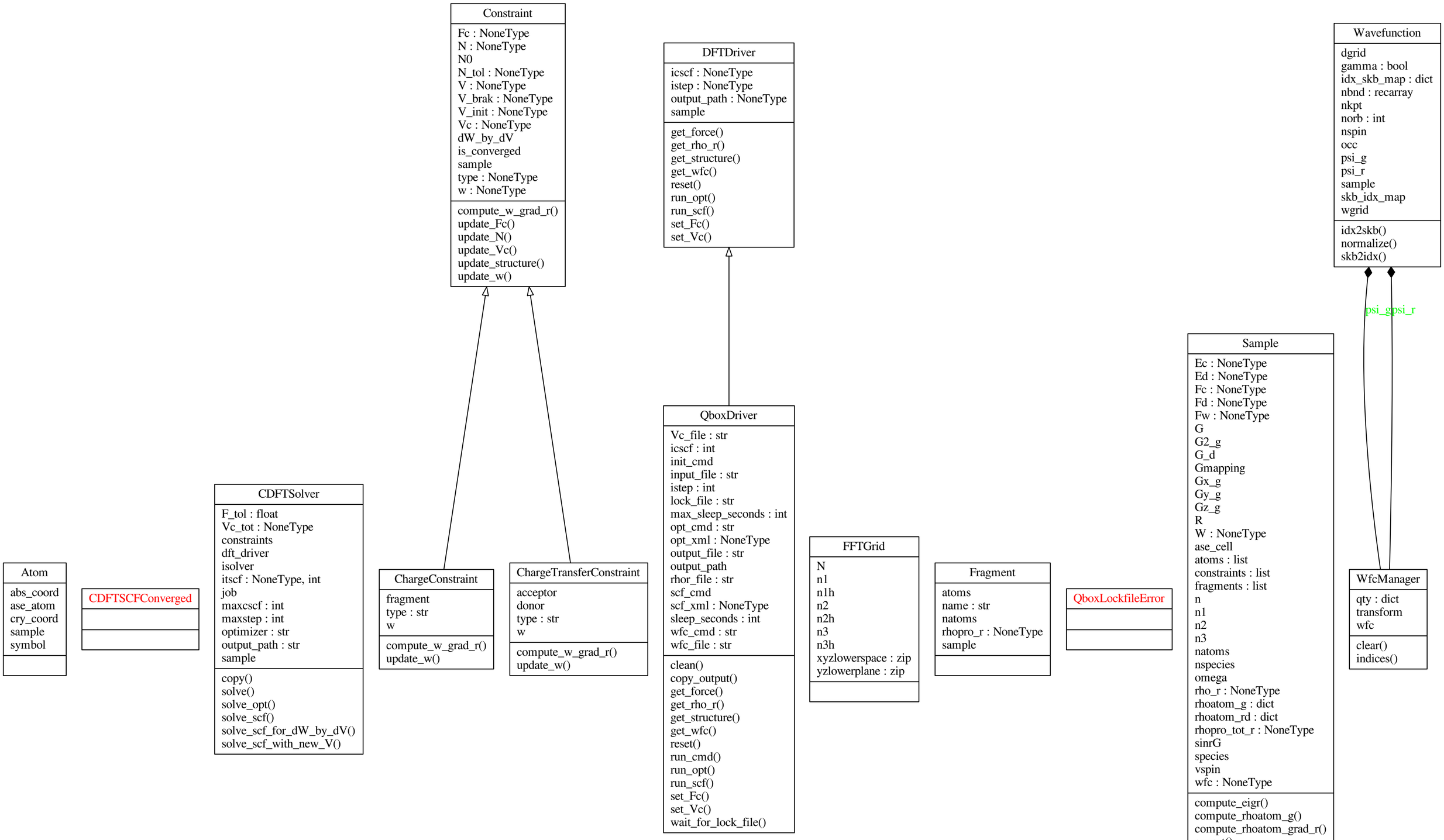
Constraint
Fc : NoneType
N : NoneType
N0
N_tol : NoneType
V : NoneType
V_brak : NoneType
V_init : NoneType
Vc : NoneType
dW_by_dV
is_converged
sample
type : NoneType
w : NoneType
compute_w_grad_r()
update_Fc()
update_N()
update_Vc()
update_structure()
update_w()
DFTDriver
icscf : NoneType
istep : NoneType
output_path : NoneType
sample
get_force()
get_rho_r()
get_structure()
get_wfc()
reset()
run_opt()
run_scf()
set_Fc()
set_Vc()
Wavefunction
dgrid
gamma : bool
idx_skb_map : dict
nbnd : recarray
nkpt
norb : int
nspin
occ
psi_g
psi_r
sample
skb_idx_map
wgrid
idx2skb()
normalize()
skb2idx()
psi_g
psi_r
Sample
Ec : NoneType
Ed : NoneType
Fc : NoneType
Fd : NoneType
Fw : NoneType
G
G2_g
G_d
Gmapping
Gx_g
Gy_g
Gz_g
R
W : NoneType
ase_cell
atoms : list
constraints : list
fragments : list
n
n1
n2
n3
natoms
nspecies
omega
rho_r : NoneType
rhoatom_g : dict
rhoatom_rd : dict
rhopro_tot_r : NoneType
sinrG
species
vspin
wfc : NoneType
compute_eigr()
compute_rhoatom_g()
compute_rhoatom_grad_r()
export()
nel()
save()
show()
update_weights()
Atom
abs_coord
ase_atom
cry_coord
sample
symbol
CDFTSCFConverged
CDFTSolver
F_tol : float
Vc_tot : NoneType
constraints
dft_driver
isolver
itscf : NoneType, int
job
maxcscf : int
maxstep : int
optimizer : str
output_path : str
sample
copy()
solve()
solve_opt()
solve_scf()
solve_scf_for_dW_by_dV()
solve_scf_with_new_V()
ChargeConstraint
fragment
type : str
w
compute_w_grad_r()
update_w()
ChargeTransferConstraint
acceptor
donor
type : str
w
compute_w_grad_r()
update_w()
QboxDriver
Vc_file : str
icscf : int
init_cmd
input_file : str
istep : int
lock_file : str
max_sleep_seconds : int
opt_cmd : str
opt_xml : NoneType
output_file : str
output_path
rhor_file : str
scf_cmd
scf_xml : NoneType
sleep_seconds : int
wfc_cmd : str
wfc_file : str
clean()
copy_output()
get_force()
get_rho_r()
get_structure()
get_wfc()
reset()
run_cmd()
run_opt()
run_scf()
set_Fc()
set_Vc()
wait_for_lock_file()
FFTGrid
N
n1
n1h
n2
n2h
n3
n3h
xyzlowerspace : zip
yzlowerplane : zip
Fragment
atoms
name : str
natoms
rhopro_r : NoneType
sample
QboxLockfileError
WfcManager
qty : dict
transform
wfc
clear()
indices()