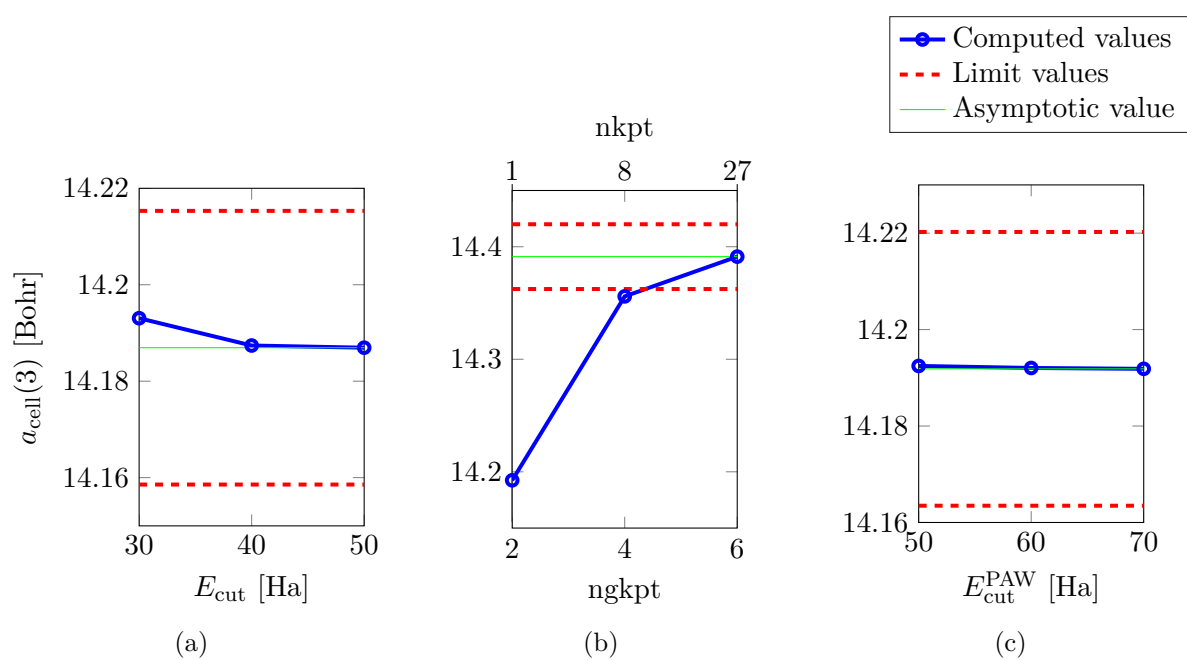


Figure D.12: Convergence study of $a_{\text{cell}}(3)$ of SrCrO_3 as a function of (a) E_{cut} , (b) the number of k points and (c) $E_{\text{cut}}^{\text{PAW}}$.