DFT_KIT

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Contents

Chapter 1

Namespace Index

1.1 Namespace List

Here is a list of all namespaces with brief descriptions:

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 3

Class Index

3.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

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_soi = {}
- dictionary Sb_qespresso_scf = {}
- dictionary Sb_qespresso_nscf_soi = {}
- 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','LMAXMIX':'4'}
- dictionary 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}
- 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.UPF',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','ED↩ IFF':'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,'rhom_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 lelfield 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 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 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 lelfield 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 tolp 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','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 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('ptdata','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('ptdata','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',ENCU↩ 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()

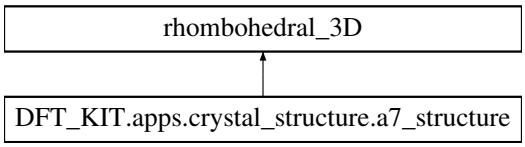
Definition at line 19 of file VASP_single_calculation.py.

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

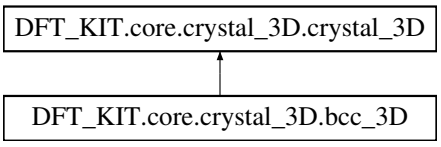
Definition at line 13 of file atom.py.

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*)

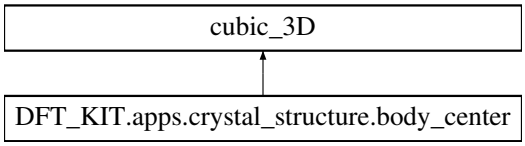
Definition at line 176 of file crystal_3D.py.

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

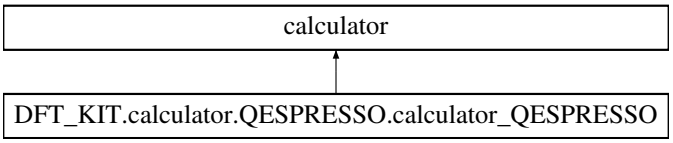
Definition at line 26 of file calculator.py.

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

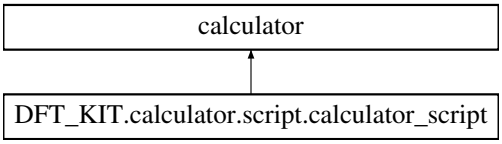
Definition at line 34 of file QESPRESSO.py.

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*)

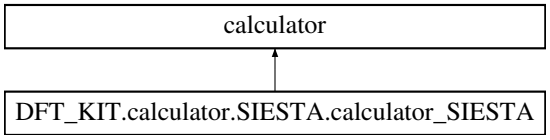
Definition at line 36 of file script.py.

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*)

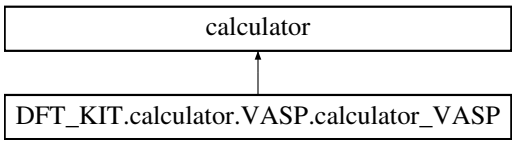
Definition at line 328 of file SIESTA.py.

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

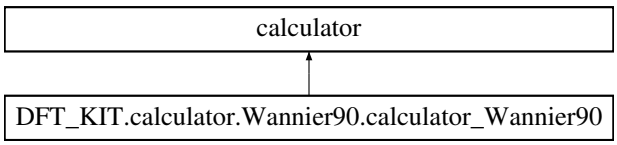
Definition at line 42 of file VASP.py.

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.

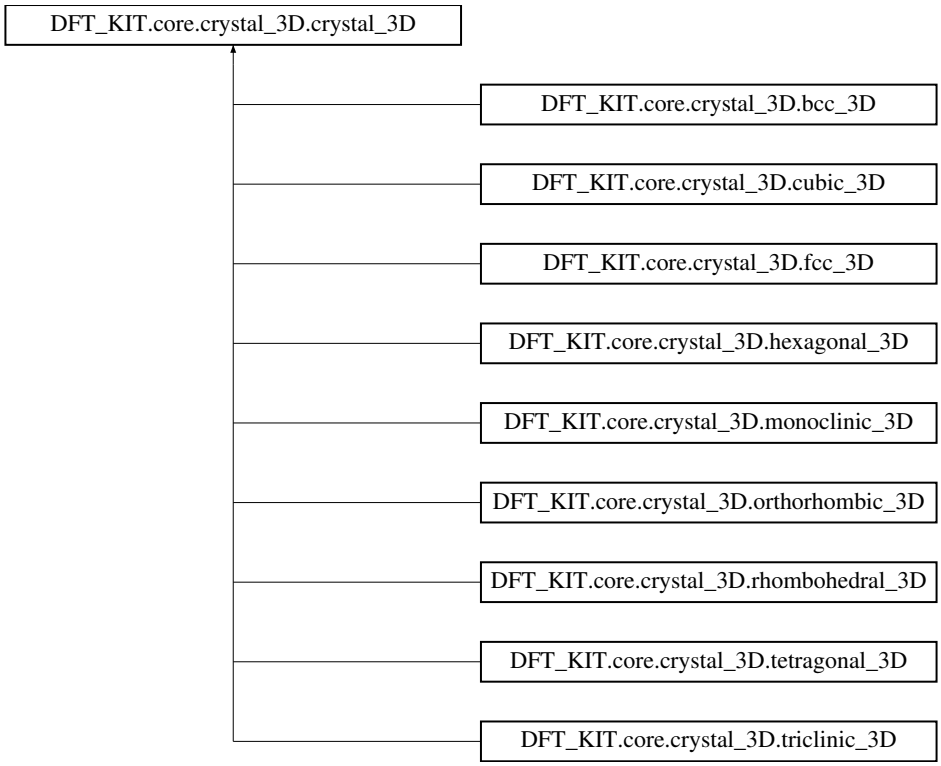
The documentation for this class was generated from the following file:

- 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 updata_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

length_unit	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

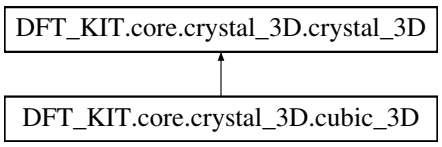
Definition at line 25 of file crystal_3D.py.

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*)

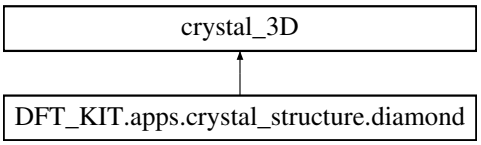
Definition at line 149 of file crystal_3D.py.

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

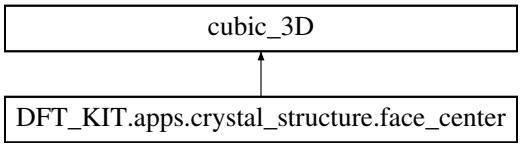
Definition at line 50 of file element.py.

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`)

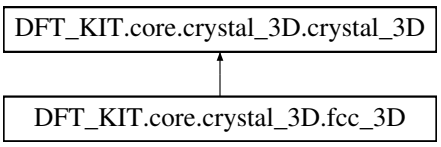
Definition at line 65 of file crystal_structure.py.

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*)

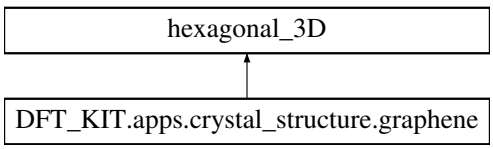
Definition at line 201 of file crystal_3D.py.

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*)

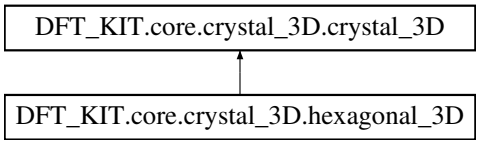
Definition at line 36 of file crystal_structure.py.

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

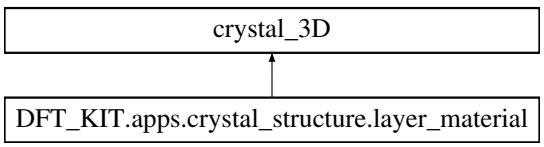
Definition at line 18 of file kpoint.py.

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)

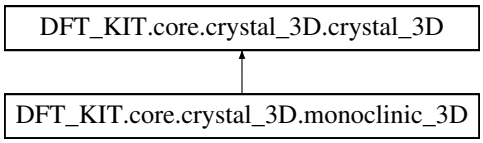
Definition at line 44 of file crystal_structure.py.

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_*)

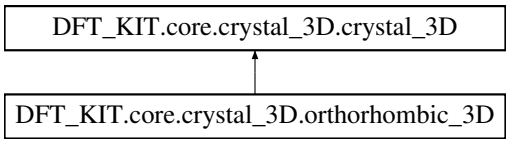
Definition at line 324 of file crystal_3D.py.

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_*)

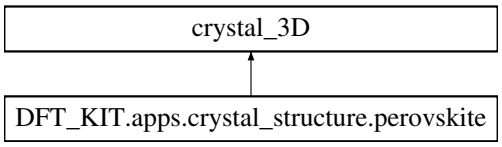
Definition at line 290 of file crystal_3D.py.

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`)

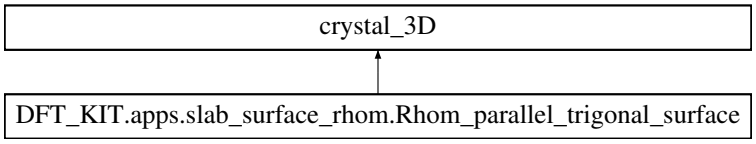
Definition at line 53 of file crystal_structure.py.

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

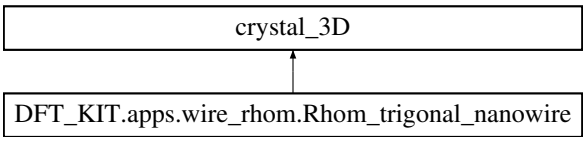
Definition at line 77 of file slab_surface_rhom.py.

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

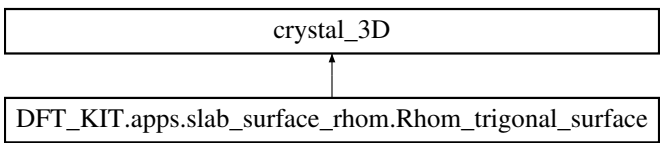
Definition at line 36 of file wire_rhom.py.

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

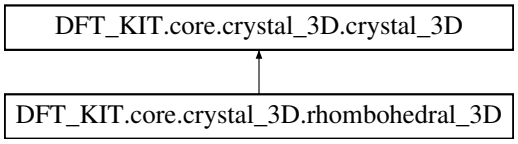
Definition at line 34 of file slab_surface_rhom.py.

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_*)

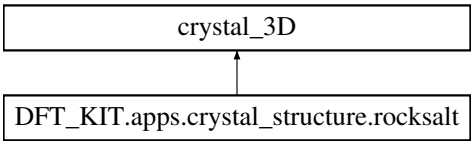
Definition at line 353 of file crystal_3D.py.

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

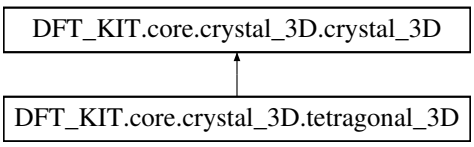
Definition at line 14 of file general_tool.py.

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_*)

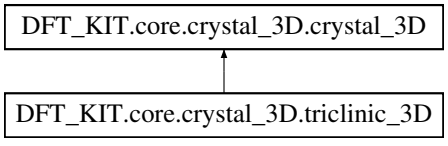
Definition at line 258 of file crystal_3D.py.

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 lelfield nberrycyc lorbm lberry gdir nppstr'
- 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,I) 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('ptdata','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')

Index