Scalar and fully relativistic pseudopotential theory. SISSA 2019-2020

January 18, 2021

1 Analysis of the W Pseudopotential

In this exercise we analyze the W pseudopotential (PP) `W.pz-spn-rrkjus_psl.1.0.0.UPF` of `pslibrary`. Our goal will be to plot the main quantities that characterize the pseudopotential and to test its transferability and the absence of ghost states. Moreover we want to test the properties of this PP in the bcc-W and in a two-dimensional hexagonal layer of W.

After unpacking the file `pslibray.1.0.0.tar.gz` that you find at the web page `https://dalcorso.github.io/pslibrary`, generate the W PP by editing the file `make.ps` and choosing as element `W.`.

1. The PP is generated by running the `ld1.x` code with the input that can be found in the directory `WORK`. Identify the parameters given in the input file by reading the documentation of the `ld1.x` code.

2. Using the code `ld1.x`, plot the all-electron and pseudo wavefunctions for the W atom. In this plot mark the cut-off radii used for each orbital angular momentum l.

3. Using the code `ld1.x`, plot the all-electron and pseudo logarithmic derivatives for the s, p, and d angular momenta at $R = 2.0$ a.u.. Compare these logarithmic derivatives and identify the range of energies in which the two are similar.

4. Perform a few transferability tests using `iswitch=2` in the `ld1.x` input by considering electronic configurations different from the one used for the PP generation: $[Xe]4f^{14}6s^2 6p^0 5d^4$. Consider only configurations whose energy differ less than 1 Ry from that of the reference configuration. For instance you can consider $5s^2 5p^6 5d^4 6s^1 6p^1$ or the ionized configuration $5s^2 5p^6 5d^3 6s^2 6p^0$. Compare the all-electron and pseudo eigenvalues on these configurations. Discuss the transferability of the PP.

5. Identify the main functions contained in the PP file: radial mesh, all-electron wavefunctions, pseudo wavefunctions, projector functions, augmentation functions. Plot them as a function of the radial mesh.

6. Now use the PP in a plane wave calculation of the lattice constant of bcc-W using the `pw.x` code of Quantum Espresso. Check the convergence of the results with the kinetic energy cut-off of the wavefunctions and of the charge density. Determine the cut-offs necessary to converge the lattice constant within 0.005 Å. Discuss also the convergence with **k**-points and smearing.

7. Repeat the same calculation for an hexagonal monolayer of W. Take a hexagonal Bravais lattice with very large c/a so that different monolayers do not interact and determine the equilibrium value of the Bravais lattice parameter a. Recheck, for this geometry, the convergence of the result with the kinetic energy cut-offs.

8. (Optional) Check if it is possible to improve the PP so that the calculations at points 7 and 8 converge with lower kinetic energy cut-offs, by changing only one parameter of the PP, such as a cut-off radius or one reference energy. Recheck the transferability of the PP. For each parameter, determine the allowed range of variation, after which either the PP cannot be generated or its transferability becomes very poor.

Hint: Consult the directory `atomic/Doc` for the description of the input variables of the `ld1.x` code.