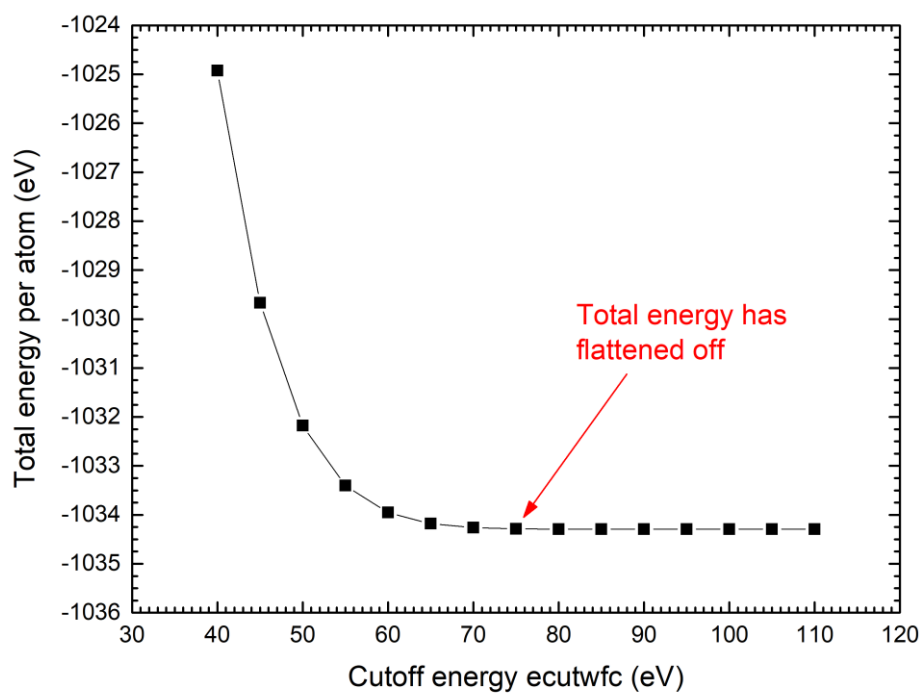


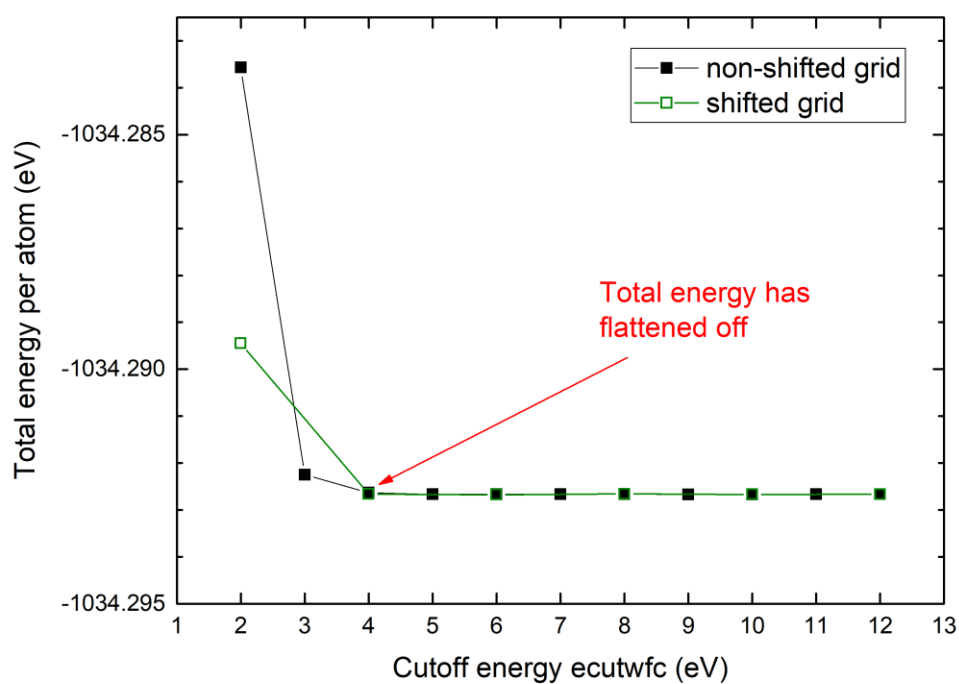
## Solutions for exercise sheet 1

### Exercise 1: Convergence test on magnesia (MgO)

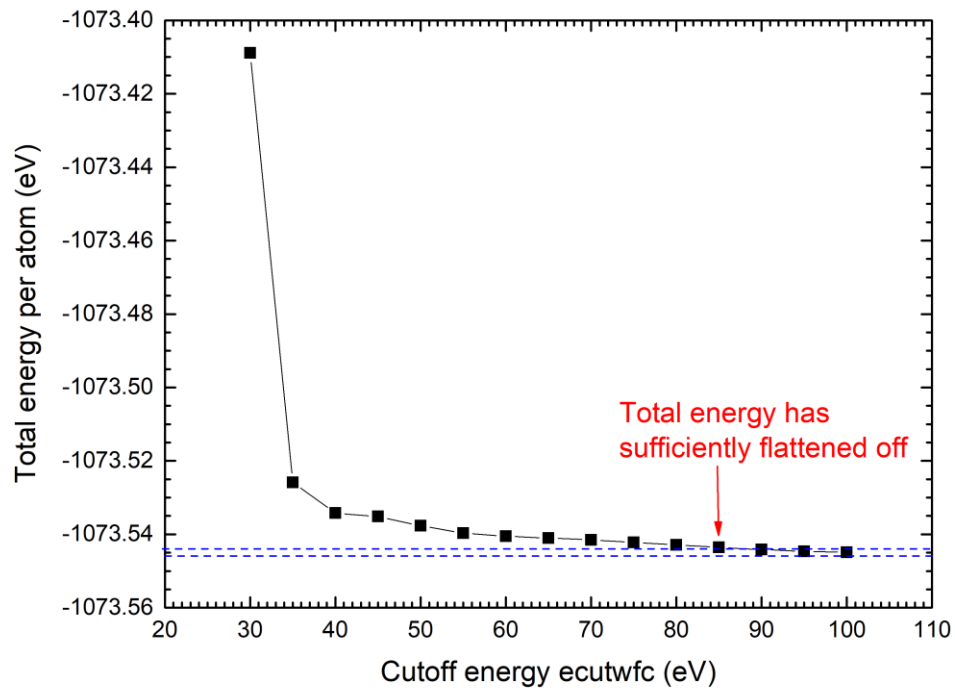
(a)



(b) & (c)



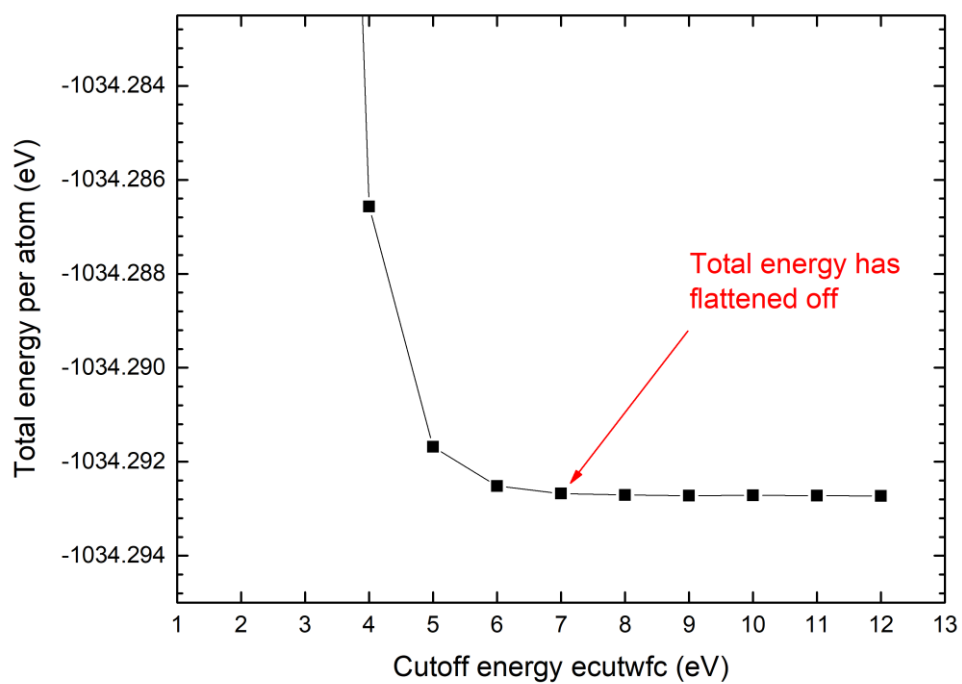
(d)



	ecutrho=4x ecutwfc	ecutrho=8x ecutwfc	ecutrho=12x ecutwfc
ecutwfc=85.0 Ry	-1073.5436 eV	-1073.54359 eV	-1073.54357 eV

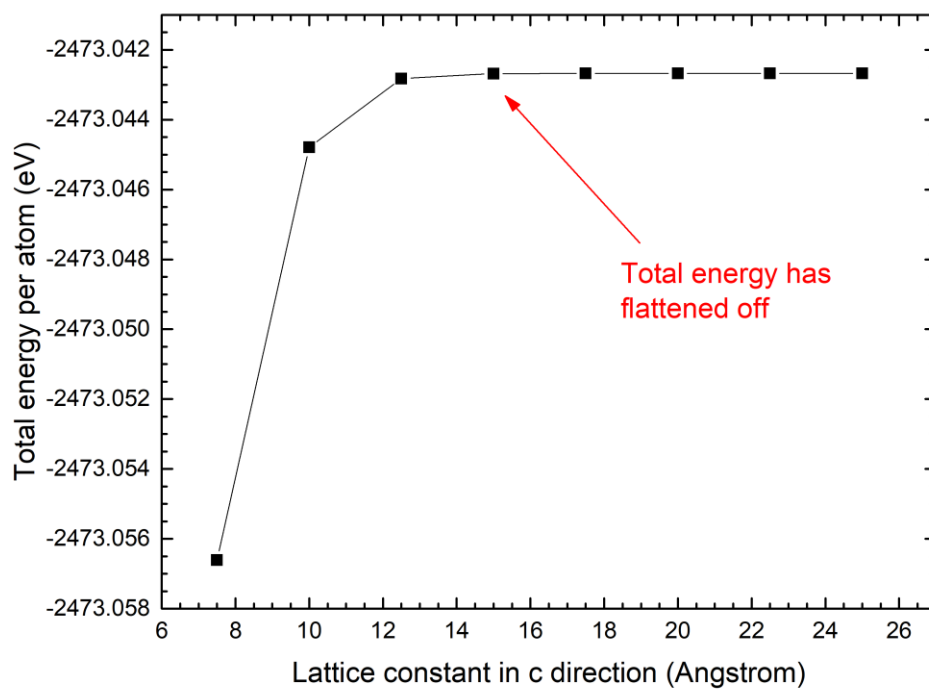
The choice of 8x  $ecutwfc$  made sense, one could have even used less (but this is usually not the case)

(e)



## Exercise 2: Convergence test on 2D antimony

(a)



(b)

