Plots of the Pd workfunction vs ecut

The first plot, Figure 1, is simply a plot of the Pd workfunction as a function of the number of plane waves – ecut – ranging from 6 to 60 Ha. The workfunction does not monotonically approach a convergent limit for values of ecut investigated, though the last 3 values with an average of

Figure 1

5.64586±0.00077 eV appear to be doing just that.

I then took the value of the workfunction at ecut = 60 (5.645031 eV) and subtracted it from all the others. Plotting this difference on a log-linear plot gives Figure 2. Note that the value of the differences for ecut = 26 and 28 are negative and therefore don’t appear in the figure. The difference covers a range of several orders of magnitude for the values of ecut investigated.

Figure 2

In the last graph, Figure 3, I have plotted the percent difference between the workfunction at ecut = 60





 Figure 3

and all the other values of the workfunction. Again values for ecut = 26 and 28 don’t appear on the graph, because they are negative.

The 1 DM file for a 3 layer slab and 7 layers of vacuum with ecut = 8. The vacuum region from a depth of 50 to 150 is very choppy.

Same run but ecut = 56. Here the vacuum region is from a depth of 90 to 300. Notice how smooth the vacuum region is compared to ecut = 8. The vacuum region is still slightly oscillating.

