

DFT_KIT

Generated by Doxygen 1.8.8

Sun Aug 31 2014 22:03:19

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Chapter 5

Namespace Documentation

5.1 DFT_KIT Namespace Reference

Namespaces

- [apps](#)
- [calculator](#)
- [core](#)
- [interface](#)

5.2 DFT_KIT.apps Namespace Reference

Namespaces

- [bismuth_antimony](#)
- [crystal_structure](#)
- [dft_cmdtool](#)
- [slab_surface_rhom](#)
- [wire_rhom](#)

5.3 DFT_KIT.apps.bismuth_antimony Namespace Reference

Variables

- dictionary [Sb_exp_1](#) = {'lattice_constant':4.489,'angle':(57.0+14.0/60.0)*np.pi/180.0,'rhom_u':0.2336}
- dictionary [Sb_exp_2](#) = {'lattice_constant':4.4898,'angle':(57.233)*np.pi/180.0,'rhom_u':0.23362}
- tuple [Sb](#) = element.element('Sb',121.760,51,5,vasp_pot='Sb',qes_pot="")
- tuple [Sb_d](#) = element.element('Sb',121.760,51,15,vasp_pot='Sb_d',qes_pot="")
- dictionary [Sb_vasp_scf](#) = {}
- dictionary [Sb_vasp_nscf_so](#) = {}
- dictionary [Sb_qespresso_scf](#) = {}
- dictionary [Sb_qespresso_nscf_so](#) = {}
- dictionary [Sb_wannier90](#) = {}
- dictionary [Bi_exp_1](#) = {'lattice_constant':4.7212,'angle':(57.0+19.0/60.0)*np.pi/180.0,'rhom_u':0.23407}
- dictionary [Bi_exp_2](#) = {'lattice_constant':4.7236,'angle':(57.35)*np.pi/180.0,'rhom_u':0.23407}
- dictionary [Bi_dft_1](#) = {'lattice_constant':4.7973,'angle':(53.0+56.0/60.0)*np.pi/180.0,'rhom_u':0.2348}
- dictionary [Bi_dft_2](#) = {'lattice_constant':4.7827,'angle':(56.0+17.0/60.0)*np.pi/180.0,'rhom_u':0.2351}

- dictionary `Bi_dft_3` = {'lattice_constant':4.8038,'angle':(53.0+36.0/60.0)*np.pi/180.0,'rhom_u':0.2347}
- tuple `Bi_exp` = element.element('Bi',208.9804,83,5,vasp_pot='Bi',qes_pot='Bi.UPF',rhom_length=4.↵
7236,angle=1.0009,rhom_u=0.23407)
- tuple `Bi_d` = element.element('Bi',208.9804,83,15,vasp_pot='Bi_d',qes_pot='')
- dictionary `Bi_vasp_slab_scf` = {}
- dictionary `Bi_vasp_slab_nscf_soi` = {}
- dictionary `Bi_vasp_crystal_scf` = {'ISTART':0,'ENCUT':250,'EDIFF':1E-6,'ISMEAR':-5,'SIGMA':0.2,'LM↵
AXMIX':4}
- dictionary `Bi_vasp_crystal_nscf_soi` = {'ISTART':0,'ICHARG':11,'ENCUT':250,'EDIFF':1E-6,'GGA_CO↵
MPAT':.FALSE., 'ISYM':0,'SAXIS':0 0 1,'LSORBIT':.TRUE., 'LMAXMIX':4,'MAGMOM':True}
- dictionary `Bi_qespresso_crystal_scf` = {}
- dictionary `Bi_qespresso_crystal_nscf_soi` = {}
- dictionary `Bi_qespresso_slab_scf` = {}
- dictionary `Bi_qespresso_slab_nscf_soi` = {}
- dictionary `Bi_wannier90` = {}

5.3.1 Variable Documentation

5.3.1.1 tuple `DFT_KIT.apps.bismuth_antimony.Bi_d` = element.element('Bi',208.9804,83,15,vasp_pot='Bi_d',qes_pot='')

Definition at line 53 of file `bismuth_antimony.py`.

5.3.1.2 dictionary `DFT_KIT.apps.bismuth_antimony.Bi_dft_1` = {'lattice_constant':4.7973,'angle':(53.0+56.0/60.0)*np.pi/180.↵
0,'rhom_u':0.2348}

Definition at line 47 of file `bismuth_antimony.py`.

5.3.1.3 dictionary `DFT_KIT.apps.bismuth_antimony.Bi_dft_2` = {'lattice_constant':4.7827,'angle':(56.0+17.0/60.0)*np.pi/180.↵
0,'rhom_u':0.2351}

Definition at line 48 of file `bismuth_antimony.py`.

5.3.1.4 dictionary `DFT_KIT.apps.bismuth_antimony.Bi_dft_3` = {'lattice_constant':4.8038,'angle':(53.0+36.0/60.0)*np.pi/180.↵
0,'rhom_u':0.2347}

Definition at line 49 of file `bismuth_antimony.py`.

5.3.1.5 tuple `DFT_KIT.apps.bismuth_antimony.Bi_exp` = element.element('Bi',208.9804,83,5,vasp_pot='Bi',qes_pot='Bi.UP↵
F',rhom_length=4.7236,angle=1.0009,rhom_u=0.23407)

Definition at line 52 of file `bismuth_antimony.py`.

5.3.1.6 dictionary `DFT_KIT.apps.bismuth_antimony.Bi_exp_1` = {'lattice_constant':4.7212,'angle':(57.0+19.0/60.0)*np.pi/180.↵
0,'rhom_u':0.23407}

Definition at line 43 of file `bismuth_antimony.py`.

5.3.1.7 dictionary `DFT_KIT.apps.bismuth_antimony.Bi_exp_2` = {'lattice_constant':4.7236,'angle':(57.35)*np.pi/180.0,'rhom_u'↵
:0.23407}

Definition at line 45 of file `bismuth_antimony.py`.

5.3.1.8 dictionary DFT_KIT.apps.bismuth_antimony.Bi_qespresso_crystal_nscf_soi = {}

Definition at line 62 of file bismuth_antimony.py.

5.3.1.9 dictionary DFT_KIT.apps.bismuth_antimony.Bi_qespresso_crystal_scf = {}

Definition at line 61 of file bismuth_antimony.py.

5.3.1.10 dictionary DFT_KIT.apps.bismuth_antimony.Bi_qespresso_slab_nscf_soi = {}

Definition at line 64 of file bismuth_antimony.py.

5.3.1.11 dictionary DFT_KIT.apps.bismuth_antimony.Bi_qespresso_slab_scf = {}

Definition at line 63 of file bismuth_antimony.py.

5.3.1.12 dictionary DFT_KIT.apps.bismuth_antimony.Bi_vasp_crystal_nscf_soi = {'ISTART':0,'ICHARG':11,'ENCUT':250,'EDIFF':1E-6,'GGA_COMPAT':.FALSE,'ISYM':0,'SAXIS':0 0 1,'LSORBIT':.TRUE,'LMAXMIX':4,'MAGMOM':True}

Definition at line 59 of file bismuth_antimony.py.

5.3.1.13 dictionary DFT_KIT.apps.bismuth_antimony.Bi_vasp_crystal_scf = {'ISTART':0,'ENCUT':250,'EDIFF':1E-6,'ISMEAR':-5,'SIGMA':0.2,'LMAXMIX':4}

Definition at line 58 of file bismuth_antimony.py.

5.3.1.14 dictionary DFT_KIT.apps.bismuth_antimony.Bi_vasp_slab_nscf_soi = {}

Definition at line 57 of file bismuth_antimony.py.

5.3.1.15 dictionary DFT_KIT.apps.bismuth_antimony.Bi_vasp_slab_scf = {}

Definition at line 56 of file bismuth_antimony.py.

5.3.1.16 dictionary DFT_KIT.apps.bismuth_antimony.Bi_wannier90 = {}

Definition at line 66 of file bismuth_antimony.py.

5.3.1.17 tuple DFT_KIT.apps.bismuth_antimony.Sb = element.element('Sb',121.760,51,5,vasp_pot='Sb',qes_pot='')

Definition at line 25 of file bismuth_antimony.py.

5.3.1.18 tuple DFT_KIT.apps.bismuth_antimony.Sb_d = element.element('Sb',121.760,51,15,vasp_pot='Sb_d',qes_pot='')

Definition at line 26 of file bismuth_antimony.py.

5.3.1.19 dictionary DFT_KIT.apps.bismuth_antimony.Sb_exp_1 = {'lattice_constant':4.489,'angle':(57.0+14.0/60.0)*np.pi/180.0,'rhomb_u':0.2336}

Definition at line 20 of file bismuth_antimony.py.

5.3.1.20 dictionary `DFT_KIT.apps.bismuth_antimony.Sb_exp_2 = {'lattice_constant':4.4898,'angle':(57.233)*np.pi/180.0,'rhom_u':0.23362}`

Definition at line 22 of file `bismuth_antimony.py`.

5.3.1.21 dictionary `DFT_KIT.apps.bismuth_antimony.Sb_qespresso_nscf_soi = {}`

Definition at line 33 of file `bismuth_antimony.py`.

5.3.1.22 dictionary `DFT_KIT.apps.bismuth_antimony.Sb_qespresso_scf = {}`

Definition at line 32 of file `bismuth_antimony.py`.

5.3.1.23 dictionary `DFT_KIT.apps.bismuth_antimony.Sb_vasp_nscf_soi = {}`

Definition at line 30 of file `bismuth_antimony.py`.

5.3.1.24 dictionary `DFT_KIT.apps.bismuth_antimony.Sb_vasp_scf = {}`

Definition at line 29 of file `bismuth_antimony.py`.

5.3.1.25 dictionary `DFT_KIT.apps.bismuth_antimony.Sb_wannier90 = {}`

Definition at line 35 of file `bismuth_antimony.py`.

5.4 DFT_KIT.apps.crystal_structure Namespace Reference

Classes

- class [a7_structure](#)
- class [body_center](#)
- class [diamond](#)
- class [face_center](#)
- class [graphene](#)
- class [layer_material](#)
- class [perovskite](#)
- class [rocksalt](#)

5.5 DFT_KIT.apps.dft_cmdtool Namespace Reference

Variables

- tuple [dft_job](#) = `job.job(False)`
- tuple [root_dir](#) = `os.getcwd()`
- tuple [numargs](#) = `len(sys.argv)`
- list [scriptfile](#) = `sys.argv[1]`
- tuple [input_cmd](#) = `dft_job.get_info('dft_cmdtool','input command',True)`
- tuple [cmd_first](#) = `input_cmd.split()`
- tuple [cmd_num](#) = `len(input_cmd.split())`
- tuple [cmds](#) = `input_cmd.split()`

5.5.1 Variable Documentation

5.5.1.1 tuple DFT_KIT.apps.dft_cmdtool.cmd_first = input_cmd.split()

Definition at line 35 of file dft_cmdtool.py.

5.5.1.2 tuple DFT_KIT.apps.dft_cmdtool.cmd_num = len(input_cmd.split())

Definition at line 36 of file dft_cmdtool.py.

5.5.1.3 tuple DFT_KIT.apps.dft_cmdtool.cmds = input_cmd.split()

Definition at line 37 of file dft_cmdtool.py.

5.5.1.4 tuple DFT_KIT.apps.dft_cmdtool.dft_job = job.job(False)

Definition at line 19 of file dft_cmdtool.py.

5.5.1.5 tuple DFT_KIT.apps.dft_cmdtool.input_cmd = dft_job.get_info('dft_cmdtool','input command',True)

Definition at line 33 of file dft_cmdtool.py.

5.5.1.6 tuple DFT_KIT.apps.dft_cmdtool.numargs = len(sys.argv)

Definition at line 25 of file dft_cmdtool.py.

5.5.1.7 tuple DFT_KIT.apps.dft_cmdtool.root_dir = os.getcwd()

Definition at line 22 of file dft_cmdtool.py.

5.5.1.8 list DFT_KIT.apps.dft_cmdtool.scriptfile = sys.argv[1]

Definition at line 29 of file dft_cmdtool.py.

5.6 DFT_KIT.apps.slab_surface_rhom Namespace Reference

Classes

- class [Rhom_parallel_trigonal_surface](#)
- class [Rhom_trigonal_surface](#)

5.7 DFT_KIT.apps.wire_rhom Namespace Reference

Classes

- class [Rhom_trigonal_nanowire](#)

5.8 DFT_KIT.calculator Namespace Reference

Namespaces

- [QESPRESSO](#)
- [script](#)
- [SIESTA](#)
- [VASP](#)
- [Wannier90](#)

5.9 DFT_KIT.calculator.QESPRESSO Namespace Reference

Classes

- class [calculator_QESPRESSO](#)

Variables

- string [QES_control_flags](#) = 'calculation title verbosity restart_mode wf_collect nstep iprint tstress tprnfor dt wfcdir lkpoint_dir max_seconds etot_conv_thr forc_conv_thr disk_io tefield dipfield lfield nberrycyc lorbm lberry gdir nppstr'
- string [QES_system_flags](#) = 'ibrav celldm A B C cosAB cosAC cosBC nbnd tot_charge tot_magnetization starting_magnetization ecutwfc ecutrho ecutfck nr1 nr2 nr3 nr1s nr2s nr3s nosym nosym_evc noinv no_t_rev force_symmorphic use_all_frac occupations one_atom_occupations starting_spin_angle degauss smearing nspin noncolin ecifixed qcutz q2sigma input_dft exx_fraction screening_parameter exxdiv_treatment x_gamma_extrapolation ecutvcut nqx1 nqx2 nqx3 lda_plus_u lda_plus_u_kind Hubbard_U Hubbard_J0 Hubbard_alpha Hubbard_beta Hubbard_J(i,ityp) starting_ns_eigenvalue(m,ispin,l) U_projection_type edir emaxpos eopreg eamp angle1 angle2 constrained_magnetization fixed_magnetization lambda report lspinorb assume_isolated esm_bc esm_w esm_efield esm_nfit vdw_corr london london_s6 london_rcut xdm xdm_a1 xdm_a2'
- string [QES_electrons_flags](#) = 'electron_maxstep scf_must_converge conv_thr adaptive_thr conv_thr_init conv_thr_multi mixing_mode mixing_beta mixing_ndim mixing_fixed_ns diagonalization ortho_para diago_thr_init diago_cg_maxiter diago_david_ndim diago_full_acc efield efield_cart startingpot startingwfc tqr'
- string [QES_ions_flags](#) = 'ion_dynamics ion_positions phase_space pot_extrapolation wfc_extrapolation remove_rigid_rot ion_temperature tempw tolp delta_t nraise refold_pos upscale bfgs_ndim trust_radius_max trust_radius_min trust_radius_ini w_1 w_2'
- string [QES_cell_flags](#) = 'cell_dynamics press wmass cell_factor press_conv_thr cell_dofree'
- list [QES_PW2WAN_flags](#) = ['write_amn','write_spn','write_mmn','write_unk']

5.9.1 Variable Documentation

5.9.1.1 string DFT_KIT.calculator.QESPRESSO.QES_cell_flags = 'cell_dynamics press wmass cell_factor press_conv_thr cell_dofree'

Definition at line 22 of file QESPRESSO.py.

5.9.1.2 string DFT_KIT.calculator.QESPRESSO.QES_control_flags = 'calculation title verbosity restart_mode wf_collect nstep iprint tstress tprnfor dt wfcdir lkpoint_dir max_seconds etot_conv_thr forc_conv_thr disk_io tefield dipfield lfield nberrycyc lorbm lberry gdir nppstr'

Definition at line 18 of file QESPRESSO.py.

5.9.1.3 `string DFT_KIT.calculator.QESPRESSO.QES_electrons_flags = 'electron_maxstep scf_must_converge conv_thr adaptive_thr conv_thr_init conv_thr_multi mixing_mode mixing_beta mixing_ndim mixing_fixed_ns diagonalization ortho_para diago_thr_init diago_cg_maxiter diago_david_ndim diago_full_acc efield efield_cart startingpot startingwfc tqr'`

Definition at line 20 of file QESPRESSO.py.

5.9.1.4 `string DFT_KIT.calculator.QESPRESSO.QES_ions_flags = 'ion_dynamics ion_positions phase_space pot_extrapolation wfc_extrapolation remove_rigid_rot ion_temperature tempw tol原因 delta_t nraise refold_pos upscale bfgs_ndim trust_radius_max trust_radius_min trust_radius_ini w_1 w_2'`

Definition at line 21 of file QESPRESSO.py.

5.9.1.5 `list DFT_KIT.calculator.QESPRESSO.QES_PW2WAN_flags = ['write_amn','write_spn','write_mmn','write_unk']`

Definition at line 25 of file QESPRESSO.py.

5.9.1.6 `string DFT_KIT.calculator.QESPRESSO.QES_system_flags = 'ibrav celldm A B C cosAB cosAC cosBC nbnd tot_charge tot_magnetization starting_magnetization ecutwfc ecutrho ecutfock nr1 nr2 nr3 nr1s nr2s nr3s nosym nosym_evc noinv no_t_rev force_symmorphic use_all_frac occupations one_atom_occupations starting_spin_angle degauss smearing nspin noncolin ecfixed qcutz q2sigma input_dft exx_fraction screening_parameter exxdiv_treatment x_gamma_extrapolation ecutvcut nqx1 nqx2 nqx3 lda_plus_u lda_plus_u_kind Hubbard_U Hubbard_J0 Hubbard_alpha Hubbard_beta Hubbard_J(i,ityp) starting_ns_eigenvalue(m,ispin,l) U_projection_type edir emaxpos eopreg eamp angle1 angle2 constrained_magnetization fixed_magnetization lambda report lspinorb assume_isolated esm_bc esm_w esm_efield esm_nfit vdw_corr london london_s6 london_rcut xdm xdm_a1 xdm_a2'`

Definition at line 19 of file QESPRESSO.py.

5.10 DFT_KIT.calculator.script Namespace Reference

Classes

- class [calculator_script](#)

Variables

- list [VASP_incar_flags](#)
- list [VASP_kpoints_flags](#) = []

5.10.1 Variable Documentation

5.10.1.1 `list DFT_KIT.calculator.script.VASP_incar_flags`

Initial value:

```
1 = ['NGX','NGY','NGZ','NGXF','NGYF','NGZF','NBANDS','NBLK','NWRITE',
2 'ISTART','ICHARG','ISPIN','MAGMOM','INIWAV','ENCUT','PREC','NELM',
3 'NELMIN','NELMDL','EDIFF','EDIFFG','NSW','NBLOCK','KBLOCK','IBRION',
4 'ISIF','IWAVER','ISYM','SYMPREC','LCORR','POTIM','TEBEG','TEEND',
5 'SMASS','NPACO','APACO','POMASS','ZVAL','RWIGS','NELECT','NUPDOWN',
6 'EMIN','EMAX','ISMEAR','SIGMA','ALGO','IALGO','LREAL','ROPT','GGA','VOSKOWN','DIPOL',
7 'AMIX','BMIX','WEIMIN','EBREAK','DEPER','TIME','LWAVE','LCHARG','LVTOT','LVHAR',
8 'LELF','LORBIT','NPAR','LSCALAPACK','LSCALU','LASYNC']
```

Definition at line 19 of file script.py.

5.10.1.2 list DFT_KIT.calculator.script.VASP_kpoints_flags = []

Definition at line 28 of file script.py.

5.11 DFT_KIT.calculator.SIESTA Namespace Reference

Classes

- class [calculator_SIESTA](#)

Variables

- list [SIESTA_flags](#)
- string [SIE_flags](#)

5.11.1 Variable Documentation

5.11.1.1 string DFT_KIT.calculator.SIESTA.SIE_flags

Definition at line 23 of file SIESTA.py.

5.11.1.2 list DFT_KIT.calculator.SIESTA.SIESTA_flags

Initial value:

```
1 = ['SystemName', 'SystemLabel', 'WriteMullikenPop', 'PAO.BasisType', 'PAO.EnergyShift',
2 'PAO.BasisSize', 'SpinPolarized', 'MeshCutoff', 'MaxSCFIterations', 'DM.MixingWeight', 'DM.Tolerance',
3 'DM.NumberPulay', 'DM.UseSaveDM', 'NeglNonOverlapInt', 'SolutionMethod', 'ElectronicTemperature',
4 'MD.TypeOfRun', 'MD.NumCGSteps', 'MD.MaxCGDispl', 'MD.MaxForceTol']
```

Definition at line 18 of file SIESTA.py.

5.12 DFT_KIT.calculator.VASP Namespace Reference

Classes

- class [calculator_VASP](#)

Variables

- list [VASP_incar_flags](#)
- list [VASP_kpoints_flags](#) = []

5.12.1 Variable Documentation

5.12.1.1 list DFT_KIT.calculator.VASP.VASP_incar_flags

Initial value:

```

1 = ['NGX','NGY','NGZ','NGXF','NGYF','NGZF','NBANDS','NBLK','NWRITE',
2 'ISTART','ICHARG','ISPIN','INIWAV','ENCUT','PREC','NELM','LSORBIT','GGA_COMPAT',
3 'NELMIN','NELMDL','EDIFF','EDIFFG','NSW','NBLOCK','KBLOCK','IBRION','SAXIS','LMAXMIX',
4 'ISIF','IWAVPR','ISYM','SYMPREC','LCORR','POTIM','TEBEG','TEEND',
5 'SMASS','NPACO','APACO','POMASS','ZVAL','RWIGS','NELECT','NUPDOWN',
6 'EMIN','EMAX','ISMEAR','SIGMA','ALGO','IALGO','LREAL','ROPT','GGA','VOSKOWN','DIPOL',
7 'AMIX','BMIX','WEIMIN','EBREAK','DEPER','TIME','LWAVE','LCHARG','LVTOT','LVHAR',
8 'LELF','LORBIT','NPAR','LSCALAPACK','LSCALU','LASYNC']

```

Definition at line 19 of file VASP.py.

5.12.1.2 list DFT_KIT.calculator.VASP.VASP_kpoints_flags = []

Definition at line 28 of file VASP.py.

5.13 DFT_KIT.calculator.Wannier90 Namespace Reference

Classes

- class [calculator_Wannier90](#)

Variables

- list [QES_wannier90_flags](#)

5.13.1 Variable Documentation

5.13.1.1 list DFT_KIT.calculator.Wannier90.QES_wannier90_flags

Initial value:

```

1 = ['num_wann','num_bands','unit_cell_cart','gamma_only','spinor','shell_list','search_shells','kmesh_tol',
   'postproc_setup','exclude_bands','restart','iprint','length_unit','wvfn_formatted',
2   'spin','devel_flag','timing_level','optimisation','translate_home_cell','write_xyz',
   'write_vdw_data','write_hr_diag','dis_win_min','dis_win_max','dis_froz_min','dis_froz_max','dis_num_iter',
   'dis_mix_ratio','dis_conv_tol',
3   'dis_conv_window','num_iter','num_cg_steps','conv_window','conv_tol','conv_noise_amp',
   'conv_noise_num','num_dump_cycles','num_print_cycles','write_r2mn','guiding_center','num_guide_cycles',
   'num_to_guide_iter','trial_step',
4   'fixed_step','use_bloch_phases','wannier_plot','wannier_plot_list',
   'wannier_plot_supercell','wannier_plot_format','wannier_plot_mode','wannier_plot_radius','bands_plot','kpoint_path',
   'bands_num_points','bands_plot_format','bands_plot_project',
5   'bands_plot_mode','bands_plot_dim','fermi_surface_plot','fermi_surface_num_points',
   'fermi_energy','fermi_energy_min','fermi_energy_max','fermi_energy_step','fermi_surface_plot_format','hr_plot',
   'hr_cutoff','dist_cutoff','dist_cutoff_mode',
6   'translation_center_frac','transport','transport_mode','tran_win_min','tran_win_max',
   'tran_energy_step','fermi_energy','tran_num_bb','tran_num_ll','tran_num_rr','tran_num_cc','tran_num_lc',
   'tran_num_cr','tran_num_cell_ll','tran_num_cell_rr','tran_num_bandc',
7   'tran_write_ht','tran_read_ht','tran_use_same_lead','tran_group_threshold','hr_cutoff',
   'dist_cutoff','dist_cutoff_mode','one_dim_axis','translation_center_frac']

```

Definition at line 24 of file Wannier90.py.

5.14 DFT_KIT.core Namespace Reference

Namespaces

- [atom](#)
- [calculator](#)
- [crystal_3D](#)

- [element](#)
- [env_parm](#)
- [env_parm_odyssey](#)
- [general_tool](#)
- [job](#)
- [kpoint](#)

5.15 DFT_KIT.core.atom Namespace Reference

Classes

- class [atom](#)

5.16 DFT_KIT.core.calculator Namespace Reference

Classes

- class [calculator](#)

5.17 DFT_KIT.core.crystal_3D Namespace Reference

Classes

- class [bcc_3D](#)
- class [crystal_3D](#)
Class for [crystal_3D](#).
- class [cubic_3D](#)
- class [fcc_3D](#)
- class [hexagonal_3D](#)
- class [monoclinic_3D](#)
- class [orthorhombic_3D](#)
- class [rhombohedral_3D](#)
- class [tetragonal_3D](#)
- class [triclinic_3D](#)

5.18 DFT_KIT.core.element Namespace Reference

Classes

- class [element](#)

Functions

- def [chem_number](#)
- def [chem_name](#)

Variables

- list `magic_numbers` = [2,10,18,36,54,86]
- list `periodic_table` = ['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al', 'Si', 'P', 'S', 'Cl', 'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At', 'Rn', 'Fr', 'Ra', 'Ac', 'Th', 'Pa', 'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm', 'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt', 'Ds', 'Rg', 'Uub', 'Uut', 'Uuq', 'Uup', 'Uuh', 'Uuo']
- list `Element_A` = [['H','Ne']]
- list `Element_B` = []
- list `Element_Lanthanides` = ['La','Ce','Pr','Nd','Pm','Sm','Eu','Gd','Tb','Dy','Ho','Er','Tm','Yb']
- list `Element_Actinides` = ['Ac','Th','Pa','U','Np','Pu','Am','Cm','Bk','Cf','Es','Fm','Md','No']

5.18.1 Function Documentation

5.18.1.1 `def DFT_KIT.core.element.chem_name (number)`

Definition at line 41 of file `element.py`.

5.18.1.2 `def DFT_KIT.core.element.chem_number (ele_name)`

Definition at line 35 of file `element.py`.

5.18.2 Variable Documentation

5.18.2.1 `list DFT_KIT.core.element.Element_A = [['H','Ne']]`

Definition at line 10 of file `element.py`.

5.18.2.2 `list DFT_KIT.core.element.Element_Actinides = ['Ac','Th','Pa','U','Np','Pu','Am','Cm','Bk','Cf','Es','Fm','Md','No']`

Definition at line 33 of file `element.py`.

5.18.2.3 `list DFT_KIT.core.element.Element_B = []`

Definition at line 20 of file `element.py`.

5.18.2.4 `list DFT_KIT.core.element.Element_Lanthanides = ['La','Ce','Pr','Nd','Pm','Sm','Eu','Gd','Tb','Dy','Ho','Er','Tm','Yb']`

Definition at line 32 of file `element.py`.

5.18.2.5 `list DFT_KIT.core.element.magic_numbers = [2,10,18,36,54,86]`

Definition at line 7 of file `element.py`.

```
5.18.2.6 list DFT_KIT.core.element.periodic_table = ['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al', 'Si', 'P', 'S', 'Cl',
'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo',
'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy',
'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At', 'Rn', 'Fr', 'Ra', 'Ac', 'Th', 'Pa',
'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm', 'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt', 'Ds', 'Rg', 'Uub', 'Uut', 'Uuq',
'Uup', 'Uuh', 'Uuo']
```

Definition at line 8 of file element.py.

5.19 DFT_KIT.core.env_parm Namespace Reference

Functions

- def [run_vasp_std](#)
- def [run_vasp_ncl](#)
- def [run_vasp_gamma](#)
- def [run_qespresso](#)
- def [run_siesta](#)

Variables

- list [modules_load](#) = []
- string [batch_cmd](#) = 'sbatch '
- string [vasp_std_path](#) = "
- string [vasp_complex_path](#) = "
- string [vasp_gamma_path](#) = "
- string [vasp_pseudo_dir](#) = '/home1/03051/sfang/Pseudo_Potential/VASP/'

5.19.1 Function Documentation

5.19.1.1 `def DFT_KIT.core.env_parm.run_qespresso(f_in, f_out)`

Definition at line 33 of file env_parm.py.

5.19.1.2 `def DFT_KIT.core.env_parm.run_siesta()`

Definition at line 45 of file env_parm.py.

5.19.1.3 `def DFT_KIT.core.env_parm.run_vasp_gamma()`

Definition at line 26 of file env_parm.py.

5.19.1.4 `def DFT_KIT.core.env_parm.run_vasp_ncl()`

Definition at line 21 of file env_parm.py.

5.19.1.5 `def DFT_KIT.core.env_parm.run_vasp_std()`

Definition at line 16 of file env_parm.py.

5.19.2 Variable Documentation

5.19.2.1 string `DFT_KIT.core.env_parm.batch_cmd` = 'sbatch '

Definition at line 9 of file `env_parm.py`.

5.19.2.2 list `DFT_KIT.core.env_parm.modules_load` = []

Definition at line 8 of file `env_parm.py`.

5.19.2.3 string `DFT_KIT.core.env_parm.vasp_complex_path` = ''

Definition at line 13 of file `env_parm.py`.

5.19.2.4 string `DFT_KIT.core.env_parm.vasp_gamma_path` = ''

Definition at line 14 of file `env_parm.py`.

5.19.2.5 string `DFT_KIT.core.env_parm.vasp_pseudo_dir` = '/home1/03051/sfang/Pseudo_Potential/VASP/'

Definition at line 15 of file `env_parm.py`.

5.19.2.6 string `DFT_KIT.core.env_parm.vasp_std_path` = ''

Definition at line 12 of file `env_parm.py`.

5.20 DFT_KIT.core.env_parm_odyssey Namespace Reference

Functions

- def `run_vasp_std`
- def `run_vasp_ncl`
- def `run_vasp_gamma`
- def `run_qespresso`
- def `run_siesta`

Variables

- list `modules_load` = []
- string `batch_cmd` = 'sbatch '
- string `vasp_std_path` = ''
- string `vasp_complex_path` = ''
- string `vasp_gamma_path` = ''
- string `vasp_pseudo_dir` = '/n/home09/sfang/Pseudo_Potential/VASP/'

5.20.1 Function Documentation

5.20.1.1 def `DFT_KIT.core.env_parm_odyssey.run_qespresso (f_in, f_out)`

Definition at line 27 of file `env_parm_odyssey.py`.

5.20.1.2 `def DFT_KIT.core.env_parm_odyssey.run_siesta ()`

Definition at line 33 of file `env_parm_odyssey.py`.

5.20.1.3 `def DFT_KIT.core.env_parm_odyssey.run_vasp_gamma ()`

Definition at line 22 of file `env_parm_odyssey.py`.

5.20.1.4 `def DFT_KIT.core.env_parm_odyssey.run_vasp_ncl ()`

Definition at line 19 of file `env_parm_odyssey.py`.

5.20.1.5 `def DFT_KIT.core.env_parm_odyssey.run_vasp_std ()`

Definition at line 16 of file `env_parm_odyssey.py`.

5.20.2 Variable Documentation

5.20.2.1 `string DFT_KIT.core.env_parm_odyssey.batch_cmd = 'sbatch '`

Definition at line 9 of file `env_parm_odyssey.py`.

5.20.2.2 `list DFT_KIT.core.env_parm_odyssey.modules_load = []`

Definition at line 8 of file `env_parm_odyssey.py`.

5.20.2.3 `string DFT_KIT.core.env_parm_odyssey.vasp_complex_path = ''`

Definition at line 13 of file `env_parm_odyssey.py`.

5.20.2.4 `string DFT_KIT.core.env_parm_odyssey.vasp_gamma_path = ''`

Definition at line 14 of file `env_parm_odyssey.py`.

5.20.2.5 `string DFT_KIT.core.env_parm_odyssey.vasp_pseudo_dir = '/n/home09/sfang/Pseudo_Potential/VASP/'`

Definition at line 15 of file `env_parm_odyssey.py`.

5.20.2.6 `string DFT_KIT.core.env_parm_odyssey.vasp_std_path = ''`

Definition at line 12 of file `env_parm_odyssey.py`.

5.21 DFT_KIT.core.general_tool Namespace Reference

Classes

- class [segments](#)

Functions

- def [bool_to_str](#)
- def [convert_vector](#)
- def [convert_array_2d](#)
- def [vec_to_str](#)
- def [get_unitvec](#)
- def [vec_length](#)
- def [vec_distance](#)
- def [generate_rotation_matrix](#)
- def [rot_x](#)
- def [rot_y](#)
- def [rot_z](#)
- def [rotation_matrix](#)
- def [get_parm](#)

5.21.1 Function Documentation

5.21.1.1 `def DFT_KIT.core.general_tool.bool_to_str (bool_)`

Definition at line 31 of file `general_tool.py`.

5.21.1.2 `def DFT_KIT.core.general_tool.convert_array_2d (arr)`

Definition at line 47 of file `general_tool.py`.

5.21.1.3 `def DFT_KIT.core.general_tool.convert_vector (vec)`

Definition at line 37 of file `general_tool.py`.

5.21.1.4 `def DFT_KIT.core.general_tool.generate_rotation_matrix ()`

Definition at line 84 of file `general_tool.py`.

5.21.1.5 `def DFT_KIT.core.general_tool.get_parm (ind_key, parms)`

Definition at line 121 of file `general_tool.py`.

5.21.1.6 `def DFT_KIT.core.general_tool.get_unitvec (vec)`

Definition at line 71 of file `general_tool.py`.

5.21.1.7 `def DFT_KIT.core.general_tool.rot_x (theta)`

Definition at line 89 of file `general_tool.py`.

5.21.1.8 `def DFT_KIT.core.general_tool.rot_y (theta)`

Definition at line 98 of file `general_tool.py`.

5.21.1.9 `def DFT_KIT.core.general_tool.rot_z (theta)`

Definition at line 107 of file `general_tool.py`.

5.21.1.10 `def DFT_KIT.core.general_tool.rotation_matrix (alpha, beta, gamma)`

Definition at line 116 of file `general_tool.py`.

5.21.1.11 `def DFT_KIT.core.general_tool.vec_distance (vec1, vec2)`

Definition at line 80 of file `general_tool.py`.

5.21.1.12 `def DFT_KIT.core.general_tool.vec_length (vec)`

Definition at line 77 of file `general_tool.py`.

5.21.1.13 `def DFT_KIT.core.general_tool.vec_to_str (vec)`

Definition at line 65 of file `general_tool.py`.

5.22 DFT_KIT.core.job Namespace Reference

Classes

- class [job](#)

5.23 DFT_KIT.core.kpoint Namespace Reference

Classes

- class [kpoint](#)

Functions

- def [generate_kgrid](#)

5.23.1 Function Documentation

5.23.1.1 `def DFT_KIT.core.kpoint.generate_kgrid (n1, n2, n3, write_weight = True)`

Definition at line 54 of file `kpoint.py`.

5.24 DFT_KIT.interface Namespace Reference

Namespaces

- [interface](#)
- [interface_script](#)

5.25 DFT_KIT.interface.interface Namespace Reference

Functions

- def [dft_kit_to_ase_atoms](#)
- def [dft_kit_to_ase_kpts](#)
- def [load_from_xml](#)
- def [read_mat_file](#)
- def [write_mat_file](#)
- def [DFT_postana_serieswrite_csv](#)

5.25.1 Function Documentation

5.25.1.1 def DFT_KIT.interface.interface.dft_kit_to_ase_atoms (*kit_atoms*)

Definition at line 9 of file interface.py.

5.25.1.2 def DFT_KIT.interface.interface.dft_kit_to_ase_kpts (*kit_kpts*)

Definition at line 13 of file interface.py.

5.25.1.3 def DFT_KIT.interface.interface.DFT_postana_serieswrite_csv (*series_*, *vars_*, *f_*)

Definition at line 33 of file interface.py.

5.25.1.4 def DFT_KIT.interface.interface.load_from_xml (*self*, *root_*, *findstr*, *data_*)

Definition at line 18 of file interface.py.

5.25.1.5 def DFT_KIT.interface.interface.read_mat_file (*fname*)

Definition at line 26 of file interface.py.

5.25.1.6 def DFT_KIT.interface.interface.write_mat_file (*fname*, *data_to_save*)

Definition at line 29 of file interface.py.

5.26 DFT_KIT.interface.interface_script Namespace Reference

Functions

- def [init_simulation](#)

5.26.1 Function Documentation

5.26.1.1 def DFT_KIT.interface.interface_script.init_simulation (*expect_num_parm*)

Definition at line 9 of file interface_script.py.

5.27 gen_period_table Namespace Reference

Variables

- `tt` = DFT_element.Bi
- `atm` = DFT_atom.atom
- tuple `f_` = open('pdata','r')
- list `ptable` = ['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al', 'Si', 'P', 'S', 'Cl', 'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At', 'Rn', 'Fr', 'Ra', 'Ac', 'Th', 'Pa', 'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm', 'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt', 'Ds', 'Rg', 'Uub', 'Uut', 'Uuq', 'Uup', 'Uuh', 'Uuo']
- list `data` = []
- tuple `tmpstr` = f_.readline()
- tuple `tmp`

5.27.1 Variable Documentation

5.27.1.1 gen_period_table.atm = DFT_atom.atom

Definition at line 10 of file gen_period_table.py.

5.27.1.2 list gen_period_table.data = []

Definition at line 17 of file gen_period_table.py.

5.27.1.3 tuple gen_period_table.f_ = open('pdata','r')

Definition at line 12 of file gen_period_table.py.

5.27.1.4 list gen_period_table.ptable = ['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al', 'Si', 'P', 'S', 'Cl', 'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At', 'Rn', 'Fr', 'Ra', 'Ac', 'Th', 'Pa', 'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm', 'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt', 'Ds', 'Rg', 'Uub', 'Uut', 'Uuq', 'Uup', 'Uuh', 'Uuo']

Definition at line 14 of file gen_period_table.py.

5.27.1.5 tuple gen_period_table.tmp

Initial value:

```
1 = tmpstr.find(' ')
2     if tmp>0:
3         tmpstr=tmpstr[0:tmp]
4         print (ptable[ind]+"_r=DFT_element(' " +ptable[ind]+"',"+tmpstr+' '+str(ind+1)+' '+str(ind+1)+'')
```

Definition at line 21 of file gen_period_table.py.

5.27.1.6 list gen_period_table.tmpstr = f_.readline()

Definition at line 19 of file gen_period_table.py.

5.27.1.7 `gen_period_table.tt = DFT_element.Bi`

Definition at line 8 of file `gen_period_table.py`.

5.28 gen_scripts Namespace Reference

Variables

- list `job_script` = `sys.argv[2]`
- tuple `num_parm` = `int(sys.argv[3])`
- `job_submit` = `False`
- tuple `root_dir` = `os.getcwd()`
- string `dir_prefix` = `'task'`
- string `job_name` = `'DFT_KIT_JOB'`
- int `num_cpu` = `2`
- string `job_queue` = `"normal"`
- string `job_time` = `"24:00:00"`
- list `module_load` = `[]`
- string `batch_fname` = `'DFT_KIT.batch'`
- string `task_dir` = `root_dir+dir_prefix+"_"`
- tuple `f_` = `open(batch_fname,'w')`

5.28.1 Variable Documentation

5.28.1.1 `string gen_scripts.batch_fname = 'DFT_KIT.batch'`

Definition at line 37 of file `gen_scripts.py`.

5.28.1.2 `string gen_scripts.dir_prefix = 'task'`

Definition at line 31 of file `gen_scripts.py`.

5.28.1.3 `tuple gen_scripts.f_ = open(batch_fname,'w')`

Definition at line 52 of file `gen_scripts.py`.

5.28.1.4 `string gen_scripts.job_name = 'DFT_KIT_JOB'`

Definition at line 32 of file `gen_scripts.py`.

5.28.1.5 `string gen_scripts.job_queue = "normal"`

Definition at line 34 of file `gen_scripts.py`.

5.28.1.6 `list gen_scripts.job_script = sys.argv[2]`

Definition at line 21 of file `gen_scripts.py`.

5.28.1.7 `gen_scripts.job_submit = False`

Definition at line 25 of file `gen_scripts.py`.

5.28.1.8 `string gen_scripts.job_time = "24:00:00"`

Definition at line 35 of file `gen_scripts.py`.

5.28.1.9 `list gen_scripts.module_load = []`

Definition at line 36 of file `gen_scripts.py`.

5.28.1.10 `int gen_scripts.num_cpu = 2`

Definition at line 33 of file `gen_scripts.py`.

5.28.1.11 `tuple gen_scripts.num_parm = int(sys.argv[3])`

Definition at line 22 of file `gen_scripts.py`.

5.28.1.12 `tuple gen_scripts.root_dir = os.getcwd()`

Definition at line 30 of file `gen_scripts.py`.

5.28.1.13 `string gen_scripts.task_dir = root_dir+dir_prefix+"_"`

Definition at line 44 of file `gen_scripts.py`.

5.29 QESPRESSO_band_structure_spinorbit Namespace Reference

5.30 QESPRESSO_single_calculation Namespace Reference

Variables

- tuple `test_job` = `job.job(subdir=False)`
- tuple `test_kgrid` = `kpoint.kpoint()`
- tuple `test_crystal` = `crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)`
- tuple `test_calc` = `QESPRESSO.calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=1)`

5.30.1 Variable Documentation

5.30.1.1 `tuple QESPRESSO_single_calculation.test_calc = QESPRESSO.calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=1)`

Definition at line 26 of file `QESPRESSO_single_calculation.py`.

5.30.1.2 `tuple QESPRESSO_single_calculation.test_crystal = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)`

Definition at line 25 of file `QESPRESSO_single_calculation.py`.

5.30.1.3 `tuple QESPRESSO_single_calculation.test_job = job.job(subdir=False)`

Definition at line 23 of file `QESPRESSO_single_calculation.py`.

5.30.1.4 tuple QESPRESSO_single_calculation.test_kgrid = kpoint.kpoint()

Definition at line 24 of file QESPRESSO_single_calculation.py.

5.31 QESPRESSO_wannier90_tb Namespace Reference

Variables

- tuple `test_job` = job.job(subdir=False)
- tuple `test_kgrid` = kpoint.kpoint()
- tuple `test_crystal` = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)
- tuple `test_calc` = QESPRESSO.calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=1)

5.31.1 Variable Documentation

5.31.1.1 tuple QESPRESSO_wannier90_tb.test_calc = QESPRESSO.calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=1)

Definition at line 25 of file QESPRESSO_wannier90_tb.py.

5.31.1.2 tuple QESPRESSO_wannier90_tb.test_crystal = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)

Definition at line 24 of file QESPRESSO_wannier90_tb.py.

5.31.1.3 tuple QESPRESSO_wannier90_tb.test_job = job.job(subdir=False)

Definition at line 22 of file QESPRESSO_wannier90_tb.py.

5.31.1.4 tuple QESPRESSO_wannier90_tb.test_kgrid = kpoint.kpoint()

Definition at line 23 of file QESPRESSO_wannier90_tb.py.

5.32 sample_run Namespace Reference

Variables

- tuple `input_parm` = interface_script.init_simulation(0)
- tuple `dft_job` = job.job(False)
- tuple `dft_lattice` = crystal_3D.cubic_3D(2.56)
- tuple `at1` = dft_lattice.add_atom(element.Bi_exp, position=np.array([0.0,0.0,0.0]),cc=3.45)
- tuple `at2` = dft_lattice.add_atom(element.Bi_exp, position=np.array([1.0,1.0,1.0]),cc=3.1415)
- tuple `dft_vasp` = VASP.calculator_VASP()

5.32.1 Variable Documentation

5.32.1.1 tuple sample_run.at1 = dft_lattice.add_atom(element.Bi_exp, position=np.array([0.0,0.0,0.0]),cc=3.45)

Definition at line 24 of file sample_run.py.

5.32.1.2 tuple `sample_run.at2 = dft_lattice.add_atom(element.Bi_exp, position=np.array([1.0,1.0,1.0]),cc=3.1415)`

Definition at line 25 of file `sample_run.py`.

5.32.1.3 tuple `sample_run.dft_job = job.job(False)`

Definition at line 20 of file `sample_run.py`.

5.32.1.4 tuple `sample_run.dft_lattice = crystal_3D.cubic_3D(2.56)`

Definition at line 23 of file `sample_run.py`.

5.32.1.5 tuple `sample_run.dft_vasp = VASP.calculator_VASP()`

Definition at line 28 of file `sample_run.py`.

5.32.1.6 tuple `sample_run.input_parm = interface_script.init_simulation(0)`

Definition at line 14 of file `sample_run.py`.

5.33 test Namespace Reference

Variables

- string [SIE_flags](#)

5.33.1 Variable Documentation

5.33.1.1 string `test.SIE_flags`

Initial value:

```
1 = 'AllocReportLevel,\
2 AtomCoorFormatOut,\
3 AtomicCoordinatesAndAtomicSpecies,\
4 AtomicCoordinatesFormat,\
5 AtomicCoordinatesOrigin,\
6 AtomicMass,\
7 BandLines,\
8 BandLinesScale,\
9 BandPoints,\
10 BasisPressure,\
11 BlockSize'
```

Definition at line 6 of file `test.py`.

5.34 test1 Namespace Reference

Variables

- tuple `test_job = DFT_job.DFT_job(subdir=False)`
- tuple `test_kgrid = DFT_kpoint.DFT_kpoint()`
- tuple `test_crystal = DFT_crystal_3D.cubic_3D(2.56)`

- tuple `test_atom1` = `test_crystal.add_atom(DFT_element.Bi, position=np.array([0.0,0.0,0.0]))`
- tuple `test_atom2` = `test_crystal.add_atom(DFT_element.Bi, position=np.array([1.0,1.0,1.0]))`
- tuple `test_atom3` = `test_crystal.add_atom(DFT_element.Sb, position=np.array([1.0,2.0,1.0]))`
- tuple `test_calc` = `DFT_calculator_VASP.DFT_calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE')`

5.34.1 Variable Documentation

5.34.1.1 tuple `test1.test_atom1` = `test_crystal.add_atom(DFT_element.Bi, position=np.array([0.0,0.0,0.0]))`

Definition at line 16 of file `test1.py`.

5.34.1.2 tuple `test1.test_atom2` = `test_crystal.add_atom(DFT_element.Bi, position=np.array([1.0,1.0,1.0]))`

Definition at line 17 of file `test1.py`.

5.34.1.3 tuple `test1.test_atom3` = `test_crystal.add_atom(DFT_element.Sb, position=np.array([1.0,2.0,1.0]))`

Definition at line 18 of file `test1.py`.

5.34.1.4 tuple `test1.test_calc` = `DFT_calculator_VASP.DFT_calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE')`

Definition at line 20 of file `test1.py`.

5.34.1.5 tuple `test1.test_crystal` = `DFT_crystal_3D.cubic_3D(2.56)`

Definition at line 15 of file `test1.py`.

5.34.1.6 tuple `test1.test_job` = `DFT_job.DFT_job(subdir=False)`

Definition at line 13 of file `test1.py`.

5.34.1.7 tuple `test1.test_kgrid` = `DFT_kpoint.DFT_kpoint()`

Definition at line 14 of file `test1.py`.

5.35 test2 Namespace Reference

Variables

- tuple `test_job` = `DFT_job.DFT_job(subdir=False)`
- tuple `test_kgrid` = `DFT_kpoint.DFT_kpoint()`
- tuple `test_crystal` = `DFT_crystal_3D.cubic_3D(2.56)`
- tuple `test_atom1` = `test_crystal.add_atom(DFT_element.Bi_exp, position=np.array([0.0,0.0,0.0]))`
- tuple `test_atom2` = `test_crystal.add_atom(DFT_element.Bi_exp, position=np.array([1.0,1.0,1.0]))`
- tuple `test_atom3` = `test_crystal.add_atom(DFT_element.Sb, position=np.array([1.0,2.0,1.0]))`
- tuple `test_calc` = `DFT_calculator_QESPRESSO.DFT_calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=0)`

5.35.1 Variable Documentation

5.35.1.1 `tuple test2.test_atom1 = test_crystal.add_atom(DFT_element.Bi_exp, position=np.array([0.0,0.0,0.0]))`

Definition at line 16 of file test2.py.

5.35.1.2 `tuple test2.test_atom2 = test_crystal.add_atom(DFT_element.Bi_exp, position=np.array([1.0,1.0,1.0]))`

Definition at line 17 of file test2.py.

5.35.1.3 `tuple test2.test_atom3 = test_crystal.add_atom(DFT_element.Sb, position=np.array([1.0,2.0,1.0]))`

Definition at line 18 of file test2.py.

5.35.1.4 `tuple test2.test_calc = DFT_calculator_QESPRESSO.DFT_calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=0)`

Definition at line 20 of file test2.py.

5.35.1.5 `tuple test2.test_crystal = DFT_crystal_3D.cubic_3D(2.56)`

Definition at line 15 of file test2.py.

5.35.1.6 `tuple test2.test_job = DFT_job.DFT_job(subdir=False)`

Definition at line 13 of file test2.py.

5.35.1.7 `tuple test2.test_kgrid = DFT_kpoint.DFT_kpoint()`

Definition at line 14 of file test2.py.

5.36 test3 Namespace Reference

Variables

- tuple `test_job` = `DFT_job.DFT_job(subdir=False)`
- tuple `test_kgrid` = `DFT_kpoint.DFT_kpoint()`
- tuple `test_crystal` = `wire_rhom.Rhom_trigonal_nanowire(DFT_element.Bi_exp,20,20,8,length_unit=1.0)`
- tuple `test_calc` = `DFT_calculator_VASP.DFT_calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE')`

5.36.1 Variable Documentation

5.36.1.1 `tuple test3.test_calc = DFT_calculator_VASP.DFT_calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE')`

Definition at line 21 of file test3.py.

5.36.1.2 tuple test3.test_crystal = wire_rhom.Rhom_trigonal_nanowire(DFT_element.Bi_exp,20,20,8,length_unit=1.0)

Definition at line 18 of file test3.py.

5.36.1.3 tuple test3.test_job = DFT_job.DFT_job(subdir=False)

Definition at line 16 of file test3.py.

5.36.1.4 tuple test3.test_kgrid = DFT_kpoint.DFT_kpoint()

Definition at line 17 of file test3.py.

5.37 VASP_band_structure Namespace Reference

Variables

- tuple [input_parm](#) = interface_script.init_simulation(0)
- tuple [test_job](#) = job.job(subdir=True)
- tuple [test_kgrid](#) = kpoint.kpoint()
- tuple [test_crystal](#) = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)
- tuple [test_calc](#) = VASP.calculator_VASP(False,[test_job](#),[test_crystal](#),[test_kgrid](#),scheme=0)

5.37.1 Variable Documentation

5.37.1.1 tuple VASP_band_structure.input_parm = interface_script.init_simulation(0)

Definition at line 15 of file VASP_band_structure.py.

5.37.1.2 tuple VASP_band_structure.test_calc = VASP.calculator_VASP(False,[test_job](#),[test_crystal](#),[test_kgrid](#),scheme=0)

Definition at line 22 of file VASP_band_structure.py.

5.37.1.3 tuple VASP_band_structure.test_crystal = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)

Definition at line 21 of file VASP_band_structure.py.

5.37.1.4 tuple VASP_band_structure.test_job = job.job(subdir=True)

Definition at line 17 of file VASP_band_structure.py.

5.37.1.5 tuple VASP_band_structure.test_kgrid = kpoint.kpoint()

Definition at line 20 of file VASP_band_structure.py.

5.38 VASP_band_structure_spinorbit Namespace Reference

Variables

- tuple [input_parm](#) = interface_script.init_simulation(0)

- tuple `test_job` = `job.job(subdir=True)`
- tuple `test_kgrid` = `kpoint.kpoint()`
- tuple `test_crystal` = `crystal_structure.a7_structure(bismuth_antimony.Bi_exp,length_unit=1.0)`
- tuple `test_calc` = `VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0)`

5.38.1 Variable Documentation

5.38.1.1 tuple `VASP_band_structure_spinorbit.input_parm` = `interface_script.init_simulation(0)`

Definition at line 14 of file `VASP_band_structure_spinorbit.py`.

5.38.1.2 tuple `VASP_band_structure_spinorbit.test_calc` = `VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0)`

Definition at line 21 of file `VASP_band_structure_spinorbit.py`.

5.38.1.3 tuple `VASP_band_structure_spinorbit.test_crystal` = `crystal_structure.a7_structure(bismuth_antimony.Bi_exp,length_unit=1.0)`

Definition at line 20 of file `VASP_band_structure_spinorbit.py`.

5.38.1.4 tuple `VASP_band_structure_spinorbit.test_job` = `job.job(subdir=True)`

Definition at line 16 of file `VASP_band_structure_spinorbit.py`.

5.38.1.5 tuple `VASP_band_structure_spinorbit.test_kgrid` = `kpoint.kpoint()`

Definition at line 19 of file `VASP_band_structure_spinorbit.py`.

5.39 VASP_ecutoff_convergence Namespace Reference

Variables

- int `expect_num_parm` = 1
- tuple `input_num_parm` = `len(sys.argv)`
- list `input_parm` = []
- tuple `e_ind` = `int(input_parm[0])`
- tuple `all_es` = `np.linspace(200,300,6)`
- list `e_now` = `all_es[e_ind]`
- tuple `test_job` = `job.job(subdir=False)`
- tuple `test_kgrid` = `kpoint.kpoint()`
- tuple `test_crystal` = `crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)`
- tuple `test_calc` = `VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE',ENCUT=`
`T=str(e_now))`

5.39.1 Variable Documentation

5.39.1.1 tuple `VASP_ecutoff_convergence.all_es` = `np.linspace(200,300,6)`

Definition at line 32 of file `VASP_ecutoff_convergence.py`.

5.39.1.2 tuple VASP_ecutoff_convergence.e_ind = int(input_parm[0])

Definition at line 31 of file VASP_ecutoff_convergence.py.

5.39.1.3 list VASP_ecutoff_convergence.e_now = all_es[e_ind]

Definition at line 33 of file VASP_ecutoff_convergence.py.

5.39.1.4 int VASP_ecutoff_convergence.expect_num_parm = 1

Definition at line 21 of file VASP_ecutoff_convergence.py.

5.39.1.5 tuple VASP_ecutoff_convergence.input_num_parm = len(sys.argv)

Definition at line 22 of file VASP_ecutoff_convergence.py.

5.39.1.6 list VASP_ecutoff_convergence.input_parm = []

Definition at line 27 of file VASP_ecutoff_convergence.py.

5.39.1.7 tuple VASP_ecutoff_convergence.test_calc = VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE',ENCUT=str(e_now))

Definition at line 38 of file VASP_ecutoff_convergence.py.

5.39.1.8 tuple VASP_ecutoff_convergence.test_crystal = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)

Definition at line 37 of file VASP_ecutoff_convergence.py.

5.39.1.9 tuple VASP_ecutoff_convergence.test_job = job.job(subdir=False)

Definition at line 35 of file VASP_ecutoff_convergence.py.

5.39.1.10 tuple VASP_ecutoff_convergence.test_kgrid = kpoint.kpoint()

Definition at line 36 of file VASP_ecutoff_convergence.py.

5.40 VASP_kgrid_convergence Namespace Reference

5.41 VASP_relaxation Namespace Reference

5.42 VASP_scan_parameters Namespace Reference

5.43 VASP_single_calculation Namespace Reference

Variables

- tuple [input_parm](#) = interface_script.init_simulation(0)

- tuple `test_job` = `job.job(subdir=False)`
- tuple `test_kgrid` = `kpoint.kpoint()`
- tuple `test_crystal` = `crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)`
- tuple `test_calc` = `VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0)`

5.43.1 Variable Documentation

5.43.1.1 tuple `VASP_single_calculation.input_parm` = `interface_script.init_simulation(0)`

Definition at line 14 of file `VASP_single_calculation.py`.

5.43.1.2 tuple `VASP_single_calculation.test_calc` = `VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0)`

Definition at line 21 of file `VASP_single_calculation.py`.

5.43.1.3 tuple `VASP_single_calculation.test_crystal` = `crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)`

Definition at line 20 of file `VASP_single_calculation.py`.

5.43.1.4 tuple `VASP_single_calculation.test_job` = `job.job(subdir=False)`

Definition at line 18 of file `VASP_single_calculation.py`.

5.43.1.5 tuple `VASP_single_calculation.test_kgrid` = `kpoint.kpoint()`

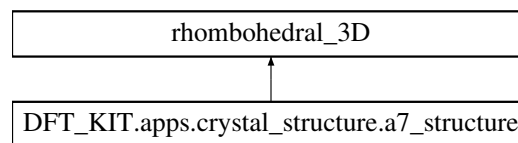
Definition at line 19 of file `VASP_single_calculation.py`.

Chapter 6

Class Documentation

6.1 DFT_KIT.apps.crystal_structure.a7_structure Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.a7_structure:



Public Member Functions

- def [__init__](#)

6.1.1 Detailed Description

Definition at line 9 of file crystal_structure.py.

6.1.2 Constructor & Destructor Documentation

6.1.2.1 def DFT_KIT.apps.crystal_structure.a7_structure.__init__(*self*, *element*, *length_unit* = 1.0, *parms*)

Definition at line 10 of file crystal_structure.py.

The documentation for this class was generated from the following file:

- apps/[crystal_structure.py](#)

6.2 DFT_KIT.core.atom.atom Class Reference

Public Member Functions

- def [__init__](#)
- def [set_magmom](#)
- def [get_magmom](#)
- def [set_position](#)

- def [get_position](#)
- def [set_parms](#)
- def [get_parms](#)
- def [remove_parm](#)

Public Attributes

- [element](#)
- [position](#)
- [magmom](#)
- [parms](#)

6.2.1 Detailed Description

Definition at line 10 of file atom.py.

6.2.2 Constructor & Destructor Documentation

6.2.2.1 `def DFT_KIT.core.atom.atom.__init__(self, element, position=np.array([0.0,0.0, parms])`

Definition at line 11 of file atom.py.

6.2.3 Member Function Documentation

6.2.3.1 `def DFT_KIT.core.atom.atom.get_magmom(self)`

Definition at line 21 of file atom.py.

6.2.3.2 `def DFT_KIT.core.atom.atom.get_parms(self, ind_parm)`

Definition at line 30 of file atom.py.

6.2.3.3 `def DFT_KIT.core.atom.atom.get_position(self)`

Definition at line 25 of file atom.py.

6.2.3.4 `def DFT_KIT.core.atom.atom.remove_parm(self, ind_parm)`

Definition at line 32 of file atom.py.

6.2.3.5 `def DFT_KIT.core.atom.atom.set_magmom(self, magmom)`

Definition at line 19 of file atom.py.

6.2.3.6 `def DFT_KIT.core.atom.atom.set_parms(self, parms)`

Definition at line 27 of file atom.py.

6.2.3.7 `def DFT_KIT.core.atom.atom.set_position (self, pos_)`

Definition at line 23 of file atom.py.

6.2.4 Member Data Documentation

6.2.4.1 `DFT_KIT.core.atom.atom.element`

Definition at line 12 of file atom.py.

6.2.4.2 `DFT_KIT.core.atom.atom.magmom`

Definition at line 14 of file atom.py.

6.2.4.3 `DFT_KIT.core.atom.atom.parms`

Definition at line 15 of file atom.py.

6.2.4.4 `DFT_KIT.core.atom.atom.position`

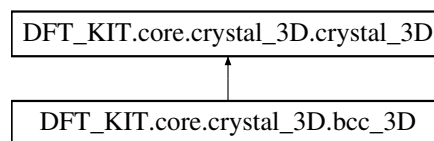
Definition at line 13 of file atom.py.

The documentation for this class was generated from the following file:

- [core/atom.py](#)

6.3 DFT_KIT.core.crystal_3D.bcc_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.bcc_3D:



Public Member Functions

- `def __init__`
- `def set_lattice`
- `def define_klabels`

Additional Inherited Members

6.3.1 Detailed Description

Definition at line 170 of file crystal_3D.py.

6.3.2 Constructor & Destructor Documentation

6.3.2.1 `def DFT_KIT.core.crystal_3D.bcc_3D.__init__(self, bcc_length, length_unit = 1.0)`

Definition at line 171 of file `crystal_3D.py`.

6.3.3 Member Function Documentation

6.3.3.1 `def DFT_KIT.core.crystal_3D.bcc_3D.define_klabels(self)`

Definition at line 183 of file `crystal_3D.py`.

6.3.3.2 `def DFT_KIT.core.crystal_3D.bcc_3D.set_lattice(self, bcc_length)`

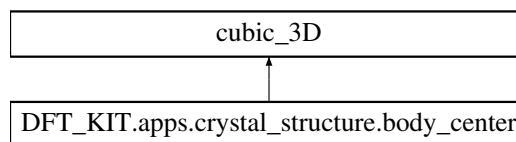
Definition at line 176 of file `crystal_3D.py`.

The documentation for this class was generated from the following file:

- [core/crystal_3D.py](#)

6.4 DFT_KIT.apps.crystal_structure.body_center Class Reference

Inheritance diagram for `DFT_KIT.apps.crystal_structure.body_center`:



Public Member Functions

- `def __init__`

6.4.1 Detailed Description

Definition at line 60 of file `crystal_structure.py`.

6.4.2 Constructor & Destructor Documentation

6.4.2.1 `def DFT_KIT.apps.crystal_structure.body_center.__init__(self, cubic_length, length_unit = 1.0)`

Definition at line 61 of file `crystal_structure.py`.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.5 DFT_KIT.core.calculator.calculator Class Reference

Public Member Functions

- def [__init__](#)
- def [run_calculation](#)
- def [get_maindir](#)
- def [set_output_dir](#)
- def [get_output_dir](#)
- def [set_parm](#)
- def [get_parm](#)
- def [load_parm](#)
- def [remove_parm](#)
- def [get_crystal](#)
- def [set_crystal](#)
- def [set_postprocess](#)
- def [clean](#)
- def [reset_simulation_data](#)

Public Attributes

- [output_dir](#)
- [crystal](#)
- [kgrid](#)
- [parms](#)
- [postprocess](#)
- [dft_job](#)
- [pre_commands](#)
- [post_commands](#)
- [output](#)

6.5.1 Detailed Description

Definition at line 12 of file calculator.py.

6.5.2 Constructor & Destructor Documentation

6.5.2.1 `def DFT_KIT.core.calculator.calculator.__init__(self, postprocess, dft_job, crystal, kgrid, parms)`

Definition at line 13 of file calculator.py.

6.5.3 Member Function Documentation

6.5.3.1 `def DFT_KIT.core.calculator.calculator.clean (self)`

Definition at line 75 of file calculator.py.

6.5.3.2 `def DFT_KIT.core.calculator.calculator.get_crystal (self)`

Definition at line 68 of file calculator.py.

6.5.3.3 `def DFT_KIT.core.calculator.calculator.get_maindir (self)`

Definition at line 47 of file calculator.py.

6.5.3.4 `def DFT_KIT.core.calculator.calculator.get_output_dir (self)`

Definition at line 52 of file calculator.py.

6.5.3.5 `def DFT_KIT.core.calculator.calculator.get_parm (self, ind_key)`

Definition at line 56 of file calculator.py.

6.5.3.6 `def DFT_KIT.core.calculator.calculator.load_parm (self, cleanup, new_parm)`

Definition at line 58 of file calculator.py.

6.5.3.7 `def DFT_KIT.core.calculator.calculator.remove_parm (self, ind_key)`

Definition at line 65 of file calculator.py.

6.5.3.8 `def DFT_KIT.core.calculator.calculator.reset_simulation_data (self)`

Definition at line 78 of file calculator.py.

6.5.3.9 `def DFT_KIT.core.calculator.calculator.run_calculation (self)`

Definition at line 32 of file calculator.py.

6.5.3.10 `def DFT_KIT.core.calculator.calculator.set_crystal (self, crystal)`

Definition at line 70 of file calculator.py.

6.5.3.11 `def DFT_KIT.core.calculator.calculator.set_output_dir (self, dir_)`

Definition at line 50 of file calculator.py.

6.5.3.12 `def DFT_KIT.core.calculator.calculator.set_parm (self, ind_key, parm_val)`

Definition at line 54 of file calculator.py.

6.5.3.13 `def DFT_KIT.core.calculator.calculator.set_postprocess (self, pp)`

Definition at line 73 of file calculator.py.

6.5.4 Member Data Documentation

6.5.4.1 `DFT_KIT.core.calculator.calculator.crystal`

Definition at line 15 of file calculator.py.

6.5.4.2 DFT_KIT.core.calculator.calculator.dft_job

Definition at line 21 of file calculator.py.

6.5.4.3 DFT_KIT.core.calculator.calculator.kgrid

Definition at line 16 of file calculator.py.

6.5.4.4 DFT_KIT.core.calculator.calculator.output

Definition at line 28 of file calculator.py.

6.5.4.5 DFT_KIT.core.calculator.calculator.output_dir

Definition at line 14 of file calculator.py.

6.5.4.6 DFT_KIT.core.calculator.calculator.parms

Definition at line 17 of file calculator.py.

6.5.4.7 DFT_KIT.core.calculator.calculator.post_commands

Definition at line 27 of file calculator.py.

6.5.4.8 DFT_KIT.core.calculator.calculator.postprocess

Definition at line 18 of file calculator.py.

6.5.4.9 DFT_KIT.core.calculator.calculator.pre_commands

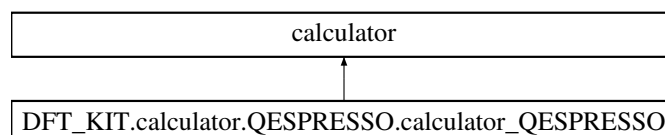
Definition at line 26 of file calculator.py.

The documentation for this class was generated from the following file:

- [core/calculator.py](#)

6.6 DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO Class Reference

Inheritance diagram for DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO:



Public Member Functions

- [def __init__](#)
- [def apply_scheme](#)

- `def run_main`
- `def qes_generate_pw2wan`
- `def generate_files`
- `def qespresso_postana_xml`
- `def post_process`
- `def run_wannier`

Public Attributes

- `wannier90_analysis`
- `write_occupations`
- `write_constraints`
- `write_atomic_forces`
- `atomic_positions_ang`

6.6.1 Detailed Description

Definition at line 29 of file QESPRESSO.py.

6.6.2 Constructor & Destructor Documentation

6.6.2.1 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.__init__(self, postprocess, dft_job, crystal, kgrid, scheme = 0, parms)`

Definition at line 30 of file QESPRESSO.py.

6.6.3 Member Function Documentation

6.6.3.1 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.apply_scheme(self, scheme)`

Definition at line 39 of file QESPRESSO.py.

6.6.3.2 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.generate_files(self)`

Definition at line 87 of file QESPRESSO.py.

6.6.3.3 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.post_process(self)`

Definition at line 224 of file QESPRESSO.py.

6.6.3.4 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.qes_generate_pw2wan(self)`

Definition at line 73 of file QESPRESSO.py.

6.6.3.5 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.qespresso_postana_xml(self)`

Definition at line 197 of file QESPRESSO.py.

6.6.3.6 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.run_main(self)`

Definition at line 68 of file QESPRESSO.py.

6.6.3.7 `def DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.run_wannier (self)`

Definition at line 227 of file QESPRESSO.py.

6.6.4 Member Data Documentation

6.6.4.1 `DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.atomic_positions_ang`

Definition at line 37 of file QESPRESSO.py.

6.6.4.2 `DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.wannier90_analysis`

Definition at line 33 of file QESPRESSO.py.

6.6.4.3 `DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.write_atomic_forces`

Definition at line 36 of file QESPRESSO.py.

6.6.4.4 `DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.write_constraints`

Definition at line 35 of file QESPRESSO.py.

6.6.4.5 `DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO.write_occupations`

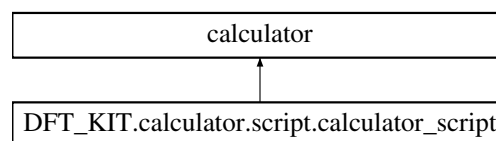
Definition at line 34 of file QESPRESSO.py.

The documentation for this class was generated from the following file:

- calculator/[QESPRESSO.py](#)

6.7 DFT_KIT.calculator.script.calculator_script Class Reference

Inheritance diagram for DFT_KIT.calculator.script.calculator_script:



Public Member Functions

- `def __init__`
- `def run_main`
- `def generate_files`
- `def post_process`

6.7.1 Detailed Description

Definition at line 30 of file script.py.

6.7.2 Constructor & Destructor Documentation

6.7.2.1 `def DFT_KIT.calculator.script.calculator_script.__init__(self, postprocess, dft_job, crystal, kgrid, parms)`

Definition at line 31 of file script.py.

6.7.3 Member Function Documentation

6.7.3.1 `def DFT_KIT.calculator.script.calculator_script.generate_files (self)`

Definition at line 40 of file script.py.

6.7.3.2 `def DFT_KIT.calculator.script.calculator_script.post_process (self)`

Definition at line 44 of file script.py.

6.7.3.3 `def DFT_KIT.calculator.script.calculator_script.run_main (self)`

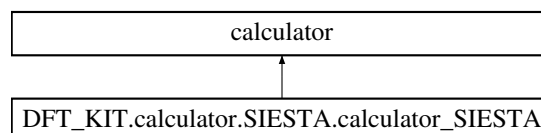
Definition at line 36 of file script.py.

The documentation for this class was generated from the following file:

- calculator/[script.py](#)

6.8 DFT_KIT.calculator.SIESTA.calculator_SIESTA Class Reference

Inheritance diagram for DFT_KIT.calculator.SIESTA.calculator_SIESTA:



Public Member Functions

- `def __init__`
- `def apply_scheme`
- `def generate_files`

6.8.1 Detailed Description

Definition at line 298 of file SIESTA.py.

6.8.2 Constructor & Destructor Documentation

6.8.2.1 `def DFT_KIT.calculator.SIESTA.calculator_SIESTA.__init__(self, postprocess, dft_job, crystal, kgrid, scheme = 0, parms)`

Definition at line 299 of file SIESTA.py.

6.8.3 Member Function Documentation

6.8.3.1 `def DFT_KIT.calculator.SIESTA.calculator_SIESTA.apply_scheme (self, scheme)`

Definition at line 302 of file SIESTA.py.

6.8.3.2 `def DFT_KIT.calculator.SIESTA.calculator_SIESTA.generate_files (self)`

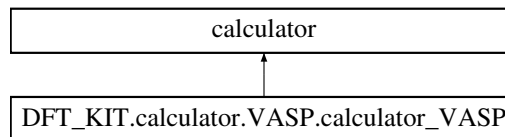
Definition at line 328 of file SIESTA.py.

The documentation for this class was generated from the following file:

- calculator/[SIESTA.py](#)

6.9 DFT_KIT.calculator.VASP.calculator_VASP Class Reference

Inheritance diagram for DFT_KIT.calculator.VASP.calculator_VASP:



Public Member Functions

- `def __init__`
- `def set_run_vasp_mode`
- `def run_main`
- `def generate_files`
- `def vasp_generate_incar`
- `def vasp_generate_poscar`
- `def vasp_generate_kpoints`
- `def apply_scheme`
- `def post_process`
- `def vasp_load_calculation_xml`
- `def vasp_postana_xml`
- `def vasp_postana_calculation`

Public Attributes

- `potcar_gen`
- `poscar_gen`
- `xc`
- `vasp_vars`
- `run_vasp_mode`
- `poscar_selective`
- `kpoint_mode`
- `vasp_band_kpoints`
- `vasp_band_kpoints_weight`
- `vasp_band_energies`
- `vasp_band_occupations`
- `vasp_dos`

6.9.1 Detailed Description

Definition at line 30 of file VASP.py.

6.9.2 Constructor & Destructor Documentation

6.9.2.1 `def DFT_KIT.calculator.VASP.calculator_VASP.__init__(self, postprocess, dft_job, crystal, kgrid, scheme = 0, parms)`

Definition at line 31 of file VASP.py.

6.9.3 Member Function Documentation

6.9.3.1 `def DFT_KIT.calculator.VASP.calculator_VASP.apply_scheme(self, scheme)`

Definition at line 177 of file VASP.py.

6.9.3.2 `def DFT_KIT.calculator.VASP.calculator_VASP.generate_files(self)`

Definition at line 57 of file VASP.py.

6.9.3.3 `def DFT_KIT.calculator.VASP.calculator_VASP.post_process(self)`

Definition at line 244 of file VASP.py.

6.9.3.4 `def DFT_KIT.calculator.VASP.calculator_VASP.run_main(self)`

Definition at line 49 of file VASP.py.

6.9.3.5 `def DFT_KIT.calculator.VASP.calculator_VASP.set_run_vasp_mode(self, mode)`

Definition at line 46 of file VASP.py.

6.9.3.6 `def DFT_KIT.calculator.VASP.calculator_VASP.vasp_generate_incar(self, f_)`

Definition at line 98 of file VASP.py.

6.9.3.7 `def DFT_KIT.calculator.VASP.calculator_VASP.vasp_generate_kpoints(self, f_)`

Definition at line 143 of file VASP.py.

6.9.3.8 `def DFT_KIT.calculator.VASP.calculator_VASP.vasp_generate_poscar(self, f_)`

Definition at line 114 of file VASP.py.

6.9.3.9 `def DFT_KIT.calculator.VASP.calculator_VASP.vasp_load_calculation_xml(self, root_cals, data_)`

Definition at line 249 of file VASP.py.

6.9.3.10 `def DFT_KIT.calculator.VASP.calculator_VASP.vasp_postana_calculation (self, item, array=False, num=-1)`

Definition at line 543 of file VASP.py.

6.9.3.11 `def DFT_KIT.calculator.VASP.calculator_VASP.vasp_postana_xml (self, parm, xmlfile='vasprun.xml')`

Definition at line 365 of file VASP.py.

6.9.4 Member Data Documentation

6.9.4.1 `DFT_KIT.calculator.VASP.calculator_VASP.kpoint_mode`

Definition at line 225 of file VASP.py.

6.9.4.2 `DFT_KIT.calculator.VASP.calculator_VASP.poscar_gen`

Definition at line 41 of file VASP.py.

6.9.4.3 `DFT_KIT.calculator.VASP.calculator_VASP.poscar_selective`

Definition at line 210 of file VASP.py.

6.9.4.4 `DFT_KIT.calculator.VASP.calculator_VASP.potcar_gen`

Definition at line 40 of file VASP.py.

6.9.4.5 `DFT_KIT.calculator.VASP.calculator_VASP.run_vasp_mode`

Definition at line 44 of file VASP.py.

6.9.4.6 `DFT_KIT.calculator.VASP.calculator_VASP.vasp_band_energies`

Definition at line 530 of file VASP.py.

6.9.4.7 `DFT_KIT.calculator.VASP.calculator_VASP.vasp_band_kpoints`

Definition at line 405 of file VASP.py.

6.9.4.8 `DFT_KIT.calculator.VASP.calculator_VASP.vasp_band_kpoints_weight`

Definition at line 410 of file VASP.py.

6.9.4.9 `DFT_KIT.calculator.VASP.calculator_VASP.vasp_band_occupations`

Definition at line 531 of file VASP.py.

6.9.4.10 `DFT_KIT.calculator.VASP.calculator_VASP.vasp_dos`

Definition at line 532 of file VASP.py.

6.9.4.11 DFT_KIT.calculator.VASP.calculator_VASP.vasp_vars

Definition at line 43 of file VASP.py.

6.9.4.12 DFT_KIT.calculator.VASP.calculator_VASP.xc

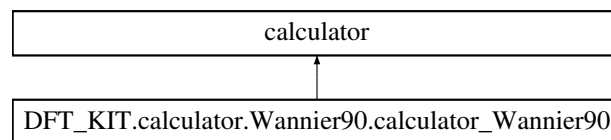
Definition at line 42 of file VASP.py.

The documentation for this class was generated from the following file:

- calculator/[VASP.py](#)

6.10 DFT_KIT.calculator.Wannier90.calculator_Wannier90 Class Reference

Inheritance diagram for DFT_KIT.calculator.Wannier90.calculator_Wannier90:



Public Member Functions

- def [__init__](#)
- def [add_projection](#)
- def [apply_scheme](#)
- def [run_main](#)
- def [generate_files](#)
- def [run_wannier](#)
- def [read_hamiltonian](#)

Public Attributes

- [projections](#)

6.10.1 Detailed Description

Definition at line 32 of file Wannier90.py.

6.10.2 Constructor & Destructor Documentation

6.10.2.1 def DFT_KIT.calculator.Wannier90.calculator_Wannier90.__init__(*self*, *postprocess*, *dft_job*, *crystal*, *kgrid*, *scheme* = 0, *parms*)

Definition at line 33 of file Wannier90.py.

6.10.3 Member Function Documentation

6.10.3.1 def DFT_KIT.calculator.Wannier90.calculator_Wannier90.add_projection(*self*, *proj*)

Definition at line 38 of file Wannier90.py.

6.10.3.2 `def DFT_KIT.calculator.Wannier90.calculator_Wannier90.apply_scheme (self, scheme)`

Definition at line 41 of file Wannier90.py.

6.10.3.3 `def DFT_KIT.calculator.Wannier90.calculator_Wannier90.generate_files (self)`

Definition at line 52 of file Wannier90.py.

6.10.3.4 `def DFT_KIT.calculator.Wannier90.calculator_Wannier90.read_hamiltonian (self)`

Definition at line 91 of file Wannier90.py.

6.10.3.5 `def DFT_KIT.calculator.Wannier90.calculator_Wannier90.run_main (self)`

Definition at line 50 of file Wannier90.py.

6.10.3.6 `def DFT_KIT.calculator.Wannier90.calculator_Wannier90.run_wannier (self)`

Definition at line 88 of file Wannier90.py.

6.10.4 Member Data Documentation

6.10.4.1 `DFT_KIT.calculator.Wannier90.calculator_Wannier90.projections`

Definition at line 36 of file Wannier90.py.

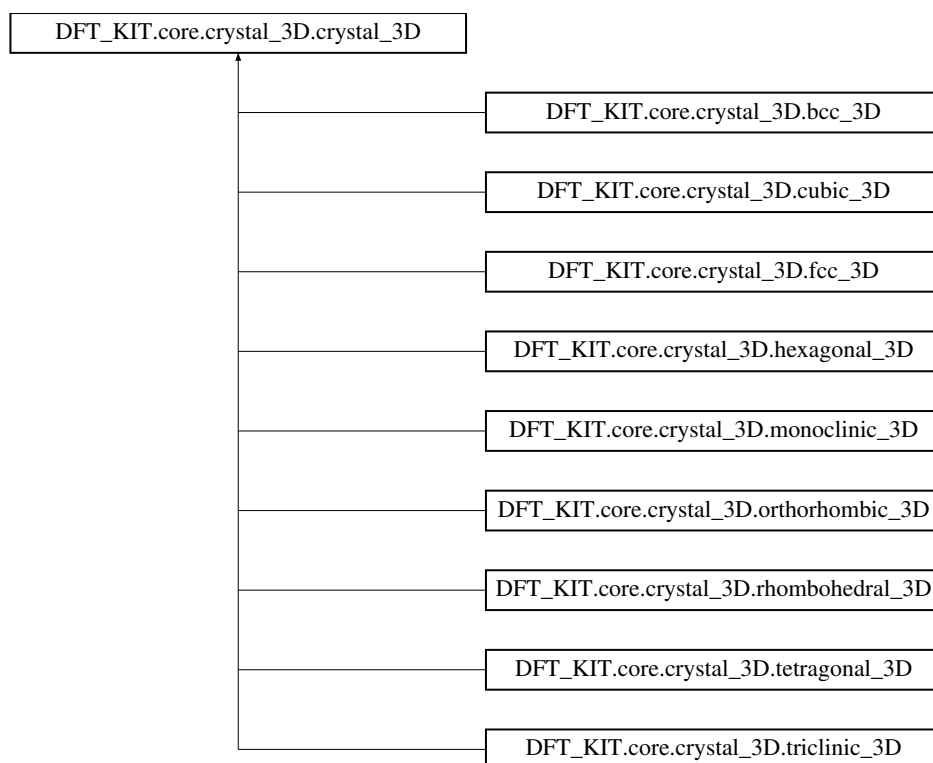
The documentation for this class was generated from the following file:

- calculator/[Wannier90.py](#)

6.11 DFT_KIT.core.crystal_3D.crystal_3D Class Reference

Class for [crystal_3D](#).

Inheritance diagram for DFT_KIT.core.crystal_3D.crystal_3D:



Public Member Functions

- def `__init__`
- def `set_coordinate`
- def `cart_coordinate`
- def `get_length_unit`
- def `set_length_units`
- def `evaluate_basic`
- def `evaluate_rec_vectors`
- def `eval_inv_primitive_vec`
- def `eval_inv_reciprocal_vec`
- def `prim_to_cart`
- def `cart_to_prim`
- def `get_prim_vec`
- def `set_prim_vec`
- def `rec_to_cart`
- def `cart_to_rec`
- def `set_rec_vec`
- def `get_rec_vec`
- def `k_distance`
- def `special_kpoints`
- def `clear_klabels`
- def `get_num_atoms`
- def `get_totnum_atoms`
- def `get_atom`
- def `get_atoms_groups`
- def `get_atoms_group`
- def `add_atom`
- def `add_atoms`
- def `update_position`

Public Attributes

- [description](#)
- [primitive_vector](#)
- [inv_primitive_vector](#)
- [reciprocal_vector](#)
- [inv_reciprocal_vector](#)
- [length_unit](#)
- [basis_atom_groups](#)
- [basis_element](#)
- [k_labels](#)
- [k_directions](#)
- [cart_coordinate](#)
- [length_units](#)

6.11.1 Detailed Description

Class for [crystal_3D](#).

Parameters

<i>length_unit</i>	define the length_unit in the calculation (1 angstrom)
--------------------	--

Definition at line 17 of file crystal_3D.py.

6.11.2 Constructor & Destructor Documentation

6.11.2.1 `def DFT_KIT.core.crystal_3D.crystal_3D.__init__(self, length_unit = 1.0, description = 'CRYSTAL generated by DFT_KIT')`

Definition at line 18 of file crystal_3D.py.

6.11.3 Member Function Documentation

6.11.3.1 `def DFT_KIT.core.crystal_3D.crystal_3D.add_atom(self, element, position = np.array([0.0, 0.0, parms])`

Definition at line 121 of file crystal_3D.py.

6.11.3.2 `def DFT_KIT.core.crystal_3D.crystal_3D.add_atoms(self, element, positions, parms)`

Definition at line 129 of file crystal_3D.py.

6.11.3.3 `def DFT_KIT.core.crystal_3D.crystal_3D.cart_coordinate(self)`

Definition at line 41 of file crystal_3D.py.

6.11.3.4 `def DFT_KIT.core.crystal_3D.crystal_3D.cart_to_prim(self, vec_)`

Definition at line 78 of file crystal_3D.py.

6.11.3.5 `def DFT_KIT.core.crystal_3D.crystal_3D.cart_to_rec(self, vec_)`

Definition at line 86 of file crystal_3D.py.

6.11.3.6 `def DFT_KIT.core.crystal_3D.crystal_3D.clear_klabels (self)`

Definition at line 98 of file `crystal_3D.py`.

6.11.3.7 `def DFT_KIT.core.crystal_3D.crystal_3D.eval_inv_primitive_vec (self)`

Definition at line 61 of file `crystal_3D.py`.

6.11.3.8 `def DFT_KIT.core.crystal_3D.crystal_3D.eval_inv_reciprocal_vec (self)`

Definition at line 68 of file `crystal_3D.py`.

6.11.3.9 `def DFT_KIT.core.crystal_3D.crystal_3D.evaluate_basic (self)`

Definition at line 51 of file `crystal_3D.py`.

6.11.3.10 `def DFT_KIT.core.crystal_3D.crystal_3D.evaluate_rec_vectors (self)`

Definition at line 56 of file `crystal_3D.py`.

6.11.3.11 `def DFT_KIT.core.crystal_3D.crystal_3D.get_atom (self, group, num)`

Definition at line 114 of file `crystal_3D.py`.

6.11.3.12 `def DFT_KIT.core.crystal_3D.crystal_3D.get_atoms_group (self, group)`

Definition at line 118 of file `crystal_3D.py`.

6.11.3.13 `def DFT_KIT.core.crystal_3D.crystal_3D.get_atoms_groups (self)`

Definition at line 116 of file `crystal_3D.py`.

6.11.3.14 `def DFT_KIT.core.crystal_3D.crystal_3D.get_length_unit (self)`

Definition at line 44 of file `crystal_3D.py`.

6.11.3.15 `def DFT_KIT.core.crystal_3D.crystal_3D.get_num_atoms (self, group)`

Definition at line 103 of file `crystal_3D.py`.

6.11.3.16 `def DFT_KIT.core.crystal_3D.crystal_3D.get_prim_vec (self, num_)`

Definition at line 80 of file `crystal_3D.py`.

6.11.3.17 `def DFT_KIT.core.crystal_3D.crystal_3D.get_rec_vec (self, vec_num)`

Definition at line 90 of file `crystal_3D.py`.

6.11.3.18 `def DFT_KIT.core.crystal_3D.crystal_3D.get_totnum_atoms (self)`

Definition at line 108 of file `crystal_3D.py`.

6.11.3.19 `def DFT_KIT.core.crystal_3D.crystal_3D.k_distance (self)`

Definition at line 94 of file `crystal_3D.py`.

6.11.3.20 `def DFT_KIT.core.crystal_3D.crystal_3D.prim_to_cart (self, vec_)`

Definition at line 76 of file `crystal_3D.py`.

6.11.3.21 `def DFT_KIT.core.crystal_3D.crystal_3D.rec_to_cart (self, vec_)`

Definition at line 84 of file `crystal_3D.py`.

6.11.3.22 `def DFT_KIT.core.crystal_3D.crystal_3D.set_coordinate (self, cart)`

Definition at line 38 of file `crystal_3D.py`.

6.11.3.23 `def DFT_KIT.core.crystal_3D.crystal_3D.set_length_units (self, leng_)`

Definition at line 47 of file `crystal_3D.py`.

6.11.3.24 `def DFT_KIT.core.crystal_3D.crystal_3D.set_prim_vec (self, num_, vec)`

Definition at line 82 of file `crystal_3D.py`.

6.11.3.25 `def DFT_KIT.core.crystal_3D.crystal_3D.set_rec_vec (self, vec_num, new_vec)`

Definition at line 88 of file `crystal_3D.py`.

6.11.3.26 `def DFT_KIT.core.crystal_3D.crystal_3D.special_kpoints (self)`

Definition at line 96 of file `crystal_3D.py`.

6.11.3.27 `def DFT_KIT.core.crystal_3D.crystal_3D.updata_position (self, pos_list)`

Definition at line 138 of file `crystal_3D.py`.

6.11.4 Member Data Documentation

6.11.4.1 `DFT_KIT.core.crystal_3D.crystal_3D.basis_atom_groups`

Definition at line 29 of file `crystal_3D.py`.

6.11.4.2 `DFT_KIT.core.crystal_3D.crystal_3D.basis_element`

Definition at line 30 of file `crystal_3D.py`.

6.11.4.3 DFT_KIT.core.crystal_3D.crystal_3D.cart_coordinate

Definition at line 36 of file crystal_3D.py.

6.11.4.4 DFT_KIT.core.crystal_3D.crystal_3D.description

Definition at line 19 of file crystal_3D.py.

6.11.4.5 DFT_KIT.core.crystal_3D.crystal_3D.inv_primitive_vector

Definition at line 22 of file crystal_3D.py.

6.11.4.6 DFT_KIT.core.crystal_3D.crystal_3D.inv_reciprocal_vector

Definition at line 26 of file crystal_3D.py.

6.11.4.7 DFT_KIT.core.crystal_3D.crystal_3D.k_directions

Definition at line 34 of file crystal_3D.py.

6.11.4.8 DFT_KIT.core.crystal_3D.crystal_3D.k_labels

Definition at line 33 of file crystal_3D.py.

6.11.4.9 DFT_KIT.core.crystal_3D.crystal_3D.length_unit

Definition at line 28 of file crystal_3D.py.

6.11.4.10 DFT_KIT.core.crystal_3D.crystal_3D.length_units

Definition at line 48 of file crystal_3D.py.

6.11.4.11 DFT_KIT.core.crystal_3D.crystal_3D.primitive_vector

Definition at line 21 of file crystal_3D.py.

6.11.4.12 DFT_KIT.core.crystal_3D.crystal_3D.reciprocal_vector

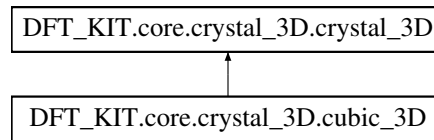
Definition at line 25 of file crystal_3D.py.

The documentation for this class was generated from the following file:

- [core/crystal_3D.py](#)

6.12 DFT_KIT.core.crystal_3D.cubic_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.cubic_3D:



Public Member Functions

- def [__init__](#)
- def [set_lattice](#)
- def [define_klabels](#)

Additional Inherited Members

6.12.1 Detailed Description

Definition at line 143 of file crystal_3D.py.

6.12.2 Constructor & Destructor Documentation

6.12.2.1 `def DFT_KIT.core.crystal_3D.cubic_3D.__init__(self, cubic_length, length_unit = 1.0)`

Definition at line 144 of file crystal_3D.py.

6.12.3 Member Function Documentation

6.12.3.1 `def DFT_KIT.core.crystal_3D.cubic_3D.define_klabels(self)`

Definition at line 155 of file crystal_3D.py.

6.12.3.2 `def DFT_KIT.core.crystal_3D.cubic_3D.set_lattice(self, cubic_length)`

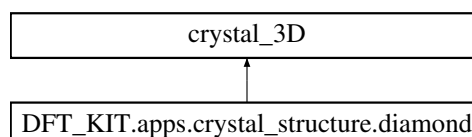
Definition at line 149 of file crystal_3D.py.

The documentation for this class was generated from the following file:

- core/[crystal_3D.py](#)

6.13 DFT_KIT.apps.crystal_structure.diamond Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.diamond:



Public Member Functions

- def [__init__](#)

6.13.1 Detailed Description

Definition at line 48 of file `crystal_structure.py`.

6.13.2 Constructor & Destructor Documentation

6.13.2.1 `def DFT_KIT.apps.crystal_structure.diamond.__init__(self, length_unit = 1.0)`

Definition at line 49 of file `crystal_structure.py`.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.14 DFT_KIT.core.element.element Class Reference

Public Member Functions

- `def __init__`

Public Attributes

- `symbol`
- `mass`
- `nucZ`
- `vale`
- `info`

6.14.1 Detailed Description

Definition at line 45 of file `element.py`.

6.14.2 Constructor & Destructor Documentation

6.14.2.1 `def DFT_KIT.core.element.element.__init__(self, symbol = None, mass = None, nucZ = None, vale = None, info)`

Definition at line 46 of file `element.py`.

6.14.3 Member Data Documentation

6.14.3.1 `DFT_KIT.core.element.element.info`

Definition at line 51 of file `element.py`.

6.14.3.2 `DFT_KIT.core.element.element.mass`

Definition at line 48 of file `element.py`.

6.14.3.3 DFT_KIT.core.element.element.nucZ

Definition at line 49 of file element.py.

6.14.3.4 DFT_KIT.core.element.element.symbol

Definition at line 47 of file element.py.

6.14.3.5 DFT_KIT.core.element.element.vale

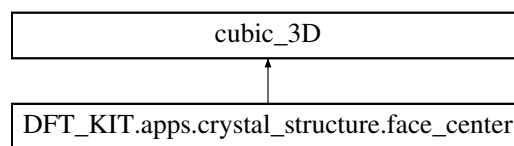
Definition at line 50 of file element.py.

The documentation for this class was generated from the following file:

- [core/element.py](#)

6.15 DFT_KIT.apps.crystal_structure.face_center Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.face_center:



Public Member Functions

- [def __init__](#)

6.15.1 Detailed Description

Definition at line 64 of file crystal_structure.py.

6.15.2 Constructor & Destructor Documentation

6.15.2.1 def DFT_KIT.apps.crystal_structure.face_center.__init__(self, cubic_length, length_unit = 1.0)

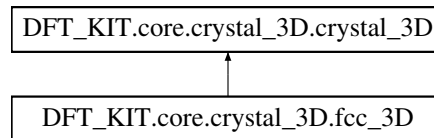
Definition at line 65 of file crystal_structure.py.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.16 DFT_KIT.core.crystal_3D.fcc_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.fcc_3D:



Public Member Functions

- def [__init__](#)
- def [set_lattice](#)
- def [define_klabels](#)

Additional Inherited Members

6.16.1 Detailed Description

Definition at line 195 of file crystal_3D.py.

6.16.2 Constructor & Destructor Documentation

6.16.2.1 `def DFT_KIT.core.crystal_3D.fcc_3D.__init__(self, fcc_length, length_unit = 1.0)`

Definition at line 196 of file crystal_3D.py.

6.16.3 Member Function Documentation

6.16.3.1 `def DFT_KIT.core.crystal_3D.fcc_3D.define_klabels(self)`

Definition at line 208 of file crystal_3D.py.

6.16.3.2 `def DFT_KIT.core.crystal_3D.fcc_3D.set_lattice(self, fcc_length)`

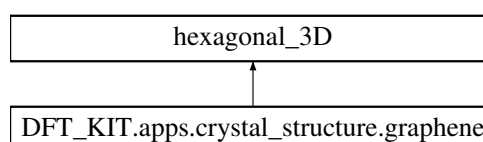
Definition at line 201 of file crystal_3D.py.

The documentation for this class was generated from the following file:

- core/[crystal_3D.py](#)

6.17 DFT_KIT.apps.crystal_structure.graphene Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.graphene:



Public Member Functions

- def [__init__](#)

6.17.1 Detailed Description

Definition at line 35 of file crystal_structure.py.

6.17.2 Constructor & Destructor Documentation

6.17.2.1 `def DFT_KIT.apps.crystal_structure.graphene.__init__(self, element, hex_a_length, hex_c_length, length_unit = 1.0, parms)`

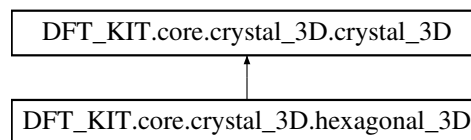
Definition at line 36 of file crystal_structure.py.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.18 DFT_KIT.core.crystal_3D.hexagonal_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.hexagonal_3D:



Public Member Functions

- `def __init__`
- `def set_lattice`
- `def define_klabels`

Additional Inherited Members

6.18.1 Detailed Description

Definition at line 222 of file crystal_3D.py.

6.18.2 Constructor & Destructor Documentation

6.18.2.1 `def DFT_KIT.core.crystal_3D.hexagonal_3D.__init__(self, hex_a_length, hex_c_length, length_unit = 1.0)`

Definition at line 223 of file crystal_3D.py.

6.18.3 Member Function Documentation

6.18.3.1 `def DFT_KIT.core.crystal_3D.hexagonal_3D.define_klabels(self)`

Definition at line 235 of file crystal_3D.py.

6.18.3.2 `def DFT_KIT.core.crystal_3D.hexagonal_3D.set_lattice (self, hex_a_length, hex_c_length)`

Definition at line 228 of file `crystal_3D.py`.

The documentation for this class was generated from the following file:

- `core/crystal_3D.py`

6.19 DFT_KIT.core.job.job Class Reference

Public Member Functions

- `def __init__`
- `def set_sysinfo`
- `def get_sysinfo`
- `def get_maindir`
- `def set_verbosity`
- `def show_verbose`
- `def show`
- `def show_error`
- `def get_info`
- `def copy_from_task`
- `def create_taskdir`
- `def get_task_dirname`
- `def set_parms`
- `def get_parms`
- `def remove_parms`
- `def next_task`
- `def make_fname`
- `def load_script`
- `def take_script_cmd`

Public Attributes

- `root_dir`
- `subdir`
- `all_dir`
- `count`
- `main_dir`
- `task_prefix`
- `verbose`
- `temp_dir`
- `scriptmode`
- `dft_script_cmds`
- `system`
- `parms`
- `sys_info`

6.19.1 Detailed Description

Definition at line 9 of file `job.py`.

6.19.2 Constructor & Destructor Documentation

6.19.2.1 `def DFT_KIT.core.job.job.__init__(self, subdir=True, system='DFT simulation', dir_task_prefix='task_', verbosity=True, parms)`

Definition at line 10 of file job.py.

6.19.3 Member Function Documentation

6.19.3.1 `def DFT_KIT.core.job.job.copy_from_task(self, from_task, fname)`

Definition at line 76 of file job.py.

6.19.3.2 `def DFT_KIT.core.job.job.create_taskdir(self)`

Definition at line 81 of file job.py.

6.19.3.3 `def DFT_KIT.core.job.job.get_info(self, src, prompt, force_enter)`

Definition at line 59 of file job.py.

6.19.3.4 `def DFT_KIT.core.job.job.get_maindir(self)`

Definition at line 45 of file job.py.

6.19.3.5 `def DFT_KIT.core.job.job.get_parms(self, ind_key)`

Definition at line 97 of file job.py.

6.19.3.6 `def DFT_KIT.core.job.job.get_sysinfo(self, ind_key)`

Definition at line 41 of file job.py.

6.19.3.7 `def DFT_KIT.core.job.job.get_task_dirname(self, task_)`

Definition at line 92 of file job.py.

6.19.3.8 `def DFT_KIT.core.job.job.load_script(self, scriptfile)`

Definition at line 111 of file job.py.

6.19.3.9 `def DFT_KIT.core.job.job.make_fname(self, prefix)`

Definition at line 107 of file job.py.

6.19.3.10 `def DFT_KIT.core.job.job.next_task(self, make_new_dir)`

Definition at line 101 of file job.py.

6.19.3.11 `def DFT_KIT.core.job.job.remove_parms (self, ind_key)`

Definition at line 99 of file job.py.

6.19.3.12 `def DFT_KIT.core.job.job.set_parms (self, ind_key, parm_val)`

Definition at line 95 of file job.py.

6.19.3.13 `def DFT_KIT.core.job.job.set_sysinfo (self, ind_key, val)`

Definition at line 39 of file job.py.

6.19.3.14 `def DFT_KIT.core.job.job.set_verbosity (self, verbosity)`

Definition at line 48 of file job.py.

6.19.3.15 `def DFT_KIT.core.job.job.show (self, src, message)`

Definition at line 55 of file job.py.

6.19.3.16 `def DFT_KIT.core.job.job.show_error (self, src, message)`

Definition at line 57 of file job.py.

6.19.3.17 `def DFT_KIT.core.job.job.show_verbose (self, src, message)`

Definition at line 50 of file job.py.

6.19.3.18 `def DFT_KIT.core.job.job.take_script_cmd (self)`

Definition at line 120 of file job.py.

6.19.4 Member Data Documentation

6.19.4.1 `DFT_KIT.core.job.job.all_dir`

Definition at line 13 of file job.py.

6.19.4.2 `DFT_KIT.core.job.job.count`

Definition at line 14 of file job.py.

6.19.4.3 `DFT_KIT.core.job.job.dft_script_cmds`

Definition at line 20 of file job.py.

6.19.4.4 `DFT_KIT.core.job.job.main_dir`

Definition at line 15 of file job.py.

6.19.4.5 DFT_KIT.core.job.job.parms

Definition at line 23 of file job.py.

6.19.4.6 DFT_KIT.core.job.job.root_dir

Definition at line 11 of file job.py.

6.19.4.7 DFT_KIT.core.job.job.scriptmode

Definition at line 19 of file job.py.

6.19.4.8 DFT_KIT.core.job.job.subdir

Definition at line 12 of file job.py.

6.19.4.9 DFT_KIT.core.job.job.sys_info

Definition at line 34 of file job.py.

6.19.4.10 DFT_KIT.core.job.job.system

Definition at line 22 of file job.py.

6.19.4.11 DFT_KIT.core.job.job.task_prefix

Definition at line 16 of file job.py.

6.19.4.12 DFT_KIT.core.job.job.temp_dir

Definition at line 18 of file job.py.

6.19.4.13 DFT_KIT.core.job.job.verbose

Definition at line 17 of file job.py.

The documentation for this class was generated from the following file:

- [core/job.py](#)

6.20 DFT_KIT.core.kpoint.kpoint Class Reference

Public Member Functions

- [def __init__](#)
- [def add_kscan_point](#)
- [def set_num_kscan](#)
- [def set_grid_mode](#)
- [def set_scan_mode](#)
- [def add_klist_point](#)
- [def generate_kgrid](#)

Public Attributes

- [kmode](#)
- [kgridtype](#)
- [kgrid](#)
- [kgrid_shift](#)
- [rec_coordinate](#)
- [num_kscan](#)
- [kscan](#)
- [klist](#)

6.20.1 Detailed Description

Definition at line 7 of file kpoint.py.

6.20.2 Constructor & Destructor Documentation

6.20.2.1 `def DFT_KIT.core.kpoint.kpoint.__init__(self, mode = 0)`

Definition at line 8 of file kpoint.py.

6.20.3 Member Function Documentation

6.20.3.1 `def DFT_KIT.core.kpoint.kpoint.add_klist_point(self, kpoint)`

Definition at line 47 of file kpoint.py.

6.20.3.2 `def DFT_KIT.core.kpoint.kpoint.add_kscan_point(self, kpoint)`

Definition at line 31 of file kpoint.py.

6.20.3.3 `def DFT_KIT.core.kpoint.kpoint.generate_kgrid(self, write_weight)`

Definition at line 51 of file kpoint.py.

6.20.3.4 `def DFT_KIT.core.kpoint.kpoint.set_grid_mode(self, grid_)`

Definition at line 35 of file kpoint.py.

6.20.3.5 `def DFT_KIT.core.kpoint.kpoint.set_num_kscan(self, num)`

Definition at line 33 of file kpoint.py.

6.20.3.6 `def DFT_KIT.core.kpoint.kpoint.set_scan_mode(self, num, kpoints)`

Definition at line 39 of file kpoint.py.

6.20.4 Member Data Documentation

6.20.4.1 DFT_KIT.core.kpoint.kpoint.kgrid

Definition at line 16 of file kpoint.py.

6.20.4.2 DFT_KIT.core.kpoint.kpoint.kgrid_shift

Definition at line 17 of file kpoint.py.

6.20.4.3 DFT_KIT.core.kpoint.kpoint.kgridtype

Definition at line 15 of file kpoint.py.

6.20.4.4 DFT_KIT.core.kpoint.kpoint.klist

Definition at line 25 of file kpoint.py.

6.20.4.5 DFT_KIT.core.kpoint.kpoint.kmode

Definition at line 12 of file kpoint.py.

6.20.4.6 DFT_KIT.core.kpoint.kpoint.kscan

Definition at line 22 of file kpoint.py.

6.20.4.7 DFT_KIT.core.kpoint.kpoint.num_kscan

Definition at line 21 of file kpoint.py.

6.20.4.8 DFT_KIT.core.kpoint.kpoint.rec_coordinate

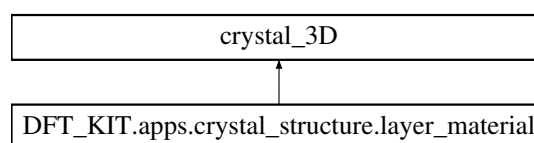
Definition at line 18 of file kpoint.py.

The documentation for this class was generated from the following file:

- [core/kpoint.py](#)

6.21 DFT_KIT.apps.crystal_structure.layer_material Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.layer_material:



Public Member Functions

- [def __init__](#)

6.21.1 Detailed Description

Definition at line 43 of file `crystal_structure.py`.

6.21.2 Constructor & Destructor Documentation

6.21.2.1 `def DFT_KIT.apps.crystal_structure.layer_material.__init__(self, length_unit = 1.0)`

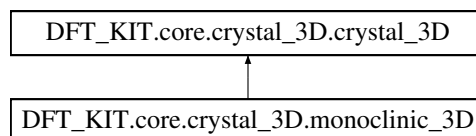
Definition at line 44 of file `crystal_structure.py`.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.22 DFT_KIT.core.crystal_3D.monoclinic_3D Class Reference

Inheritance diagram for `DFT_KIT.core.crystal_3D.monoclinic_3D`:



Public Member Functions

- `def __init__`
- `def set_lattice`

Additional Inherited Members

6.22.1 Detailed Description

Definition at line 319 of file `crystal_3D.py`.

6.22.2 Constructor & Destructor Documentation

6.22.2.1 `def DFT_KIT.core.crystal_3D.monoclinic_3D.__init__(self, a = 0.0, b = 0.0, c = 0.0, angle = 0.0, length_unit = 1.0)`

Definition at line 320 of file `crystal_3D.py`.

6.22.3 Member Function Documentation

6.22.3.1 `def DFT_KIT.core.crystal_3D.monoclinic_3D.set_lattice(self, a, b, c, angle)`

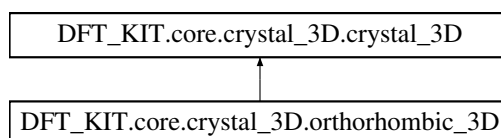
Definition at line 324 of file `crystal_3D.py`.

The documentation for this class was generated from the following file:

- [core/crystal_3D.py](#)

6.23 DFT_KIT.core.crystal_3D.orthorhombic_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.orthorhombic_3D:



Public Member Functions

- def [__init__](#)
- def [set_lattice](#)
- def [define_klabels](#)

Additional Inherited Members

6.23.1 Detailed Description

Definition at line 284 of file crystal_3D.py.

6.23.2 Constructor & Destructor Documentation

6.23.2.1 `def DFT_KIT.core.crystal_3D.orthorhombic_3D.__init__(self, a_ = 0.0, b_ = 0.0, c_ = 0.0, length_unit = 1.0)`

Definition at line 285 of file crystal_3D.py.

6.23.3 Member Function Documentation

6.23.3.1 `def DFT_KIT.core.crystal_3D.orthorhombic_3D.define_klabels(self)`

Definition at line 296 of file crystal_3D.py.

6.23.3.2 `def DFT_KIT.core.crystal_3D.orthorhombic_3D.set_lattice(self, a_, b_, c_)`

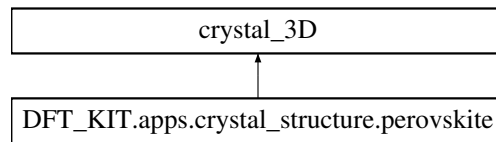
Definition at line 290 of file crystal_3D.py.

The documentation for this class was generated from the following file:

- [core/crystal_3D.py](#)

6.24 DFT_KIT.apps.crystal_structure.perovskite Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.perovskite:



Public Member Functions

- [def __init__](#)

6.24.1 Detailed Description

Definition at line 52 of file crystal_structure.py.

6.24.2 Constructor & Destructor Documentation

6.24.2.1 `def DFT_KIT.apps.crystal_structure.perovskite.__init__(self, length_unit = 1.0)`

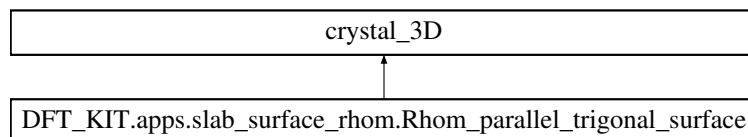
Definition at line 53 of file crystal_structure.py.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.25 DFT_KIT.apps.slab_surface_rhom.Rhom_parallel_trigonal_surface Class Reference

Inheritance diagram for DFT_KIT.apps.slab_surface_rhom.Rhom_parallel_trigonal_surface:



Public Member Functions

- [def __init__](#)

Public Attributes

- [ref_crystal](#)

6.25.1 Detailed Description

Definition at line 59 of file slab_surface_rhom.py.

6.25.2 Constructor & Destructor Documentation

6.25.2.1 `def DFT_KIT.apps.slab_surface_rhom.Rhom_parallel_trigonal_surface.__init__(self, element, num_layers, vacuum_layers, length_unit = 1.0, description = 'Trigonal Surface', parms)`

Definition at line 60 of file slab_surface_rhom.py.

6.25.3 Member Data Documentation

6.25.3.1 `DFT_KIT.apps.slab_surface_rhom.Rhom_parallel_trigonal_surface.ref_crystal`

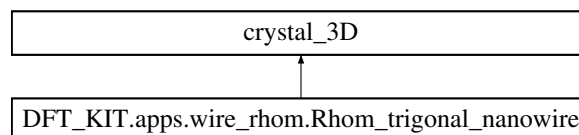
Definition at line 77 of file slab_surface_rhom.py.

The documentation for this class was generated from the following file:

- [apps/slab_surface_rhom.py](#)

6.26 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire Class Reference

Inheritance diagram for DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire:



Public Member Functions

- `def __init__`

Public Attributes

- [ref_crystal](#)
- [Lx](#)
- [Ly](#)
- [Lz](#)
- [radius](#)
- [hex_a1](#)
- [hex_a2](#)
- [all_points](#)

6.26.1 Detailed Description

Definition at line 12 of file wire_rhom.py.

6.26.2 Constructor & Destructor Documentation

6.26.2.1 `def DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.__init__(self, element, Lx, Ly, radius, length_unit = 1.0, description = 'Trigonal Nanowire', parms)`

Definition at line 13 of file wire_rhom.py.

6.26.3 Member Data Documentation

6.26.3.1 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.all_points

Definition at line 106 of file wire_rhom.py.

6.26.3.2 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.hex_a1

Definition at line 60 of file wire_rhom.py.

6.26.3.3 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.hex_a2

Definition at line 61 of file wire_rhom.py.

6.26.3.4 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.Lx

Definition at line 46 of file wire_rhom.py.

6.26.3.5 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.Ly

Definition at line 47 of file wire_rhom.py.

6.26.3.6 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.Lz

Definition at line 48 of file wire_rhom.py.

6.26.3.7 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.radius

Definition at line 49 of file wire_rhom.py.

6.26.3.8 DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire.ref_crystal

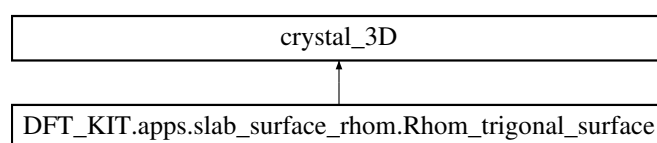
Definition at line 36 of file wire_rhom.py.

The documentation for this class was generated from the following file:

- apps/[wire_rhom.py](#)

6.27 DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface Class Reference

Inheritance diagram for DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface:



Public Member Functions

- def [__init__](#)

Public Attributes

- [ref_crystal](#)
- [num_layers](#)
- [vacuum_layers](#)
- [rhom_constant](#)
- [angle](#)
- [rhom_u](#)

6.27.1 Detailed Description

Definition at line 9 of file slab_surface_rhom.py.

6.27.2 Constructor & Destructor Documentation

6.27.2.1 `def DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.__init__(self, element, num_layers, vacuum_layers, length_unit = 1.0, description = 'Trigonal Surface', parms)`

Definition at line 10 of file slab_surface_rhom.py.

6.27.3 Member Data Documentation

6.27.3.1 `DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.angle`

Definition at line 36 of file slab_surface_rhom.py.

6.27.3.2 `DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.num_layers`

Definition at line 33 of file slab_surface_rhom.py.

6.27.3.3 `DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.ref_crystal`

Definition at line 27 of file slab_surface_rhom.py.

6.27.3.4 `DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.rhom_constant`

Definition at line 35 of file slab_surface_rhom.py.

6.27.3.5 `DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.rhom_u`

Definition at line 37 of file slab_surface_rhom.py.

6.27.3.6 `DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface.vacuum_layers`

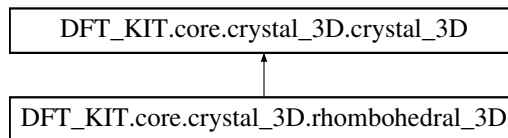
Definition at line 34 of file slab_surface_rhom.py.

The documentation for this class was generated from the following file:

- [apps/slab_surface_rhom.py](#)

6.28 DFT_KIT.core.crystal_3D.rhombohedral_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.rhombohedral_3D:



Public Member Functions

- def [__init__](#)
- def [set_lattice](#)
- def [define_klabels](#)

Additional Inherited Members

6.28.1 Detailed Description

Definition at line 345 of file crystal_3D.py.

6.28.2 Constructor & Destructor Documentation

6.28.2.1 def DFT_KIT.core.crystal_3D.rhombohedral_3D.__init__(self, rhom_length, angle, length_unit = 1.0)

Definition at line 346 of file crystal_3D.py.

6.28.3 Member Function Documentation

6.28.3.1 def DFT_KIT.core.crystal_3D.rhombohedral_3D.define_klabels(self)

Definition at line 367 of file crystal_3D.py.

6.28.3.2 def DFT_KIT.core.crystal_3D.rhombohedral_3D.set_lattice(self, rhom_length, angle_)

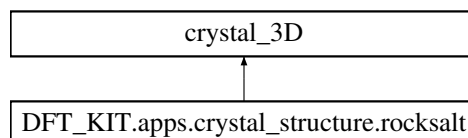
Definition at line 353 of file crystal_3D.py.

The documentation for this class was generated from the following file:

- core/[crystal_3D.py](#)

6.29 DFT_KIT.apps.crystal_structure.rocksalt Class Reference

Inheritance diagram for DFT_KIT.apps.crystal_structure.rocksalt:



Public Member Functions

- [def __init__](#)

6.29.1 Detailed Description

Definition at line 56 of file `crystal_structure.py`.

6.29.2 Constructor & Destructor Documentation

6.29.2.1 `def DFT_KIT.apps.crystal_structure.rocksalt.__init__(self, length_unit = 1.0)`

Definition at line 57 of file `crystal_structure.py`.

The documentation for this class was generated from the following file:

- [apps/crystal_structure.py](#)

6.30 DFT_KIT.core.general_tool.segments Class Reference

Public Member Functions

- [def __init__](#)
- [def get_ordering](#)
- [def print_ordering](#)
- [def swap_groups](#)
- [def invert_group](#)

Public Attributes

- [ordering](#)
- [subnum](#)
- [sets](#)
- [tmp1](#)
- [tmp2](#)
- [tmp0](#)

6.30.1 Detailed Description

Definition at line 8 of file `general_tool.py`.

6.30.2 Constructor & Destructor Documentation

6.30.2.1 `def DFT_KIT.core.general_tool.segments.__init__(self, num_, sets_)`

Definition at line 9 of file `general_tool.py`.

6.30.3 Member Function Documentation

6.30.3.1 `def DFT_KIT.core.general_tool.segments.get_ordering(self)`

Definition at line 16 of file `general_tool.py`.

6.30.3.2 `def DFT_KIT.core.general_tool.segments.invert_group (self, group_)`

Definition at line 25 of file `general_tool.py`.

6.30.3.3 `def DFT_KIT.core.general_tool.segments.print_ordering (self)`

Definition at line 18 of file `general_tool.py`.

6.30.3.4 `def DFT_KIT.core.general_tool.segments.swap_groups (self, group1, group2)`

Definition at line 20 of file `general_tool.py`.

6.30.4 Member Data Documentation

6.30.4.1 `DFT_KIT.core.general_tool.segments.ordering`

Definition at line 10 of file `general_tool.py`.

6.30.4.2 `DFT_KIT.core.general_tool.segments.sets`

Definition at line 12 of file `general_tool.py`.

6.30.4.3 `DFT_KIT.core.general_tool.segments.subnum`

Definition at line 11 of file `general_tool.py`.

6.30.4.4 `DFT_KIT.core.general_tool.segments.tmp0`

Definition at line 15 of file `general_tool.py`.

6.30.4.5 `DFT_KIT.core.general_tool.segments.tmp1`

Definition at line 13 of file `general_tool.py`.

6.30.4.6 `DFT_KIT.core.general_tool.segments.tmp2`

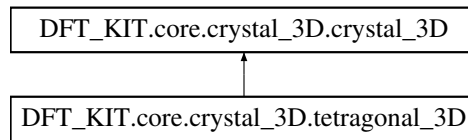
Definition at line 14 of file `general_tool.py`.

The documentation for this class was generated from the following file:

- [core/general_tool.py](#)

6.31 DFT_KIT.core.crystal_3D.tetragonal_3D Class Reference

Inheritance diagram for `DFT_KIT.core.crystal_3D.tetragonal_3D`:



Public Member Functions

- `def __init__`
- `def set_lattice`
- `def define_klabels`

Additional Inherited Members

6.31.1 Detailed Description

Definition at line 252 of file `crystal_3D.py`.

6.31.2 Constructor & Destructor Documentation

6.31.2.1 `def DFT_KIT.core.crystal_3D.tetragonal_3D.__init__(self, a_ = 0.0, c_ = 0.0, length_unit = 1.0)`

Definition at line 253 of file `crystal_3D.py`.

6.31.3 Member Function Documentation

6.31.3.1 `def DFT_KIT.core.crystal_3D.tetragonal_3D.define_klabels(self)`

Definition at line 264 of file `crystal_3D.py`.

6.31.3.2 `def DFT_KIT.core.crystal_3D.tetragonal_3D.set_lattice(self, a_, c_)`

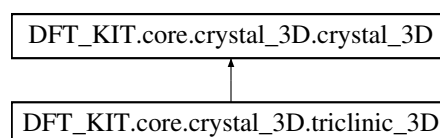
Definition at line 258 of file `crystal_3D.py`.

The documentation for this class was generated from the following file:

- `core/crystal_3D.py`

6.32 DFT_KIT.core.crystal_3D.triclinic_3D Class Reference

Inheritance diagram for DFT_KIT.core.crystal_3D.triclinic_3D:



Public Member Functions

- [def __init__](#)
- [def set_lattice_constant](#)

Additional Inherited Members

6.32.1 Detailed Description

Definition at line 331 of file `crystal_3D.py`.

6.32.2 Constructor & Destructor Documentation

6.32.2.1 `def DFT_KIT.core.crystal_3D.triclinic_3D.__init__(self, a_ = 0.0, b_ = 0.0, c_ = 0.0, angle_ = 0.0, length_unit = 1.0)`

Definition at line 333 of file `crystal_3D.py`.

6.32.3 Member Function Documentation

6.32.3.1 `def DFT_KIT.core.crystal_3D.triclinic_3D.set_lattice_constant(self, a_, b_, c_, angle_)`

Definition at line 337 of file `crystal_3D.py`.

The documentation for this class was generated from the following file:

- `core/crystal_3D.py`

Chapter 7

File Documentation

7.1 `__init__.py` File Reference

Namespaces

- [DFT_KIT](#)

7.2 `apps/__init__.py` File Reference

Namespaces

- [DFT_KIT.apps](#)

7.3 `calculator/__init__.py` File Reference

Namespaces

- [DFT_KIT.calculator](#)

7.4 `core/__init__.py` File Reference

Namespaces

- [DFT_KIT.core](#)

7.5 `interface/__init__.py` File Reference

Namespaces

- [DFT_KIT.interface](#)

7.6 `apps/bismuth_antimony.py` File Reference

Namespaces

- [DFT_KIT.apps.bismuth_antimony](#)

Variables

- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_exp_1](#) = {'lattice_constant':4.489,'angle':(57.0+14.0/60.↵
0)*np.pi/180.0,'rhom_u':0.2336}
- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_exp_2](#) = {'lattice_constant':4.4898,'angle':(57.233)*np.↵
pi/180.0,'rhom_u':0.23362}
- tuple [DFT_KIT.apps.bismuth_antimony.Sb](#) = element.element('Sb',121.760,51,5,vasp_pot='Sb',qes_pot="↵
)
- tuple [DFT_KIT.apps.bismuth_antimony.Sb_d](#) = element.element('Sb',121.760,51,15,vasp_pot='Sb_d',qes_↵
pot=")
- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_vasp_scf](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_vasp_nscf_soi](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_qespresso_scf](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_qespresso_nscf_soi](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Sb_wannier90](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_exp_1](#) = {'lattice_constant':4.7212,'angle':(57.0+19.0/60.↵
0)*np.pi/180.0,'rhom_u':0.23407}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_exp_2](#) = {'lattice_constant':4.7236,'angle':(57.35)*np.↵
pi/180.0,'rhom_u':0.23407}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_dft_1](#) = {'lattice_constant':4.7973,'angle':(53.0+56.0/60.↵
0)*np.pi/180.0,'rhom_u':0.2348}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_dft_2](#) = {'lattice_constant':4.7827,'angle':(56.0+17.0/60.↵
0)*np.pi/180.0,'rhom_u':0.2351}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_dft_3](#) = {'lattice_constant':4.8038,'angle':(53.0+36.0/60.↵
0)*np.pi/180.0,'rhom_u':0.2347}
- tuple [DFT_KIT.apps.bismuth_antimony.Bi_exp](#) = element.element('Bi',208.9804,83,5,vasp_pot='Bi',qes_↵
pot='Bi.UPF',rhom_length=4.7236,angle=1.0009,rhom_u=0.23407)
- tuple [DFT_KIT.apps.bismuth_antimony.Bi_d](#) = element.element('Bi',208.9804,83,15,vasp_pot='Bi_d',qes_↵
pot=")
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_vasp_slab_scf](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_vasp_slab_nscf_soi](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_vasp_crystal_scf](#) = {'ISTART':0,'ENCUT':250,'EDIFF':1E-↵
6,'ISMEAR':5,'SIGMA':0.2,'LMAXMIX':4}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_vasp_crystal_nscf_soi](#) = {'ISTART':0,'ICHARG':11,'ENCU↵
T':250,'EDIFF':1E-6,'GGA_COMPAT':.FALSE,'ISYM':0,'SAXIS':0 0 1,'LSORBIT':.TRUE,'LMAXMIX'↵
:'4','MAGMOM':True}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_qespresso_crystal_scf](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_qespresso_crystal_nscf_soi](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_qespresso_slab_scf](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_qespresso_slab_nscf_soi](#) = {}
- dictionary [DFT_KIT.apps.bismuth_antimony.Bi_wannier90](#) = {}

7.7 apps/crystal_structure.py File Reference

Classes

- class [DFT_KIT.apps.crystal_structure.a7_structure](#)
- class [DFT_KIT.apps.crystal_structure.graphene](#)
- class [DFT_KIT.apps.crystal_structure.layer_material](#)
- class [DFT_KIT.apps.crystal_structure.diamond](#)
- class [DFT_KIT.apps.crystal_structure.perovskite](#)

- class [DFT_KIT.apps.crystal_structure.rocksalt](#)
- class [DFT_KIT.apps.crystal_structure.body_center](#)
- class [DFT_KIT.apps.crystal_structure.face_center](#)

Namespaces

- [DFT_KIT.apps.crystal_structure](#)

7.8 apps/dft_cmdtool.py File Reference

Namespaces

- [DFT_KIT.apps.dft_cmdtool](#)

Variables

- tuple [DFT_KIT.apps.dft_cmdtool.dft_job](#) = job.job(False)
- tuple [DFT_KIT.apps.dft_cmdtool.root_dir](#) = os.getcwd()
- tuple [DFT_KIT.apps.dft_cmdtool.numargs](#) = len(sys.argv)
- list [DFT_KIT.apps.dft_cmdtool.scriptfile](#) = sys.argv[1]
- tuple [DFT_KIT.apps.dft_cmdtool.input_cmd](#) = dft_job.get_info('dft_cmdtool','input command',True)
- tuple [DFT_KIT.apps.dft_cmdtool.cmd_first](#) = input_cmd.split()
- tuple [DFT_KIT.apps.dft_cmdtool.cmd_num](#) = len(input_cmd.split())
- tuple [DFT_KIT.apps.dft_cmdtool.cmds](#) = input_cmd.split()

7.9 apps/slab_surface_rhom.py File Reference

Classes

- class [DFT_KIT.apps.slab_surface_rhom.Rhom_trigonal_surface](#)
- class [DFT_KIT.apps.slab_surface_rhom.Rhom_parallel_trigonal_surface](#)

Namespaces

- [DFT_KIT.apps.slab_surface_rhom](#)

7.10 apps/wire_rhom.py File Reference

Classes

- class [DFT_KIT.apps.wire_rhom.Rhom_trigonal_nanowire](#)

Namespaces

- [DFT_KIT.apps.wire_rhom](#)

7.11 calculator/QESPRESSO.py File Reference

Classes

- class [DFT_KIT.calculator.QESPRESSO.calculator_QESPRESSO](#)

Namespaces

- [DFT_KIT.calculator.QESPRESSO](#)

Variables

- string [DFT_KIT.calculator.QESPRESSO.QES_control_flags](#) = 'calculation title verbosity restart_mode wf↵
_collect nstep iprint tstress tprnfor dt wfcdir lkpoint_dir max_seconds etot_conv_thr forc_conv_thr disk_io
tefield dipfield lfield nberrycyc lorbm lberry gdir npostr'
- string [DFT_KIT.calculator.QESPRESSO.QES_system_flags](#) = 'ibrav celldm A B C cosAB cosAC cosB↵
C nbnd tot_charge tot_magnetization starting_magnetization ecutwfc ecutrho ecutfock nr1 nr2 nr3 nr1s
nr2s nr3s nosym nosym_evc noinv no_t_rev force_symmorphic use_all_frac occupations one_atom↵
occupations starting_spin_angle degauss smearing nspin noncolin ecfixed qcutz q2sigma input_dft exx↵
_fraction screening_parameter exxdiv_treatment x_gamma_extrapolation ecutvcut nqx1 nqx2 nqx3 lda↵
plus_u lda_plus_u_kind Hubbard_U Hubbard_J0 Hubbard_alpha Hubbard_beta Hubbard_J(i,ityp) starting↵
_ns_eigenvalue(m,ispin,l) U_projection_type edir emaxpos eopreg eamp angle1 angle2 constrained↵
magnetization fixed_magnetization lambda report lspinorb assume_isolated esm_bc esm_w esm_efield
esm_nfit vdw_corr london london_s6 london_rcut xdm xdm_a1 xdm_a2'
- string [DFT_KIT.calculator.QESPRESSO.QES_electrons_flags](#) = 'electron_maxstep scf_must_converge
conv_thr adaptive_thr conv_thr_init conv_thr_multi mixing_mode mixing_beta mixing_ndim mixing_fixed↵
_ns diagonalization ortho_para diago_thr_init diago_cg_maxiter diago_david_ndim diago_full_acc efield
efield_cart startingpot startingwfc tqr'
- string [DFT_KIT.calculator.QESPRESSO.QES_ions_flags](#) = 'ion_dynamics ion_positions phase_space pot↵
_extrapolation wfc_extrapolation remove_rigid_rot ion_temperature tempw tolp delta_t nraise refold_pos up↵
scale bfgs_ndim trust_radius_max trust_radius_min trust_radius_ini w_1 w_2'
- string [DFT_KIT.calculator.QESPRESSO.QES_cell_flags](#) = 'cell_dynamics press wmass cell_factor press↵
conv_thr cell_dofree'
- list [DFT_KIT.calculator.QESPRESSO.QES_PW2WAN_flags](#) = ['write_amn','write_spn','write_mmn','write↵
unk']

7.12 calculator/script.py File Reference

Classes

- class [DFT_KIT.calculator.script.calculator_script](#)

Namespaces

- [DFT_KIT.calculator.script](#)

Variables

- list [DFT_KIT.calculator.script.VASP_incar_flags](#)
- list [DFT_KIT.calculator.script.VASP_kpoints_flags](#) = []

7.13 calculator/SIESTA.py File Reference

Classes

- class [DFT_KIT.calculator.SIESTA.calculator_SIESTA](#)

Namespaces

- [DFT_KIT.calculator.SIESTA](#)

Variables

- list [DFT_KIT.calculator.SIESTA.SIESTA_flags](#)
- string [DFT_KIT.calculator.SIESTA.SIE_flags](#)

7.14 calculator/VASP.py File Reference

Classes

- class [DFT_KIT.calculator.VASP.calculator_VASP](#)

Namespaces

- [DFT_KIT.calculator.VASP](#)

Variables

- list [DFT_KIT.calculator.VASP.VASP_incar_flags](#)
- list [DFT_KIT.calculator.VASP.VASP_kpoints_flags](#) = []

7.15 calculator/Wannier90.py File Reference

Classes

- class [DFT_KIT.calculator.Wannier90.calculator_Wannier90](#)

Namespaces

- [DFT_KIT.calculator.Wannier90](#)

Variables

- list [DFT_KIT.calculator.Wannier90.QES_wannier90_flags](#)

7.16 core/atom.py File Reference

Classes

- class [DFT_KIT.core.atom.atom](#)

Namespaces

- [DFT_KIT.core.atom](#)

7.17 core/calculator.py File Reference

Classes

- class [DFT_KIT.core.calculator.calculator](#)

Namespaces

- [DFT_KIT.core.calculator](#)

7.18 core/crystal_3D.py File Reference

Classes

- class [DFT_KIT.core.crystal_3D.crystal_3D](#)
Class for crystal_3D.
- class [DFT_KIT.core.crystal_3D.cubic_3D](#)
- class [DFT_KIT.core.crystal_3D.bcc_3D](#)
- class [DFT_KIT.core.crystal_3D.fcc_3D](#)
- class [DFT_KIT.core.crystal_3D.hexagonal_3D](#)
- class [DFT_KIT.core.crystal_3D.tetragonal_3D](#)
- class [DFT_KIT.core.crystal_3D.orthorhombic_3D](#)
- class [DFT_KIT.core.crystal_3D.monoclinic_3D](#)
- class [DFT_KIT.core.crystal_3D.triclinic_3D](#)
- class [DFT_KIT.core.crystal_3D.rhombohedral_3D](#)

Namespaces

- [DFT_KIT.core.crystal_3D](#)

7.19 core/element.py File Reference

Classes

- class [DFT_KIT.core.element.element](#)

Namespaces

- [DFT_KIT.core.element](#)

Functions

- def [DFT_KIT.core.element.chem_number](#)
- def [DFT_KIT.core.element.chem_name](#)

Variables

- list [DFT_KIT.core.element.magic_numbers](#) = [2,10,18,36,54,86]
- list [DFT_KIT.core.element.periodic_table](#) = ['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al', 'Si', 'P', 'S', 'Cl', 'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At', 'Rn', 'Fr', 'Ra', 'Ac', 'Th', 'Pa', 'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm', 'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt', 'Ds', 'Rg', 'Uub', 'Uut', 'Uuq', 'Uup', 'Uuh', 'Uuo']
- list [DFT_KIT.core.element.Element_A](#) = [['H','Ne']]
- list [DFT_KIT.core.element.Element_B](#) = []
- list [DFT_KIT.core.element.Element_Lanthanides](#) = ['La','Ce','Pr','Nd','Pm','Sm','Eu','Gd','Tb','Dy','Ho','Er','Tm','Yb']
- list [DFT_KIT.core.element.Element_Actinides](#) = ['Ac','Th','Pa','U','Np','Pu','Am','Cm','Bk','Cf','Es','Fm','Md','No']

7.20 core/env_parm.py File Reference

Namespaces

- [DFT_KIT.core.env_parm](#)

Functions

- def [DFT_KIT.core.env_parm.run_vasp_std](#)
- def [DFT_KIT.core.env_parm.run_vasp_ncl](#)
- def [DFT_KIT.core.env_parm.run_vasp_gamma](#)
- def [DFT_KIT.core.env_parm.run_qespresso](#)
- def [DFT_KIT.core.env_parm.run_siesta](#)

Variables

- list [DFT_KIT.core.env_parm.modules_load](#) = []
- string [DFT_KIT.core.env_parm.batch_cmd](#) = 'sbatch '
- string [DFT_KIT.core.env_parm.vasp_std_path](#) = ''
- string [DFT_KIT.core.env_parm.vasp_complex_path](#) = ''
- string [DFT_KIT.core.env_parm.vasp_gamma_path](#) = ''
- string [DFT_KIT.core.env_parm.vasp_pseudo_dir](#) = '/home1/03051/sfang/Pseudo_Potential/VASP/'

7.21 core/env_parm_odyssey.py File Reference

Namespaces

- [DFT_KIT.core.env_parm_odyssey](#)

Functions

- def [DFT_KIT.core.env_parm_odyssey.run_vasp_std](#)
- def [DFT_KIT.core.env_parm_odyssey.run_vasp_ncl](#)
- def [DFT_KIT.core.env_parm_odyssey.run_vasp_gamma](#)
- def [DFT_KIT.core.env_parm_odyssey.run_qespresso](#)
- def [DFT_KIT.core.env_parm_odyssey.run_siesta](#)

Variables

- list [DFT_KIT.core.env_parm_odyssey.modules_load](#) = []
- string [DFT_KIT.core.env_parm_odyssey.batch_cmd](#) = 'sbatch '
- string [DFT_KIT.core.env_parm_odyssey.vasp_std_path](#) = ""
- string [DFT_KIT.core.env_parm_odyssey.vasp_complex_path](#) = ""
- string [DFT_KIT.core.env_parm_odyssey.vasp_gamma_path](#) = ""
- string [DFT_KIT.core.env_parm_odyssey.vasp_pseudo_dir](#) = '/n/home09/sfang/Pseudo_Potential/VASP/'

7.22 core/general_tool.py File Reference

Classes

- class [DFT_KIT.core.general_tool.segments](#)

Namespaces

- [DFT_KIT.core.general_tool](#)

Functions

- def [DFT_KIT.core.general_tool.bool_to_str](#)
- def [DFT_KIT.core.general_tool.convert_vector](#)
- def [DFT_KIT.core.general_tool.convert_array_2d](#)
- def [DFT_KIT.core.general_tool.vec_to_str](#)
- def [DFT_KIT.core.general_tool.get_unitvec](#)
- def [DFT_KIT.core.general_tool.vec_length](#)
- def [DFT_KIT.core.general_tool.vec_distance](#)
- def [DFT_KIT.core.general_tool.generate_rotation_matrix](#)
- def [DFT_KIT.core.general_tool.rot_x](#)
- def [DFT_KIT.core.general_tool.rot_y](#)
- def [DFT_KIT.core.general_tool.rot_z](#)
- def [DFT_KIT.core.general_tool.rotation_matrix](#)
- def [DFT_KIT.core.general_tool.get_parm](#)

7.23 core/job.py File Reference

Classes

- class [DFT_KIT.core.job.job](#)

Namespaces

- [DFT_KIT.core.job](#)

7.24 core/kpoint.py File Reference

Classes

- class [DFT_KIT.core.kpoint.kpoint](#)

Namespaces

- [DFT_KIT.core.kpoint](#)

Functions

- `def DFT_KIT.core.kpoint.generate_kgrid`

7.25 examples/gen_scripts.py File Reference

Namespaces

- [gen_scripts](#)

Variables

- list [gen_scripts.job_script](#) = sys.argv[2]
- tuple [gen_scripts.num_parm](#) = int(sys.argv[3])
- [gen_scripts.job_submit](#) = False
- tuple [gen_scripts.root_dir](#) = os.getcwd()
- string [gen_scripts.dir_prefix](#) = 'task'
- string [gen_scripts.job_name](#) = 'DFT_KIT_JOB'
- int [gen_scripts.num_cpu](#) = 2
- string [gen_scripts.job_queue](#) = "normal"
- string [gen_scripts.job_time](#) = "24:00:00"
- list [gen_scripts.module_load](#) = []
- string [gen_scripts.batch_fname](#) = 'DFT_KIT.batch'
- string [gen_scripts.task_dir](#) = root_dir+dir_prefix+"_"
- tuple [gen_scripts.f_](#) = open(batch_fname,'w')

7.26 examples/QESPRESSO_band_structure_spinorbit.py File Reference

Namespaces

- [QESPRESSO_band_structure_spinorbit](#)

7.27 examples/QESPRESSO_single_calculation.py File Reference

Namespaces

- [QESPRESSO_single_calculation](#)

Variables

- tuple [QESPRESSO_single_calculation.test_job](#) = job.job(subdir=False)
- tuple [QESPRESSO_single_calculation.test_kgrid](#) = kpoint.kpoint()
- tuple [QESPRESSO_single_calculation.test_crystal](#) = crystal_structure.a7_structure(element.Bi_exp,length↵_unit=1.0)
- tuple [QESPRESSO_single_calculation.test_calc](#) = QESPRESSO.calculator_QESPRESSO(False,test_↵job,test_crystal,test_kgrid,scheme=1)

7.28 examples/QESPRESSO_wannier90_tb.py File Reference

Namespaces

- [QESPRESSO_wannier90_tb](#)

Variables

- tuple [QESPRESSO_wannier90_tb.test_job](#) = job.job(subdir=False)
- tuple [QESPRESSO_wannier90_tb.test_kgrid](#) = kpoint.kpoint()
- tuple [QESPRESSO_wannier90_tb.test_crystal](#) = crystal_structure.a7_structure(element.Bi_exp,length_↵unit=1.0)
- tuple [QESPRESSO_wannier90_tb.test_calc](#) = QESPRESSO.calculator_QESPRESSO(False,test_job,test_↵_crystal,test_kgrid,scheme=1)

7.29 examples/sample_run.py File Reference

Namespaces

- [sample_run](#)

Variables

- tuple [sample_run.input_parm](#) = interface_script.init_simulation(0)
- tuple [sample_run.dft_job](#) = job.job(False)
- tuple [sample_run.dft_lattice](#) = crystal_3D.cubic_3D(2.56)
- tuple [sample_run.at1](#) = dft_lattice.add_atom(element.Bi_exp, position=np.array([0.0,0.0,0.0]),cc=3.45)
- tuple [sample_run.at2](#) = dft_lattice.add_atom(element.Bi_exp, position=np.array([1.0,1.0,1.0]),cc=3.1415)
- tuple [sample_run.dft_vasp](#) = VASP.calculator_VASP()

7.30 examples/VASP_band_structure.py File Reference

Namespaces

- [VASP_band_structure](#)

Variables

- tuple [VASP_band_structure.input_parm](#) = interface_script.init_simulation(0)
- tuple [VASP_band_structure.test_job](#) = job.job(subdir=True)
- tuple [VASP_band_structure.test_kgrid](#) = kpoint.kpoint()
- tuple [VASP_band_structure.test_crystal](#) = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)
- tuple [VASP_band_structure.test_calc](#) = VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0)

7.31 examples/VASP_band_structure_spinorbit.py File Reference

Namespaces

- [VASP_band_structure_spinorbit](#)

Variables

- tuple [VASP_band_structure_spinorbit.input_parm](#) = interface_script.init_simulation(0)
- tuple [VASP_band_structure_spinorbit.test_job](#) = job.job(subdir=True)
- tuple [VASP_band_structure_spinorbit.test_kgrid](#) = kpoint.kpoint()
- tuple [VASP_band_structure_spinorbit.test_crystal](#) = crystal_structure.a7_structure(bismuth_antimony.Bi_exp,length_unit=1.0)
- tuple [VASP_band_structure_spinorbit.test_calc](#) = VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0)

7.32 examples/VASP_ecutoff_convergence.py File Reference

Namespaces

- [VASP_ecutoff_convergence](#)

Variables

- int [VASP_ecutoff_convergence.expect_num_parm](#) = 1
- tuple [VASP_ecutoff_convergence.input_num_parm](#) = len(sys.argv)
- list [VASP_ecutoff_convergence.input_parm](#) = []
- tuple [VASP_ecutoff_convergence.e_ind](#) = int(input_parm[0])
- tuple [VASP_ecutoff_convergence.all_es](#) = np.linspace(200,300,6)
- list [VASP_ecutoff_convergence.e_now](#) = all_es[e_ind]
- tuple [VASP_ecutoff_convergence.test_job](#) = job.job(subdir=False)
- tuple [VASP_ecutoff_convergence.test_kgrid](#) = kpoint.kpoint()
- tuple [VASP_ecutoff_convergence.test_crystal](#) = crystal_structure.a7_structure(element.Bi_exp,length_unit=1.0)
- tuple [VASP_ecutoff_convergence.test_calc](#) = VASP.calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE',ENCUT=str(e_now))

7.33 examples/VASP_kgrid_convergence.py File Reference

Namespaces

- [VASP_kgrid_convergence](#)

7.34 examples/VASP_relaxation.py File Reference

Namespaces

- [VASP_relaxation](#)

7.35 examples/VASP_scan_parameters.py File Reference

Namespaces

- [VASP_scan_parameters](#)

7.36 examples/VASP_single_calculation.py File Reference

Namespaces

- [VASP_single_calculation](#)

Variables

- tuple [VASP_single_calculation.input_parm](#) = [interface_script.init_simulation\(0\)](#)
- tuple [VASP_single_calculation.test_job](#) = [job.job\(subdir=False\)](#)
- tuple [VASP_single_calculation.test_kgrid](#) = [kpoint.kpoint\(\)](#)
- tuple [VASP_single_calculation.test_crystal](#) = [crystal_structure.a7_structure\(element.Bi_exp,length_unit=1.0\)](#)
- tuple [VASP_single_calculation.test_calc](#) = [VASP.calculator_VASP\(False,test_job,test_crystal,test_kgrid,scheme=0\)](#)

7.37 interface/interface.py File Reference

Namespaces

- [DFT_KIT.interface.interface](#)

Functions

- def [DFT_KIT.interface.interface.dft_kit_to_ase_atoms](#)
- def [DFT_KIT.interface.interface.dft_kit_to_ase_kpts](#)
- def [DFT_KIT.interface.interface.load_from_xml](#)
- def [DFT_KIT.interface.interface.read_mat_file](#)
- def [DFT_KIT.interface.interface.write_mat_file](#)
- def [DFT_KIT.interface.interface.DFT_postana_serieswrite_csv](#)

7.38 interface/interface_script.py File Reference

Namespaces

- [DFT_KIT.interface.interface_script](#)

Functions

- def [DFT_KIT.interface.interface_script.init_simulation](#)

7.39 temp/gen_period_table.py File Reference

Namespaces

- [gen_period_table](#)

Variables

- `gen_period_table.tt` = `DFT_element.Bi`
- `gen_period_table.atm` = `DFT_atom.atom`
- tuple `gen_period_table.f_` = `open('pdata','r')`
- list `gen_period_table.ptable` = `['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al', 'Si', 'P', 'S', 'Cl', 'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn', 'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At', 'Rn', 'Fr', 'Ra', 'Ac', 'Th', 'Pa', 'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm', 'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt', 'Ds', 'Rg', 'Uub', 'Uut', 'Uuq', 'Uup', 'Uuh', 'Uuo']`
- list `gen_period_table.data` = `[]`
- tuple `gen_period_table.tmpstr` = `f_.readline()`
- tuple `gen_period_table.tmp`

7.40 temp/test.py File Reference

Namespaces

- `test`

Variables

- string `test.SIE_flags`

7.41 temp/test1.py File Reference

Namespaces

- `test1`

Variables

- tuple `test1.test_job` = `DFT_job.DFT_job(subdir=False)`
- tuple `test1.test_kgrid` = `DFT_kpoint.DFT_kpoint()`
- tuple `test1.test_crystal` = `DFT_crystal_3D.cubic_3D(2.56)`
- tuple `test1.test_atom1` = `test_crystal.add_atom(DFT_element.Bi, position=np.array([0.0,0.0,0.0]))`
- tuple `test1.test_atom2` = `test_crystal.add_atom(DFT_element.Bi, position=np.array([1.0,1.0,1.0]))`
- tuple `test1.test_atom3` = `test_crystal.add_atom(DFT_element.Sb, position=np.array([1.0,2.0,1.0]))`
- tuple `test1.test_calc` = `DFT_calculator_VASP.DFT_calculator_VASP(False,test_job,test_crystal,test_↵
kgrid,scheme=0,xc='PBE')`

7.42 temp/test2.py File Reference

Namespaces

- `test2`

Variables

- tuple `test2.test_job` = `DFT_job.DFT_job(subdir=False)`
- tuple `test2.test_kgrid` = `DFT_kpoint.DFT_kpoint()`
- tuple `test2.test_crystal` = `DFT_crystal_3D.cubic_3D(2.56)`
- tuple `test2.test_atom1` = `test_crystal.add_atom(DFT_element.Bi_exp, position=np.array([0.0,0.0,0.0]))`
- tuple `test2.test_atom2` = `test_crystal.add_atom(DFT_element.Bi_exp, position=np.array([1.0,1.0,1.0]))`
- tuple `test2.test_atom3` = `test_crystal.add_atom(DFT_element.Sb, position=np.array([1.0,2.0,1.0]))`
- tuple `test2.test_calc` = `DFT_calculator_QESPRESSO.DFT_calculator_QESPRESSO(False,test_job,test_crystal,test_kgrid,scheme=0)`

7.43 temp/test3.py File Reference

Namespaces

- `test3`

Variables

- tuple `test3.test_job` = `DFT_job.DFT_job(subdir=False)`
- tuple `test3.test_kgrid` = `DFT_kpoint.DFT_kpoint()`
- tuple `test3.test_crystal` = `wire_rhom.Rhom_trigonal_nanowire(DFT_element.Bi_exp,20,20,8,length_unit=1.0)`
- tuple `test3.test_calc` = `DFT_calculator_VASP.DFT_calculator_VASP(False,test_job,test_crystal,test_kgrid,scheme=0,xc='PBE')`

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