Can MgO and CaO grow on each other?

Group 4

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Contents

Chapter 1

Getting started

Group 4 term 3

1. Generate a lattice using `lattice.f90`
2. Run the simulation using `run_castep.sh`
3. Find the convex hull using `convex_hull.py`

To run on Physlogin use `run_castep_ebor.sh`.

For full documentation, see `latex/refman.pdf`.

Generate your own copy of this documentation, including an interactive HTML version, by running `makedoc.sh` (requires `doxygen`).

Chapter 2

Todo List

Subprogram lattice

Produce a pair of sheets with a vacuum between them

Chapter 3

Namespace Index

3.1 Namespace List

Here is a list of all namespaces 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 constants Module Reference

Module contains definitions of useful constants.

Variables

- integer, parameter dp =selected_real_kind(15, 300)

  Double-precision real kind.
- real(kind=dp), parameter pi = 4.0_dp∗atan(1.0_dp)

  The circle constant, pi.
- real(kind=dp), parameter tau = 2.0_dp∗pi

  2∗pi

5.1.1 Detailed Description

Module contains definitions of useful constants.

5.1.2 Variable Documentation

5.1.2.1 integer, parameter constants::dp =selected_real_kind(15, 300)

Double-precision real kind.

Definition at line 8 of file constants.f90.

5.1.2.2 real(kind=dp), parameter constants::pi = 4.0_dp∗atan(1.0_dp)

The circle constant, pi.

Definition at line 11 of file constants.f90.

5.1.2.3 real(kind=dp), parameter constants::tau = 2.0_dp∗pi

2∗pi

Definition at line 12 of file constants.f90.

5.2 convex_hull Namespace Reference

Variables

- string file_name = 'madeup.dat'
- data = np.genfromtxt(file_name, usecols = (0, 1))
- n = len(data)
- convex_hull = open('convex_hull.dat', 'w')
- int hv_new = 0
- float theta_max = -2.0
- int theta = -1
- max_loc = i

5.2.1 Variable Documentation

5.2.1.1 convex_hull.convex_hull = open('convex_hull.dat', 'w')

Definition at line 18 of file convex_hull.py.

5.2.1.2 convex_hull.data = np.genfromtxt(file_name, usecols = (0, 1))

Definition at line 12 of file convex_hull.py.

5.2.1.3 string convex_hull.file_name = 'madeup.dat'

Definition at line 11 of file convex_hull.py.

5.2.1.4 convex_hull.hv_new = 0

Definition at line 22 of file convex_hull.py.

5.2.1.5 convex_hull.max_loc = i

Definition at line 35 of file convex_hull.py.

5.2.1.6 convex_hull.n = len(data)

Definition at line 15 of file convex_hull.py.

5.2.1.7 int convex_hull.theta = -1

Definition at line 31 of file convex_hull.py.

5.2.1.8 convex_hull.theta_max = -2.0

Definition at line 27 of file convex_hull.py.

Chapter 6

File Documentation

6.1 constants.f90 File Reference

Modules

- module constants

  Module contains definitions of useful constants.

Variables

- integer, parameter constants::dp =selected_real_kind(15, 300)

  Double-precision real kind.
- real(kind=dp), parameter constants::pi = 4.0_dp∗atan(1.0_dp)

  The circle constant, pi.
- real(kind=dp), parameter constants::tau = 2.0_dp∗pi

  2∗pi

6.2 convex_hull.py File Reference

Namespaces

- convex_hull

Variables

- string convex_hull.file_name = 'madeup.dat'
- convex_hull.data = np.genfromtxt(file_name, usecols = (0, 1))
- convex_hull.n = len(data)
- convex_hull.convex_hull = open('convex_hull.dat', 'w')
- int convex_hull.hv_new = 0
- float convex_hull.theta_max = -2.0
- int convex_hull.theta = -1
- convex_hull.max_loc = i

6.3 lattice.f90 File Reference

Functions/Subroutines

- program lattice

  Fortran 2003 program to generate an initial lattice.
- subroutine sheet_init (L, V, sheet)

  Initialises a thin sheet of randomly-arranged atoms.
- subroutine cube_init (L, cube, prop)

  Initialises a cube of randomly-arranged atoms.
- subroutine write_cube (cube, L, prop, fileno)

  Writes a generated cube to a CASTEP cell file.
- subroutine write_sheet (sheet, L, V, fileno)

  Writes a generated sheet to a CASTEP cell file.

6.3.1 Function/Subroutine Documentation

6.3.1.1 subroutine lattice::cube_init (integer, intent(in) *L,* integer, dimension(:,:,:), intent(inout), allocatable *cube,* real(kind=dp), intent(inout) *prop*)

Initialises a cube of randomly-arranged atoms.

Parameters

in	*L*	(integer) length of a side of the cube
out	*cube*	(integer array) the generated cube
in	*prop*	(real) proportion of metal ions that are calcium

Definition at line 92 of file lattice.f90.

6.3.1.2 program lattice ( )

Fortran 2003 program to generate an initial lattice.

Todo Produce a pair of sheets with a vacuum between them

This program creates a CASTEP cell file consisting of a random arrangement of Ca and Mg atoms in a crystal structure with oxygen, according to a user specification.

Definition at line 8 of file lattice.f90.

6.3.1.3 subroutine lattice::sheet_init (integer, intent(in) *L,* integer, intent(in) *V,* integer, dimension(:,:,:), intent(inout), allocatable *sheet*)

Initialises a thin sheet of randomly-arranged atoms.

Parameters

in	*L*	(integer) length of a side of the sheet
in	*V*	(integer) total height of the structure
out	*sheet*	(integer array) the generated sheet

Definition at line 54 of file lattice.f90.

6.3.1.4 subroutine lattice::write_cube (integer, dimension(:,:,:), intent(in), allocatable *cube,* integer, intent(in) *L,* real(kind=dp), intent(in) *prop,* integer, intent(in) *fileno*)

Writes a generated cube to a CASTEP cell file.

Parameters

in	*cube*	(integer array) the cube of atoms
in	*L*	(real) length of a side of the cube
in	*prop*	(real) proportion of metal ions that are calcium
in	*fileno*	(integer) the memory unit corresponding to the file to which to write

Definition at line 161 of file lattice.f90.

6.3.1.5 subroutine lattice::write_sheet (integer, dimension(:,:,:), intent(in), allocatable *sheet,* integer, intent(in) *L,* integer, intent(in) *V,* integer, intent(in) *fileno*)

Writes a generated sheet to a CASTEP cell file.

Parameters

in	*sheet*	(integer array) the sheet of atoms
in	*L*	(real) length of a side of the sheet
in	*V*	(integer) total height of the structure
in	*fileno*	(integer) the memory unit corresponding to the file to which to write

Definition at line 228 of file lattice.f90.

6.4 README.md File Reference

Index