PWDFT.jl Developer's Note

Fadjar Fathurrahman

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1 Describing an atomic system

All atomic systems are assumed to be periodic.

The definition of type `Atoms` is given below.

```
mutable struct Atoms
    Natoms::Int64
    Nspecies::Int64
    positions::Array{Float64,2}
    atm2species::Array{Int64,1}
    atsymbs::Array{String,1}
    SpeciesSymbols::Array{String,1}
    LatVecs::Array{Float64,2}
    Zvals::Array{Float64,1}
end
```

Information about `LatVecs` and `Zvals` are also available from `PWGrid` and `PsPots`. They are included to reduce number of required arguments to several functions.

Currently, the following functions are provided to initialize an `Atoms`:

```
atoms = Atoms() # dummy constructor
atoms = init_atoms_xyz(filexyz; in_bohr=false, verbose=false)
atoms = init_atoms_xyz_string(filexyz; in_bohr=false, verbose=false)
```

Note that, `LatVecs` must be set manually by:

```
atoms.LatVecs = 16*eye(3) # for example
```

`Zvals` is set when constructing `PWHamiltonian`.

Equation

$$\frac{\alpha}{\beta} \tag{1}$$

2 k-points (Bloch wave vectors)

Monkhorst-Pack grid (used for Brillouin-zone integration)

$$\sum_{i=1,2,3} \frac{2n_i - N_i - 1}{2N_i} \mathbf{b}_i \tag{2}$$

where $n_i = 1, 2, ..., N_i$ size $= (N_1, N_2, N_3)$ and the $\mathbf{b}_i$'s are reciprocal lattice vectors.

Please see file `kpoint_grid.f90` in `PW/src`.