

PWDFT.jl: Density Functional Theory Calculations with Julia

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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:

```
-----  
Final Kohn-Sham energies:  
-----  
  
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  
-----  
Electronic energy:     -1.4326847047  
NN          energy:      0.3131700043  
-----  
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= 0.000000000000000E+00  
>>>>>>> Etot= -1.11951439795224E+00
```