PWDFT.jl: Density Functional Theory Calculations with Julia

Fadjar Fathurrahman

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

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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

```
using PWDFT
atoms = init_atoms_xyz("H2.xyz")
pspfiles = ["../pseudopotentials/pade_gth/H-q1.gth"]
LatVecs = 16.0*diagm( ones(3) )
ecutwfc = 15.0 # in Hartree
Ham = PWHamiltonian( atoms, pspfiles, ecutwfc, LatVecs )
Ham.energies.NN = calc_E_NN( Ham.pw, atoms, [1.0] )
KS_solve_SCF!( Ham, update_psi="CheFSI" )
```