Atomic dataset generation – atompaw

User's guide: /home/natalie/ForPHY752/pgms/graphatom/doc/atompaw-usersguide.pdf

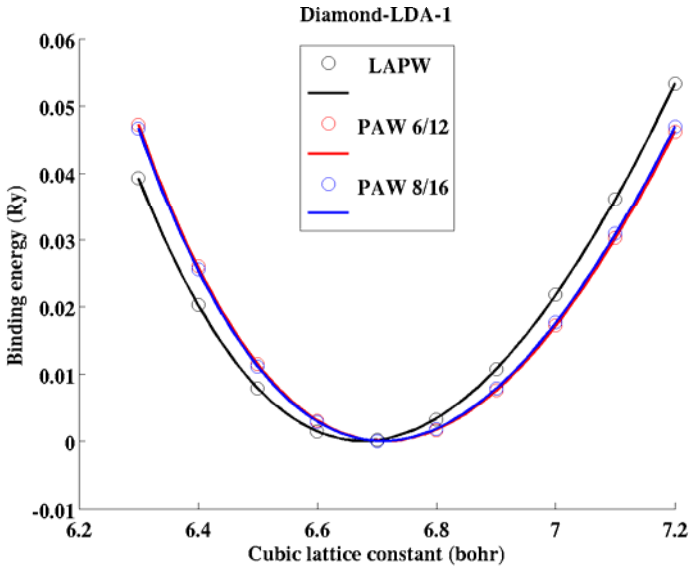
Input file for *atompaw*

In red, mandatory arguments
In green, optional arguments

Keywords are in normal font
Numbers are in italics

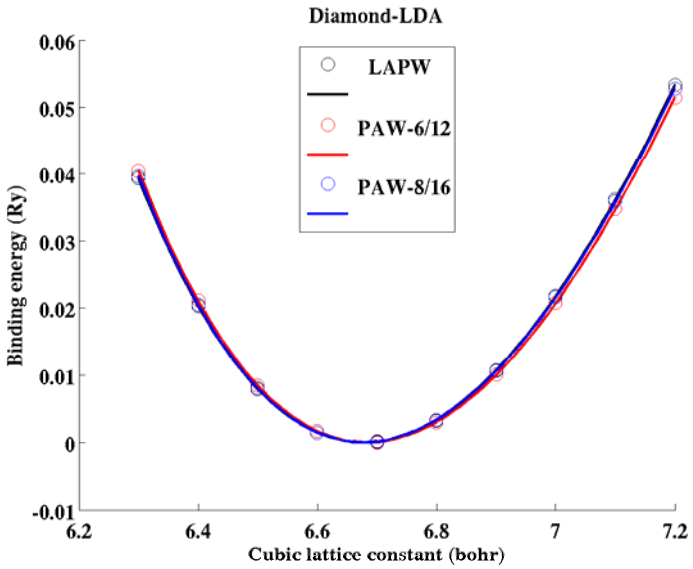
```
Atom_name Z
XC_functional rel_keyword nucleus_keyword grid_keyword logderivrange
n_s^max n_p^max n_d^max n_f^max n_g^max
n l occ_n1                          } One line for each empty or
n l occ_n2                          } partially occupied (n,l) state
...
0 0 0
c or v                              } One line for each (n,l) state
c or v                              }   l=0 states first
c or v                              }   then l=1 states...
c or v                              }
c or v                              }
...
                                    Atomic all-electrons computation
l_max
r_paw r_shape r_vloc r_core
y                                   } Repeated for each additional l=0 partial-wave
E_ref                               }
n
y                                   } Repeated for each additional l=1 partial-wave
E_ref                               }
n                                   } One paragraph for each 0 ≤ l ≤ l_max
...
y                                   } Repeated for each additional l=l_max partial-
E_ref                               }
n
projector_keyword ps_scheme ortho_scheme shapefunction
l_loc E_loc Vloc_scheme
rc_1                                } If projector_keyword ≠ "Bloechl"
rc_2                                } One line for each partial-wave
...
rc_basis_size
                                    Partial-waves basis generation
1
n l occ_n1                          } One line for each empty or
n l occ_n2                          } partially occupied (n,l) state
...                                 } As many times as desired
0 0 0
                                    Test configurations
2                                   Output for ABINIT
coreWF_keyword proj_optim_keyword comp_in_XC_keyword reduced_grid_keyword
3                                   Output for PWscf
UPF_grid_keywords
0
                                    Output for various codes
```

Atomic datasets for PAW calculations
Example: Diamond




```
C  6
LDA-PW  loggrid 2001
2 2 0 0 0 0
2 1 2
0 0 0
c
v
v
1
1.3
n
n
VANDERBILT
2 0
1.30
1.30
0
```

Atomic datasets for PAW calculations
Example: Diamond




```
C  6
LDA-PW  loggrid 2001
2 2 0 0 0 0
2 1 2
0 0 0
c
v
v
1
1.3
y
16
n
y
10
n
VANDERBILT
2 0
1.30
1.30
1.30
1.30
0
```

Murnaghan Equation:

$$E(V) = E_0 + \frac{B_0 V}{B_0'}\left(\frac{(V_0/V)^{B_0'}}{B_0' - 1} + 1\right) - \frac{B_0 V_0}{B_0' - 1}.$$

Many substances have a fairly constant B'_0 of about 3.5.

F.D. Murnaghan, 'The Compressibility of Media under Extreme Pressures', in *Proceedings of the National Academy of Sciences*, vol. 30, pp. 244–247, 1944.