Practical Density Functional Theory

I. Abdolhosseini Sarsari[1],

[1] Department of Physics
Isfahan University of Technology

April 29, 2015

Collaborators at IUT : M. Alaei and S. J. Hashemifar

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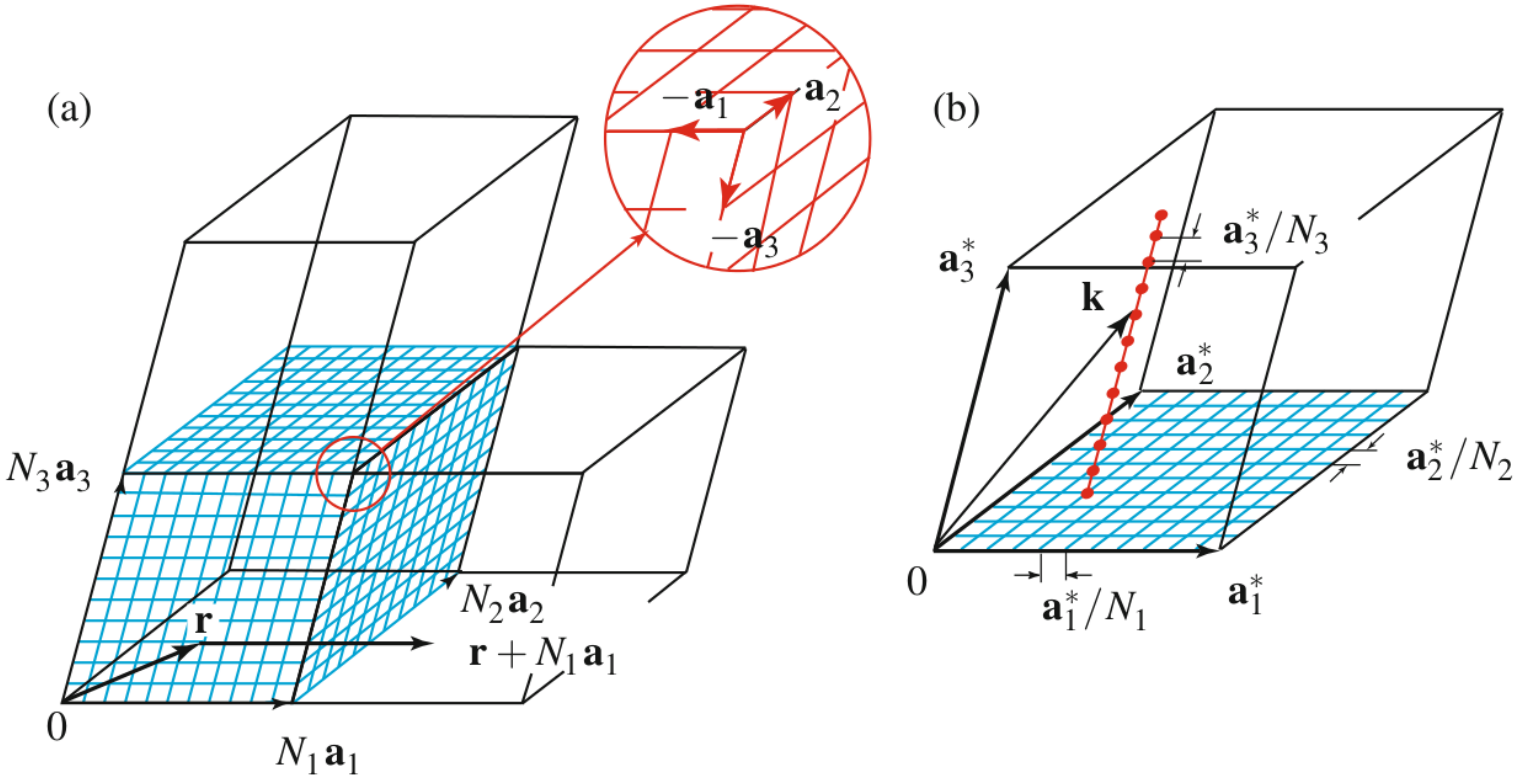
Properties like the electron density, total energy, etc. can be evaluated by integration over k inside the BZ.

$$\bar{f}_i = \frac{1}{\Omega}\int_{BZ} d\vec{k} f_i(\vec{k})$$

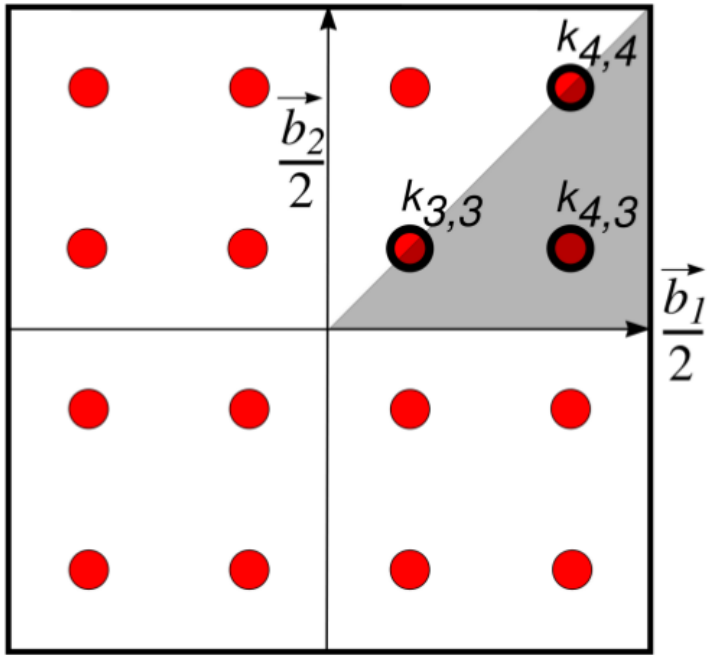
$$\bar{f}_i = \frac{1}{N_k}\Sigma_{\vec{k}} f_i(\vec{k})$$

$$\bar{f}_i = \Sigma_k w_{\vec{k}} f_i(\vec{k})$$



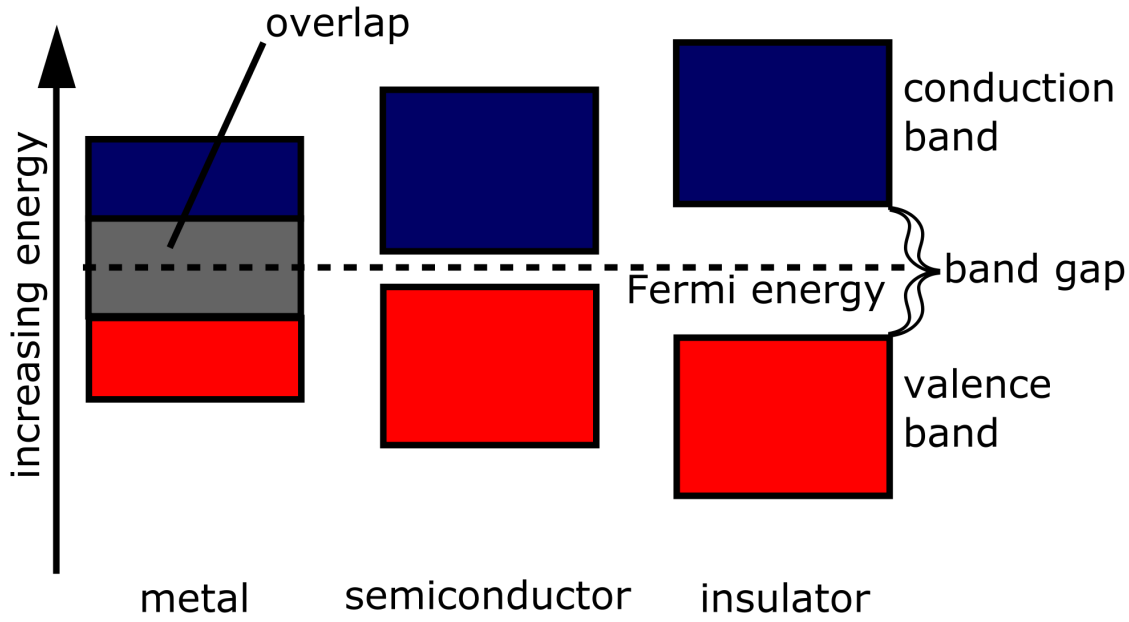
Example:

$$\bar{f}_i = \Sigma_k w_{\vec{k}} f_i(\vec{k})$$



$$\bar{f}_i = \frac{1}{4} f_i(\vec{k}_{4,4}) + \frac{1}{4} f_i(\vec{k}_{3,3}) + \frac{1}{2} f_i(\vec{k}_{4,3})$$

$$\bar{f}_i = \Sigma_{\vec{k}} w_{\vec{k}} f_i(\vec{k}) \theta(\epsilon_i(\vec{k}) - \epsilon_F)$$



- In a Semiconductor: density of states vanish smoothly before the gap.
- In a Metal: Brillouin zone can be divided into regions that are occupied and unoccupied by electrons.

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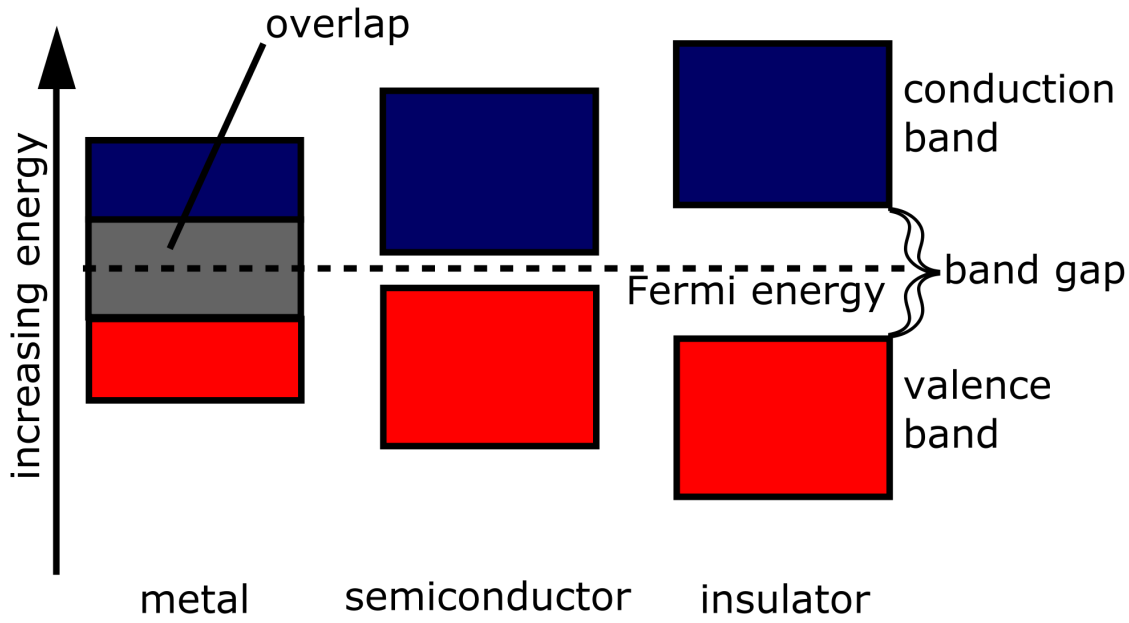

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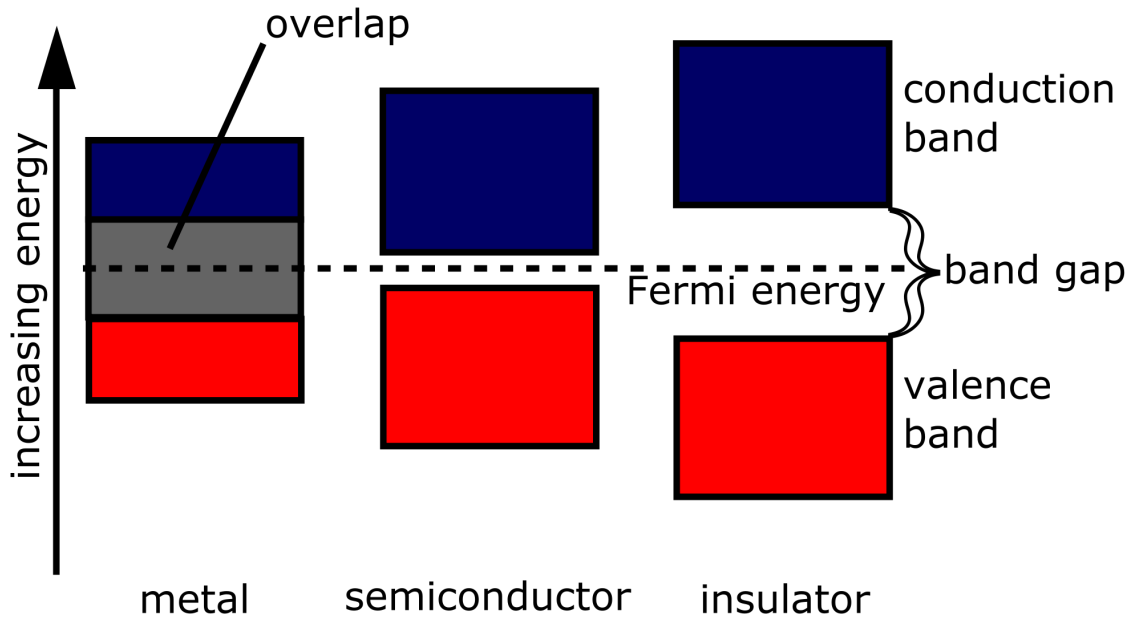

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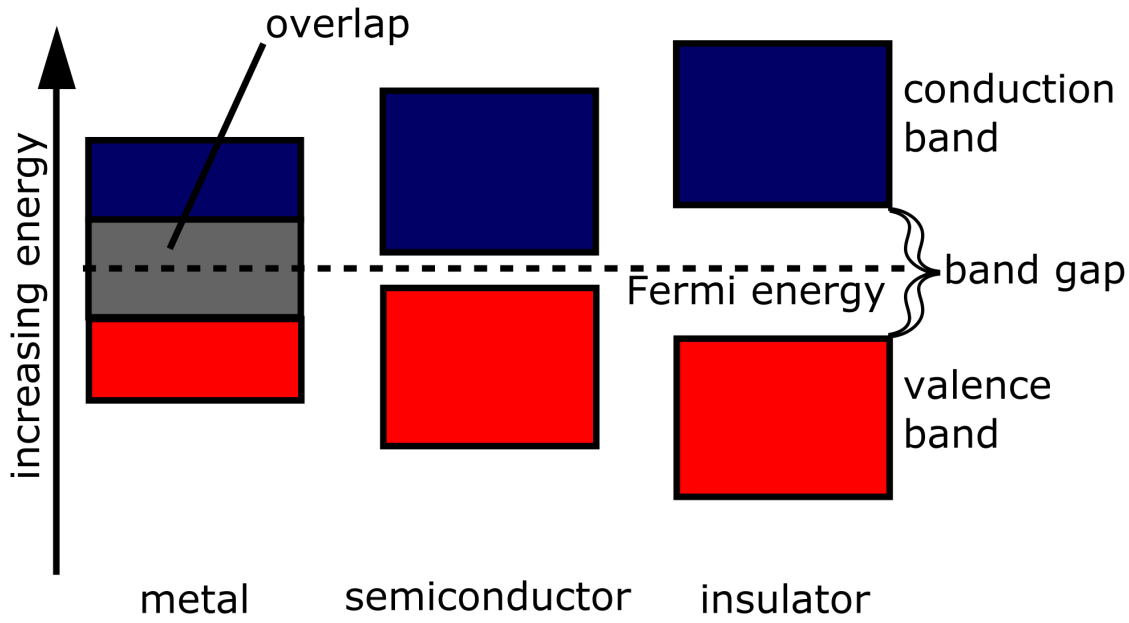

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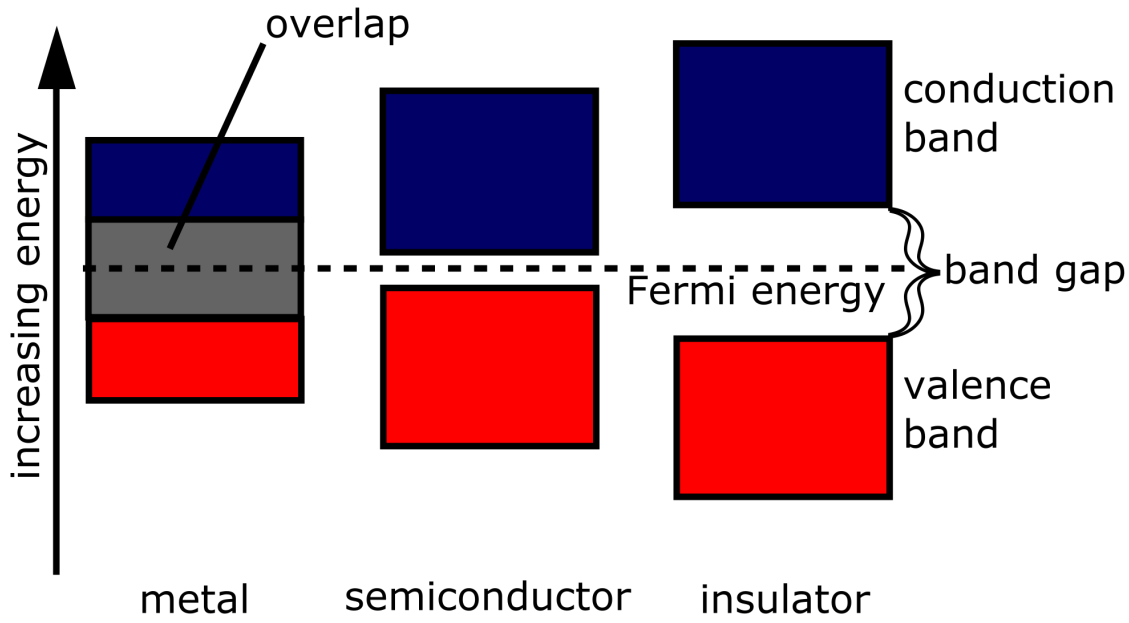

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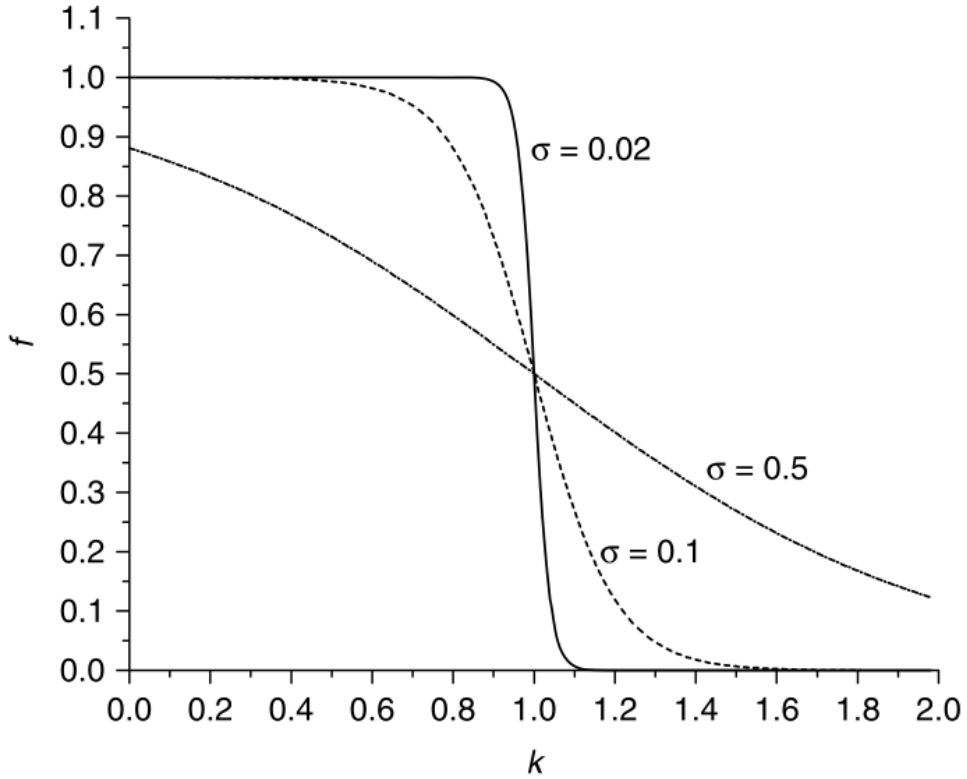
Tetrahedron method

The idea of these methods is to force the function being integrated to be continuous by smearing out the discontinuity.
An example of a smearing function: Fermi-Dirac function.

$$f(\frac{k-k_0}{\sigma}) = [exp(\frac{k-k_0}{\sigma}) + 1]^{-1}$$



Smearing method parameters

- Fermi-Dirac smearing
  Reduced occupancies below ϵ_F are not compensated new occupancies above ϵ_F .
- Gaussian smearing
  Smearing parameter, σ has no physical interpretation.
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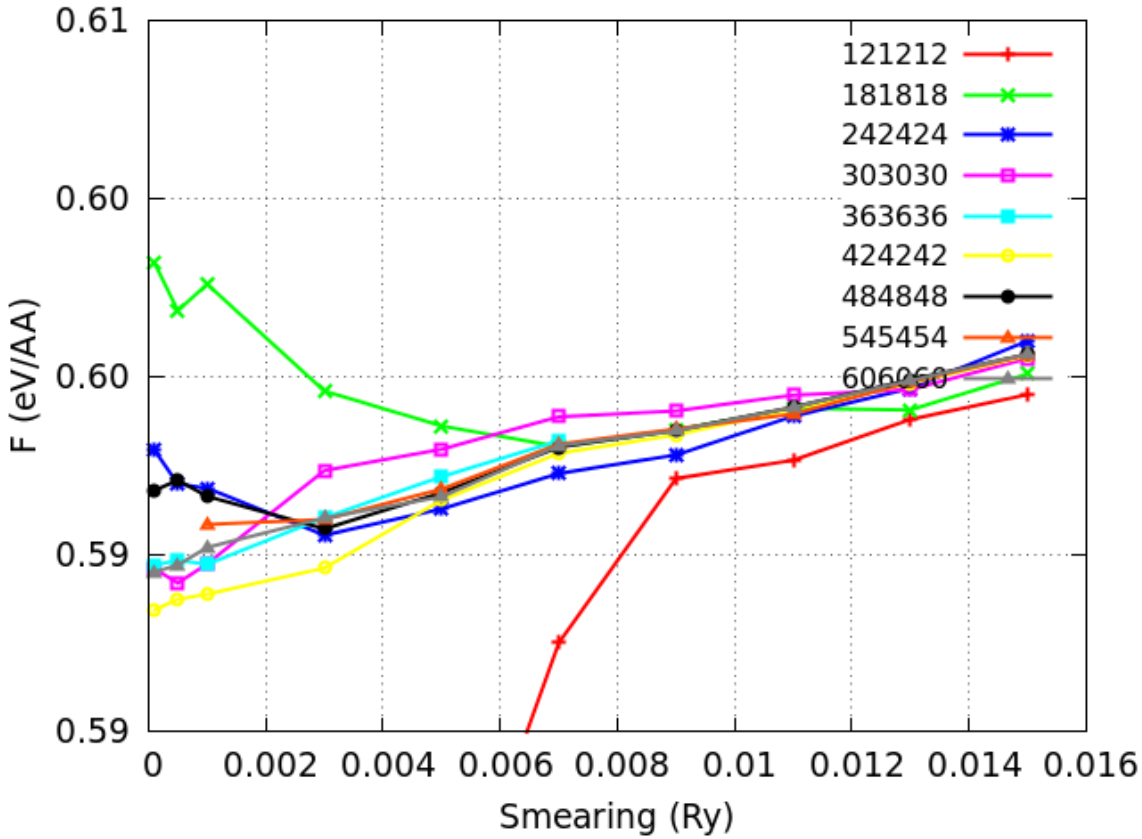

Figure: Force acting on an iron atom in a 2-atom unit cell, plotted as a function of smearing and for different Monkhorst-Pack samplings of the Brillouin Zone (different colored curves). The 2-atom simple cubic cell breaks symmetry with a displacement along the (111) direction by 5 percent of the initial 1NN atomic distance. Here we use a PAW pseudo potential (pslibrary 0.2.1) with a PBE parametrization for the XC functional and Marzari-Vanderbilt smearing [Marzari Lectures].