

Can MgO and CaO grow on each other?

Group 4

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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 <https://github.com/mges501York/Group-4-Term-3/blob/master/latex/refman.pdf>. Generate your own copy of this documentation 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:

constants	Module contains definitions of useful constants	9
convex_hull	10

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

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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

<i>L</i>	(input, integer) length of a side of the cube
<i>cube</i>	(output, integer array) the generated cube
<i>prop</i>	(input, 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

<i>L</i>	(input, integer) length of a side of the sheet
<i>V</i>	(input, integer) total height of the structure
<i>sheet</i>	(output, 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

<i>cube</i>	(input, integer array) the cube of atoms
<i>L</i>	(input, real) length of a side of the cube
<i>prop</i>	(input, real) proportion of metal ions that are calcium
<i>fileno</i>	(input, 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

<i>sheet</i>	(input, integer array) the sheet of atoms
<i>L</i>	(input, real) length of a side of the sheet
<i>V</i>	(input, integer) total height of the structure
<i>fileno</i>	(input, 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

6.5 run_castep.sh File Reference

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