ABACUS-module_ORB

Release 0.1

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Namespace std

1.3.2 Classes and Structs

Class LCAO_Orbitals

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **LCAO_Orbitals**

advices for reconstructions:

each set of orbitals should have: lmax, dr, dk, rmax, lmax, etc.

the orbitals include : NAO, non-local projectors, descriptors, etc.

mohan note 2021-02-13

Public Functions

LCAO_Orbitals()

~LCAO_Orbitals()

void **Read_Orbitals**(ofstream &ofs_in, const int &ntype_in, const int &lmax_in, const int &out_descriptor, const int &out_r_matrix, const bool &force_flag, const int &my_rank)

void **Read_PAO**(ofstream &ofs_in, const int &it, const bool &force_flag, const int &my_rank)

void **Set_NonLocal**(const int &it, int &n_projectors)
in order to get rid of the .NONLOCAL file.

void **Read_NonLocal**(const int &it, int &n_projectors, const int &my_rank)
read in the NONLOCAL projector from file.

void **Read_Descriptor**(ofstream &ofs_in, const bool &force_flag, const int &my_rank)

inline const double &**get_ecutwfc**(void) const

inline const int &**get_kmesh**(void) const

inline const double &**get_dk**(void) const

inline const double &**get_dR**(void) const

inline const double &**get_Rmax**(void) const

inline const int &**get_lmax**(void) const

inline const int &**get_lmax_d**(void) const
lmax of descriptor basis

inline const int &**get_nchimax**(void) const

inline const int &**get_nchimax_d**(void) const
nchimax of descriptor basis

inline const int &**get_ntype**(void) const

inline const double &**get_dr_uniform**(void) const

inline const double &**get_rcutmax_Phi**(void) const

inline const double &**get_rcutmax_Beta**(void) const

Public Members

Numerical_Orbital ***Phi**
numerical atomic orbitals

Numerical_Nonlocal ***Beta**
nonlocal projectors (1-dimension array)

Numerical_Orbital ***Alpha**
descriptor bases, saved as one-type atom orbital

double **ecutwfc**

double **dk**

double **dR**

double **Rmax**

int ***nproj**

int **nprojmax**

double **dr_uniform**

bool **read_in_flag**

std::vector<string> **orbital_file**

std::vector<string> **nonlocal_file**

string **descriptor_file**

Class Numerical_Nonlocal

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **Numerical_Nonlocal**

CLASS

Note : contain nonlocal ps(:pseudopotential) information about atoms

Feature : set and store information about ps infomation related to atoms

AUTHOR : liaochen

DATE : 2008-03-04

Public Functions

Numerical_Nonlocal()

~Numerical_Nonlocal()

inline const int &**getLmax**() const

inline const int &**getType**() const

inline const string &**getLabel**() const

inline const string &**getType_ps**() const

void **set_type_info**(const int &type_in, const string &label_in, const string &type_ps_in, const int &lmax_in, const int &nproj_in, const *Numerical_Nonlocal_Lm* *ps_orbital_in)

inline const double &**get_rcut_max**(void) const

Public Members

Numerical_Nonlocal_Lm ***Proj**

length: nproj(only store radial function)

Class Numerical_Nonlocal_Lm

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **Numerical_Nonlocal_Lm**

CLASS

Note : contain information about each projector all features of projector's shape

AUTHOR : liaochen

DATE : 2008-03-04

Public Functions

Numerical_Nonlocal_Lm()

use Polynomial_Interpolation_xy, Spherical_Bessel use SplineD2

~Numerical_Nonlocal_Lm()

inline const int &**getL**() const

inline const int &**getType**() const

inline const double &**getRcut**() const

inline const double *__getRadial__() const

inline const double &**getRadial**(const int &ir) const

inline const double *__getBeta_r__() const

inline const double &**getBeta_r**(const int &ir) const

inline const double &**getDk**() const

inline const double *__getKpoint__() const

inline const double &**getKpoint**(const int &ik) const

inline const double *__getBeta_k__() const

inline const double &**getBeta_k**(const int &ik) const

Numerical_Nonlocal_Lm &**operator=**(const *Numerical_Nonlocal_Lm* &nol)

void **set_NL_proj**(const string &label, const int &index_atom_type_in, const int &angular_momentum_l_in, const int &nr_in, const double *rab_in, const double *r_radial_in, const double *beta_r_in, const int &nk_in, const double &dk_in, const double &dr_uniform_in)

void **plot**(const int &my_rank) const

Public Members

double ***beta_uniform**

double ***dbeta_uniform**

int **nr_uniform**

double **dr_uniform**

Class Numerical_Orbital

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **Numerical_Orbital**

CLASS Num_Orbital

Note : contain information about atoms

Feature : set and store information about atoms

Public Functions

Numerical_Orbital()

~Numerical_Orbital()

inline const int &**getLmax**() const

inline const double &**getRcut**() const

inline const int &**getType**() const

inline const int &**getTotal_nchi**() const

inline const int &**getNchi**(const int l) const

inline const string &**getLabel**() const

inline const *Numerical_Orbital_Lm* &**PhiLN**(const int &L, const int &N) const

void **set_orbital_info**(const int &type_in, const string &label_in, const int &lmax_in, const int *nchi_in, const int &total_nchi)
set information about Numerical Orbital

Public Static Functions

static inline double &**get_distance**()
about the distance between two atoms.

static inline double **getX**()

static inline double **getY**()

static inline double **getZ**()

static inline Vector3<double> &**getR1**()

static inline Vector3<double> &**getR2**()

static inline Vector3<double> &**getdR**()

static inline void **set_position**(const Vector3<double> R1_in, const Vector3<double> R2_in)

Class Numerical_Orbital_Lm

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **Numerical_Orbital_Lm**
CLASS Num_orbital_lm

Note : contain information about each orbital : psi(l,m) all features of orbital's shape

Public Types

enum **Psi_Type**
Values:

enumerator **Psi**

enumerator **Psif**

enumerator **Psik**

enumerator **Psik2**

Public Functions

Numerical_Orbital_Lm()

~Numerical_Orbital_Lm()

void **set_orbital_info**(const string &label_in, const int &index_atom_type_in, const int &angular_momentum_l_in, const int &index_chi_in, const int &nr_in, const double *rab_in, const double *r_radial_in, const *Psi_Type* &psi_type, const double *psi_in, const int &nk_in, const double &dk_in, const double &dr_uniform, bool flag_plot, bool flag_sbpool, const bool &force_flag)

EXPLAIN : set information about *Numerical_Orbital_Lm*.

inline const string &**getLabel**() const

inline const int &**getType**() const

inline const int &**getL**() const

inline const int &**getChi**() const

inline const double *__getPsiuniform__() const

inline const double *__getDpsiuniform__() const

inline const int &**getNruniform**() const

inline const double &**getDruniform**() const

inline const int &**getNr**() const

inline const int &**getNk**() const

inline const double &**getRcut**() const

inline const double &**getKcut**() const

inline const double *__getRadial__() const

inline const vector<double> &**get_r_radial**() const

inline const double &**getRadial**(const int ir) const

inline const double *getRab() const

inline const vector<double> &get_rab() const

inline const double &getRab(const int ir) const

inline const double &getDk() const

inline const double *getKpoint() const

inline const double &getKpoint(const int ik) const

inline const vector<double> &get_k_radial() const

inline const double *getPsi() const

inline const double &getPsi(const int ir) const

inline const vector<double> &get_psi() const

inline const double *getPsi_r() const

inline const double &getPsi_r(const int ir) const

inline const double *getPsif() const

inline const double &getPsif(const int ik) const

inline const vector<double> &get_psif() const

inline const double *getPsi_k() const

inline const double &getPsi_k(const int ik) const

inline const vector<double> &get_psi_k() const

inline const double *getPsi_k2() const

inline const double &getPsi_k2(const int ik) const

inline const vector<double> &get_psi_k2() const

Public Members

vector<double> **psi_uniform**

vector<double> **dpsi_uniform**

int **nr_uniform**

double **dr_uniform**

double **zty**
the valus of psi at 0.

Class ORB_control

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **ORB_control**

Public Functions

ORB_control()

~ORB_control()

void **set_orb_tables**(ofstream &ofs_in, *ORB_gen_tables* &OGT, *LCAO_Orbitals* &orb, const int &ntype, const int &lmax, const double &lcao_ecut_in, const double &lcao_dk_in, const double &lcao_dr_in, const double &lcao_rmax_in, const double &lat0, const int &out_descriptor, const int &out_r_matrix, const int &Lmax_exx, const bool &force_flag, const int &my_rank)
Generate the S(overlap),T,NL matrix.

Parameters

- **ntype** – number of speceies, mohan add 2021-04-26
- **lmax** – value of Lmax for basis, mohan add 2021-04-26

void **clear_after_ions**(*ORB_gen_tables* &OGT, *LCAO_Orbitals* &orb, const int &out_descriptor)

Class ORB_gaunt_table

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **ORB_gaunt_table**

Public Functions

ORB_gaunt_table()

~ORB_gaunt_table()

void **init_Gaunt_CH**(const int &Lmax)
Method 2: using WIgner 3j symbols $Y(l1, m1), Y(l2, m2), Y(L, M)$

double **Get_Gaunt_CH**(const int &l1, const int &m1, const int &l2, const int &m2, const int &l3, const int &m3)

double **Get_Gaunt_SH**(const int &l1, const int &mm1, const int &l2, const int &mm2, const int &l3, const int &mm3)
M defined here are restricted within 0 to 2l+1

should be transformed first

Input value, m1, m2, m3 are restricted within 0 to 2l+1, and should be transformed first.

double **Calc_Gaunt_CH**(const int &l1, const int &m1, const int &l2, const int &m2, const int &l3, const int &m3)

void **init_Ylm_Gaunt**(const int &lmax, const double &s1, const double &e1, const double &s2, const double &e2)
(1) Make Ylm_Gaunt Table.

double **Cal_Gaunt_single**(const int &l1, const int &m1, const int &l2, const int &m2, const int &l, const int &m, const double &s1, const double &e1, const double &s2, const double &e2)
(2) Use Ylm_Gaunt to calculate Gaunt Coefficinets element

void **init_Gaunt**(const int &lmax)
(3) Make the whole Gaunt Coefficients table

Public Members

realArray **Gaunt_Coefficients**
MEthod 2

Directly Calculate integral of $S(l_1, m_1), S(l_2, m_2), S(L, M)$

Public Static Functions

static int **get_lm_index**(const int l, const int m)

static int **Index_M**(const int &m)

Class ORB_gen_tables

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **ORB_gen_tables**
used to be 'Use_Overlap_Table', now the name is '*ORB_gen_tables*'

Public Functions

ORB_gen_tables()

~ORB_gen_tables()

void **gen_tables**(ofstream &ofs_in, const int &job0, *LCAO_Orbitals* &orb, const int &Lmax_exx, const int &out_descriptor)
call in hamilt_linear::init_before_ions.

Parameters **out_descriptor** – whether to generate descriptors

inline void **set_unit**(const double &v)

void **snap_psipsi**(double olm[], const int &job, const char &dtype, const Vector3<double> &R1, const int &I1, const int &l1, const int &m1, const int &n1, const Vector3<double> &R2, const int &I2, const int &l2, const int &m2, const int &n2, const int &nspin, complex<double> *olm1 = NULL) const

Parameters

- **job** – 0 for matrix element of either S or T, 1 for its derivatives
- **dtype** – derivative type, 'S' for overlap, 'T' for kinetic energy, 'D' for descriptor in deepks

void **snap_psibeta**(double nlm[], const int &job, const Vector3<double> &R1, const int &I1, const int &l1, const int &m1, const int &n1, const Vector3<double> &R2, const int &I2, const int &l2, const int &m2, const int &n2, const Vector3<double> &Rnl, const int &type, const matrix &dion, const int &nspin, const ComplexArray &d_so, const int &count_soc, int *index1_soc, int *index2_soc, const int &nproj_in, complex<double> *nlm1 = NULL, const int is = 0) const

Parameters **job** – job = 0 for vnl matrix elements, job = 1 for its derivatives

Public Members

ORB_table_phi **MOT**
set as public because in hamilt_linear, we need to destroy the tables: SR,TR,NR after ionic optimization is done.

ORB_table_beta **tbeta**

ORB_table_alpha **talpha**
if we want to add table for descriptors, we should consider here mohan 2021-02-09

Friends

friend class ORB_control

Class ORB_table_alpha

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **ORB_table_alpha**

Public Functions

ORB_table_alpha()

~ORB_table_alpha()

void **allocate**(const int &ntype, const int &lmax_in, const int &kmesh_in, const double &Rmax_in, const double &dR_in, const double &dk_in)

void **init_DS_Opair**(void)
O stands for orbitals.

void **init_DS_2Lplus1**(void)

void **init_Table_Alpha**(Sph_Bessel_Recursive::D2 *pSB)

void **Destroy_Table_Alpha**(void)

Public Members

double *****Table_DSR**
overlap between lcao basis phi and descriptor basis alpha

bool **destroy_nr**

IntArray **DS_Opair**

int ***DS_2Lplus1**

int **Rmesh**

int **ntype**

int **lmax**

Public Static Functions

static int **get_rmesh**(const double &R1, const double &R2)

Public Static Attributes

static double **dr** = -1.0

Class ORB_table_beta

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **ORB_table_beta**

Public Functions

ORB_table_beta()

~ORB_table_beta()

void **allocate**(const int &ntype, const int &lmax_in, const int &kmesh_in, const double &Rmax_in, const double &dR_in, const double &dk_in)

void **init_NL_Tpair**(void)
NL stands for 'nonlocal', T stands for atom type. O stands for orbitals.

void **init_NL_Opair**(*LCAO_Orbitals* &orb)

void **init_Table_Beta**(Sph_Bessel_Recursive::D2 *pSB)

void **Destroy_Table_Beta**(*LCAO_Orbitals* &orb)

Public Members

double *****Table_NR**

bool **destroy_nr**

int **NL_nTpairs**

IntArray **NL_Tpair**

IntArray **NL_Opair**

IntArray **NL_L2plus1**

int **Rmesh**

Public Static Functions

static int **get_rmesh**(const double &R1, const double &R2)

Public Static Attributes

static double **dr** = -1.0

Class ORB_table_phi

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Class Documentation

class **ORB_table_phi**

Public Functions

ORB_table_phi()

~ORB_table_phi()

void **allocate**(const int &ntype, const int &lmax_in, const int &kmesh_in, const double &Rmax_in, const double &dR_in, const double &dk_in)

Parameters

- **ntype** – number of atom types
- **lmax_in** – max L used to calculate overlap
- **kmesh_in** – kpoints, for integration in k space
- **Rmax_in** – max value of radial table
- **dR_in** – delta R, for making radial table
- **dk_in** – delta k, for integration in k space

void **init_Table**(const int &job, *LCAO_Orbitals* &orb)

void **Destroy_Table**(*LCAO_Orbitals* &orb)

void **init_Lmax**(const int orb_num, const int mode, int &Lmax_used, int &Lmax, const int &Lmax_exx) const

make table of Spherical bessel

Sph_Bes : jlx[kmesh][Rmesh][L], L should be 2*Lmax, which is max L of all type

void **init_Table_Spherical_Bessel**(const int orb_num, const int mode, int &Lmax_used, int &Lmax, const int &Lmax_exx)

void **init_OV_Tpair**(*LCAO_Orbitals* &orb)

make the index, in order to get the element from Table_SR and Table_TR quickly. OV stands for 'overlap'

T stands for atom type.

void **init_OV_Opair**(*LCAO_Orbitals* &orb)

O stands for orbitals.

void **cal_ST_Phi12_R**(const int &job, const int &l, const *Numerical_Orbital_Lm* &n1, const *Numerical_Orbital_Lm* &n2, const int &rmesh, double *rs, double *drs) const

void **cal_ST_Phi12_R**(const int &job, const int &l, const *Numerical_Orbital_Lm* &n1, const *Numerical_Orbital_Lm* &n2, const set<size_t> &radials, double *rs, double *drs) const

Public Members

double *****Table_SR
Five dimension:

(1) 0: normal (S(R)) ; 1: derivative(dS/dR)

(2) pairs type number.

(3) pairs chi

(4) Max angular momentum: L.

(5) Distance between atoms: R.

double *****Table_TR

bool **destroy_sr**

bool **destroy_tr**

Sph_Bessel_Recursive::D2 ***pSB** = nullptr

int **OV_nTpairs**

IntArray **OV_Tpair**

IntArray **OV_Opair**

IntArray **OV_L2plus1**

int **Rmesh**

Public Static Functions

static int **get_rmesh**(const double &R1, const double &R2)

Public Static Attributes

static double **dr** = -1.0

1.3.3 Functions

Function calculate

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Function Documentation

Warning: doxygenfunction: Cannot find function “calculate” in doxygen xml output for project “ABACUS-module_ORB” from directory: ../../doxygen/xml/

Function main

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Function Documentation

Warning: doxygenfunction: Cannot find function “main” in doxygen xml output for project “ABACUS-module_ORB” from directory: ../../doxygen/xml/

1.3.4 Variables

Variable conf::author

- Defined in file_source_conf.py

Variable Documentation

```
conf.author = 'mohan'
```

Variable conf::breathe_default_project

- Defined in file_source_conf.py

Variable Documentation

```
conf.breathe_default_project = "ABACUS-module_ORB"
```

Variable conf::breathe_projects

- Defined in file_source_conf.py

Variable Documentation

conf.**breathe_projects = { "ABACUS-module_ORB": "../../doxygen/xml/" }**

Variable conf::chinese

- Defined in file_source_conf.py

Variable Documentation

conf.**chinese = any([language_user in ('zh_CN', 'zh_TW'),project_language in ('zh_CN', 'zh_TW'),])**

Variable conf::context

- Defined in file_source_conf.py

Variable Documentation

conf.**context**

Variable conf::copyright

- Defined in file_source_conf.py

Variable Documentation

conf.**copyright = '2021, x'**

Variable conf::exclude_patterns

- Defined in file_source_conf.py

Variable Documentation

conf.**exclude_patterns = []**

Variable conf::exhale_args

- Defined in file_source_conf.py

Variable Documentation

```
conf.exhale_args = {# These arguments are required"containmentFolder":
"./ORB_api","rootFileName":  "library_root.rst","rootFileTitle":  "ORB
API","doxygenStripFromPath":  "..",# Suggested optional arguments"createTreeView":
True,# TIP: if using the sphinx-bootstrap-theme, you need# "treeViewIsBootstrap":
True,"exhaleExecutesDoxygen":  True,"exhaleDoxygenStdin":  "INPUT = ../../.."}
```

Variable conf::extensions

- Defined in file_source_conf.py

Variable Documentation

```
conf.extensions = [ 'sphinx.ext.todo', 'breathe', 'exhale', 'sphinx.ext.mathjax',
"sphinx_rtd_theme", 'myst_parser']
```

Variable conf::highlight_language

- Defined in file_source_conf.py

Variable Documentation

```
conf.highlight_language = 'cpp'
```

Variable conf::html_baseurl

- Defined in file_source_conf.py

Variable Documentation

```
conf.html_baseurl = context['canonical_url']
```

Variable conf::html_context

- Defined in file_source_conf.py

Variable Documentation

conf.**html_context = context**

Variable conf::html_static_path

- Defined in file_source_conf.py

Variable Documentation

conf.**html_static_path = ['_static']**

Variable conf::html_style

- Defined in file_source_conf.py

Variable Documentation

conf.**html_style = None**

Variable conf::html_theme

- Defined in file_source_conf.py

Variable Documentation

conf.**html_theme = "sphinx_rtd_theme"**

Variable conf::html_theme_options

- Defined in file_source_conf.py

Variable Documentation

conf.**html_theme_options = {}**

Variable conf::html_theme_path

- Defined in file_source_conf.py

Variable Documentation

conf.**html_theme_path = [theme.get_html_theme_path()]**

Variable conf::japanese

- Defined in file_source_conf.py

Variable Documentation

conf.**japanese = any([language_user == 'ja',project_language == 'ja',])**

Variable conf::language_user

- Defined in file_source_conf.py

Variable Documentation

conf.**language_user = globals().get('language', None)**

Variable conf::latex_elements

- Defined in file_source_conf.py

Variable Documentation

conf.**latex_elements = latex_elements_user or latex_elements_rtd**

Variable conf::latex_elements_rtd

- Defined in file_source_conf.py

Variable Documentation

```
conf.latex_elements_rtd = {'preamble':  '\\usepackage[UTF8]{ctex}\n',}
```

Variable conf::latex_elements_user

- Defined in file_source_conf.py

Variable Documentation

```
conf.latex_elements_user = globals().get('latex_elements', None)
```

Variable conf::latex_engine

- Defined in file_source_conf.py

Variable Documentation

```
conf.latex_engine = latex_engine_user or 'xelatex'
```

Variable conf::latex_engine_user

- Defined in file_source_conf.py

Variable Documentation

```
conf.latex_engine_user = globals().get('latex_engine', None)
```

Variable conf::latex_use_xindy

- Defined in file_source_conf.py

Variable Documentation

conf.**latex_use_xindy = False**

Variable conf::primary_domain

- Defined in file_source_conf.py

Variable Documentation

conf.**primary_domain = 'cpp'**

Variable conf::project

- Defined in file_source_conf.py

Variable Documentation

conf.**project = 'ABACUS-module_ORB'**

Variable conf::project_language

- Defined in file_source_conf.py

Variable Documentation

conf.**project_language = 'en'**

Variable conf::PY3

- Defined in file_source_conf.py

Variable Documentation

conf.**PY3 = 3**

Variable conf::readthedocs_build_url

- Defined in file_source_conf.py

Variable Documentation

```
conf.readthedocs_build_url = 'https://readthedocs.org/projects/myabacus/builds/14216766/'
```

Variable conf::readthedocs_vcs_url

- Defined in file_source_conf.py

Variable Documentation

```
conf.readthedocs_vcs_url = 'None'
```

Variable conf::release

- Defined in file_source_conf.py

Variable Documentation

```
conf.release = '0.1'
```

Variable conf::string_types

- Defined in file_source_conf.py

Variable Documentation

```
conf.string_types = str if PY3 else basestring
```

Variable conf::SUFFIX

- Defined in file_source_conf.py

Variable Documentation

conf.**SUFFIX = source_suffix**

Variable conf::templates_path

- Defined in file_source_conf.py

Variable Documentation

conf.**templates_path = ['_templates']**

Variable conf::theme

- Defined in file_source_conf.py

Variable Documentation

conf.**theme = importlib.import_module('sphinx_rtd_theme')**

Variable conf::using_rtd_theme

- Defined in file_source_conf.py

Variable Documentation

conf.**using_rtd_theme = (('html_theme' in globals() andhtml_theme in ['default'] and# Allow people to bail with a hack of having an html_style'html_style' not in globals()) or 'html_theme' not in globals())**

Variable conf::websupport2_base_url

- Defined in file_source_conf.py

Variable Documentation

conf.**websupport2_base_url = 'https://readthedocs.org/websupport'**

Variable conf::websupport2_static_url

- Defined in file_source_conf.py

Variable Documentation

```
conf.websupport2_static_url = 'https://assets.readthedocs.org/static/'
```

Variable ORB

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Variable Documentation

LCAO_Orbitals **ORB**

PLEASE avoid using 'ORB' as global variable.

PLEASE avoid using 'ORB' as global variable

mohan note 2021 - 03 - 23

Variable ORB

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Variable Documentation

LCAO_Orbitals **ORB**

PLEASE avoid using 'ORB' as global variable.

PLEASE avoid using 'ORB' as global variable

mohan note 2021 - 03 - 23

Variable UOT

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Variable Documentation

ORB_gen_tables **UOT**

here is a member of *ORB_gen_tables* class

PLEASE try to get rid of UOT, which is a global variable mohan add 2021-03-30

Variable UOT

- Defined in file__home_docs_checkouts_readthedocs.org_user_builds_myabacus_checkouts_latest_ABACUS.develop_source_mo

Variable Documentation

ORB_gen_tables **UOT**
here is a member of *ORB_gen_tables* class

PLEASE try to get rid of UOT, which is a global variable mohan add 2021-03-30

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