PWDFT.jl: Density Functional Theory Calculations with Julia

Fadjar Fathurrahman

Engineering Physics Department
Research Center for Nanoscience and Nanotechnology
Institut Teknologi Bandung

20 April 2018

Codes for DFT

- using Fortran, C, C++: ABINIT, VASP, Quantum Espresso
- Python: GPAW

PWDFT.jl

- A package for doing DFT calculations using Julia
- plane wave basis + pseudopotentials (norm-conserving)
- LDA and GGA functionals can be used (via LibXC)
- symmetry detection (via SPGLIB)
- algorithms: SCF and Emin (PCG and DCM)

Aim

- Friendly-to-develop DFT package
- quick development for testing various algorithms

Example: hydrogen molecule in a box

```
using PWDFT
atoms = Atoms( xyz_file="H2.xyz",
               LatVecs=gen_lattice_sc(16.0) )
pspfiles = ["../pseudopotentials/pade_gth/H-q1.gth"]
ecutwfc = 15.0
Ham = Hamiltonian( atoms, pspfiles, ecutwfc )
KS_solve_SCF!( Ham )
```

Converged Kohn-Sham energy components

PWDFT.jl's result:

```
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Final Kohn-Sham energies:
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Kinetic    energy:       1.0100082964
Ps_loc     energy:      -2.7127874818
Ps_nloc    energy:       0.0000000000
Hartree    energy:       0.9015209348
XC         energy:      -0.6314251867
PspCore    energy:      -0.0000012675
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Electronic energy:      -1.4326847047
NN         energy:       0.3131700043
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Total      energy:      -1.1195147004
```

ABINIT's result:

```
 Components of total free energy (in Hartree) :

    Kinetic energy  =  1.01004059294567E+00
    Hartree energy  =  9.01545039301481E-01
    XC energy       = -6.31436384237843E-01
    Ewald energy    =  3.13170052325859E-01
    PspCore energy  = -1.26742500464741E-06
    Loc. psp. energy= -2.71283243086241E+00
    NL   psp  energy=  0.00000000000000E+00
    >>>>>>>>> Etotal= -1.11951439795224E+00
```

SCF options

Various mixing methods

Various diagonalization schemes

ChebySCF

Direct energy minimization

For systems with band gaps:

Conjugate gradient