Study of the relaxation of the Al (100) surface via Ab Initio simulations

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1 Introduction

The aim of this report is use Ab Initio (AI) methods to study the surface of an Aluminum crystal. In order to do this the Quantum Espresso [1] will be used to first find the bulk value of the lattice constant for Al and then simulate a surface to study its relaxation from the bulk configuration.

2 Estimation of the bulk lattice constant

The Al crystal has an fcc structure and the idea to find the bulk lattice constant a is to simulate the crystal at different values of a and for each of them compute the pressure P resulting on the system. At this point data can be fitted with the Murnaghan equation of state:

$$P(V) = \frac{K_0}{K_0'}\left(\left(\frac{V}{V_0}\right)^{-K_0'} - 1\right)$$

where V is the volume of the unit cell and V_0 the one at equilibrium, while the bulk modulus is $K = -V\left(\frac{\partial P}{\partial V}\right)_T \approx K_0 + K_0' P$

2.1 Optimization of the simulation parameters

References

[1] P. Giannozzi et al. *Quantum Espresso* `http://www.quantum-espresso.org`

[2] Wikipedia *Murnaghan equation of state* `https://en.wikipedia.org/wiki/Murnaghan_equation_of_state`