## Hamiltonian struct definition mutable struct Hamiltonian pw::PWGrid potentials::Potentials energies::Energies rhoe::Array{Float64,2} electrons::Electrons atoms::Atoms sym\_info::SymmetryInfo rhoe\_symmetrizer::RhoeSymmetrizer pspots::Array{PsPot\_GTH,1} pspotNL::PsPotNL xcfunc::String ik::Int64 ispin::Int64 end