OpenKIMTests

0.1

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Contents

Chapter 1

Class Index

1.1 Class Hierarchy

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

Chapter 2

Class Index

2.1 Class List

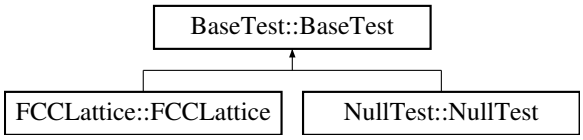
Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 3

Class Documentation

3.1 BaseTest::BaseTest Class Reference

Inheritance diagram for BaseTest::BaseTest:



Public Member Functions

- def **__init__**
- def XMLWriter
- def getASEPotentialByName
- def TestResults
- def Verify
- def main

Public Attributes

- **potentialname**
- **potential**
- **element**
- **verify**
- **write**
- **TestDependencies**

3.1.1 Detailed Description

```
This is the Base Test from which all other Tests inherit.
```

Definition at line 18 of file BaseTest.py.

3.1.2 Member Function Documentation

3.1.2.1 def BaseTest::BaseTest::getASEPotentialByName (*self, name*)

```
A little helper method to call ASE potentials by name.

In the future, to be extended to include KIM potentials
```

Definition at line 96 of file BaseTest.py.

3.1.2.2 def BaseTest::BaseTest::main (*self*)

```
Main is called when the Test is run from the command line. currently runs tests
and passes the dictionary of results to the XMLWriter Method
```

Definition at line 116 of file BaseTest.py.

3.1.2.3 def BaseTest::BaseTest::TestResults (*self*)

```
The Test Results method, runs the test and packages the result in a dictionary
```

Reimplemented in FCCLattice::FCCLattice, and NullTest::NullTest.

Definition at line 106 of file BaseTest.py.

3.1.2.4 def BaseTest::BaseTest::Verify (*self*)

```
Optional verify method, creates an easy to check visual verification of test results
```

Reimplemented in FCCLattice::FCCLattice, and NullTest::NullTest.

Definition at line 111 of file BaseTest.py.

3.1.2.5 def BaseTest::BaseTest::XMLWriter (*self, resultsdict*)

```
This method packages the results dictionary into our standard XML
Format.  The layout is roughly as follows

<test id='TestName'>
    <config>
<potential> PotentialName </potential>
<element> Element Symbol </element>
    </config>
    <results>
<FirstResultKey> FirstResultValue </FirstResultKey>
<SecondResultKey> SecondResultValue </SecondResultKey>
...
    </results>
</test>
```

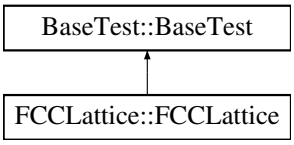
Definition at line 30 of file BaseTest.py.

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

- tests/BaseTest.py

3.2 FCCLattice::FCCLattice Class Reference

Inheritance diagram for FCCLattice::FCCLattice:



Public Member Functions

- def __init__
- def FCCEnergy
- def TestResults
- def Verify

3.2.1 Detailed Description

```
FCCLattice test returns the optimal fcc lattice constant and energy per atom
```

Definition at line 16 of file FCCLattice.py.

3.2.2 Member Function Documentation

3.2.2.1 def FCCLattice::FCCLattice::__init__ (*self, potentialname, element, TestDependencies = [], args, kwargs*)

```
Pass the initialization arguments to the BaseTest initializer
```

Definition at line 19 of file FCCLattice.py.

3.2.2.2 def FCCLattice::FCCLattice::FCCEnergy (*self, a*)

```
This function computes the energy of the crystal formation given
a certain lattice constant

It uses the ase helper function bulk to create a 1 atom periodic boundary
condition crystal with a specific structure
```

Definition at line 24 of file FCCLattice.py.

3.2.2.3 def FCCLattice::FCCLattice::TestResults (*self*)

```
FCC Lattice Test Result

uses scipy fmin (a simplex method minimization tool), to find the optimal
lattice constant, and corresponding energy per atom
```

Reimplemented from BaseTest::BaseTest.

Definition at line 39 of file FCCLattice.py.

3.2.2.4 def FCCLattice::FCCLattice::Verify (*self*)

```
Simple verification script.  Creates a plot that shows the
crystal energy in the neighborhood of the computed minimum, along
with the computed minimum, as a check
```

Reimplemented from BaseTest::BaseTest.

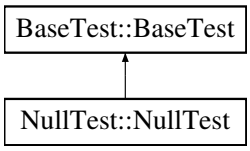
Definition at line 58 of file FCCLattice.py.

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

- tests/FCCLattice.py

3.3 NullTest::NullTest Class Reference

Inheritance diagram for NullTest::NullTest:



Public Member Functions

- def **__init__**
- def TestResults
- def Verify

3.3.1 Detailed Description

```
NullTest does nothing, but serves as an example test.

    It inherits its functionality from BaseTest, and serves as a template for future
tests.

Simply copy NullTest.py, and rename the file, and class name, and rewrite TestResults
```

Definition at line 11 of file NullTest.py.

3.3.2 Member Function Documentation

3.3.2.1 def NullTest::NullTest::TestResults (*self*)

```
Required module, the TestResults Module returns a dictionary of result.

of the form { 'NameOfValue' : value, 'NameOfSecondValue' : secondvalue }

This is where your test code goes.  Feel free to write other methods if necessary.
```

Reimplemented from BaseTest::BaseTest.

Definition at line 25 of file NullTest.py.

3.3.2.2 def NullTest::NullTest::Verify (*self*)

```
Optional verify script to be used to generate a visual output for

quick check that everything is going alright
```

Reimplemented from BaseTest::BaseTest.

Definition at line 36 of file NullTest.py.

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

- tests/NullTest.py

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