
easyInterface

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easyInterface is a library to interface crystallographic calculators to front end applications, JuPyter notebooks and scripting interfaces.

The code of the project is on Github: [easyInterface](#)

FEATURES OF EASYINTERFACE

Boom!

PROJECTS USING EASYINTERFACE

easyInterface is currently being used in the following projects:

- [easyDiffraction](#) - A scientific software for modelling and analysis of the neutron diffraction data

INSTALLATION

3.1 Install via pip

You can do a direct install via pip by using:

```
$ pip install easyInterface
```

3.2 Install as an easyInterface developer

You can get the latest development source from our [Github repository](#). You need `setuptools` installed in your system to install `easyInterface`. For example, you can do:

```
$ git clone https://github.com/easyDiffraction/easyInterface
$ cd easyInterface
$ pip install -r requirements.txt
$ pip install -e .
```

3.3 Main Contents

3.3.1 Introduction to easyInterface

Here we can see some examples of `easyInterface` in action

3.3.2 Scripted Examples

This section gathers examples which don't produce any figures. These examples show the basic features of `easyInterface`.

Note: Click [here](#) to download the full example code or to run this example in your browser via Binder

Creating a interface

This demonstrates an example of how to load an example and create a interface to a `crispy` calculator. Information about the project is then displayed.

```
import os

from easyInterface.Diffraction.Calculators import CryspyCalculator
from easyInterface.Diffraction.Interface import CalculatorInterface

main_rcif = os.path.join('examples', 'Fe3O4_powder-1d_neutrons-pol_5C1(LLB)', 'main.
↪cif')
calculator = CryspyCalculator(main_rcif)

interface = CalculatorInterface(calculator)

print(interface.project_dict)

print(interface.phasesIds())

print(interface.getPhase(interface.phasesIds()[0]))
```

Total running time of the script: (0 minutes 0.000 seconds)

Note: Click [here](#) to download the full example code or to run this example in your browser via Binder

Creating a QT interface

This demonstrates an example of how to load an example and create a QT interface to a cryspy calculator. Information about the project is then displayed.

```
import os

from easyInterface.Diffraction.Calculators import CryspyCalculator
from easyInterface.Diffraction.QtInterface import QtCalculatorInterface

main_rcif = os.path.join('examples', 'Fe3O4_powder-1d_neutrons-pol_5C1(LLB)', 'main.
↪cif')
calculator = CryspyCalculator(main_rcif)

interface = QtCalculatorInterface(calculator, None)

print(interface.project_dict)

print(interface.phasesIds())

print(interface.getPhase(interface.phasesIds()[0]))
```

Total running time of the script: (0 minutes 0.000 seconds)

Note: Click [here](#) to download the full example code or to run this example in your browser via Binder

Performing a fit

This demonstrates an example of how to load an example and create an interface to a cryspy calculator and then fit a value.

```
import os
from easyInterface.Diffraction.Calculators import CryspyCalculator
from easyInterface.Diffraction.Interface import CalculatorInterface

main_rcif = os.path.join('examples', 'PbSO4_powder-1d_neutrons-unpol_D1A(ILL)', 'main.
↪cif')
calculator = CryspyCalculator(main_rcif)

interface = CalculatorInterface(calculator)

print(interface.project_dict)

phase_ids = interface.phasesIds()

print(phase_ids)

phase = interface.getPhase(phase_ids[0])
phase['phasename'] = 'PbSO5'
interface.addPhase(phase)
interface.removePhase('PbSO5')

phase = interface.getPhase(phase_ids[0])
interface.setPhaseValue(phase_ids[0], ['atoms', 'Pb', 'fract_x'], 0.18)
interface.setPhases(phase)
print(phase)

interface.setPhaseRefine(phase_ids[0], ['atoms', 'Pb', 'fract_x'], True)

calc = interface.getCalculations()
print(calc)

res = interface.refine()

print(res)
```

Total running time of the script: (0 minutes 0.000 seconds)

3.3.3 Interface and Calculators

easyInterface Interface

class easyInterface.Diffraction.Interface.**CalculatorInterface** (*calculator*)

Interface to calculators in the *easyInterface.Diffraction.Calculator* class.

addExperimentDefinition (*exp_path*)

Add an experiment to be simulated from a cif file. Note that this will not have any crystallographic phases associated with it.

Parameters *exp_path* (str) – Path to a experiment file (.cif)

addPhase (*phase*)

Add a new phases from a cif file to the list of existing crystal phases.

Parameters `phase` (*Phase*) –

addPhaseDefinition (*phase_path*)

Add a new phases from a cif file to the list of existing crystal phases.

Parameters `phase_path` (*str*) – Path to a phase definition file (*.cif*)

Example:

```
interface = CalculatorInterface(calculator)
phase_path = '~/Experiments/new_phase.cif'
interface.addPhaseDefinition(phase_path)
```

asCifDict ()

...

Return type *dict*

asDict ()

Return data dict.

Return type *dict*

experimentsCount ()

Returns number of experiments in the project.

Return type *int*

experimentsIds ()

Returns labels of the experiments in the project.

Return type *list*

property final_chi_square

Calculates the final chi squared of the simulation. Where the final chi squared is the chi squared divided by the number of data points.

Return type *float*

Returns Final chi squared

getPhase (*phase_name*)

Returns a phase from the project dictionary by name if one is supplied. If the phase name is none then all phases are returned. If the phase name does not exist **KeyError** is thrown.

Parameters `phase_name` (*Optional[str]*) – Name of the phase to be returned or None for all phases

Return type *Phase*

Returns Copy of the project dictionaries phase object with name `phase_name`

Raises **KeyError** – The supplied key is not a valid phase name

phasesCount ()

Returns number of phases in the project.

Return type *int*

phasesIds ()

Returns labels of the phases in the project.

Return type *list*

refine ()

refinement ...

Return type dict

saveCifs (*save_dir*)

Write project cif files (*main.cif*, *experiments.cif* and *phases.cif*) to a user supplied directory. This contains all information needed to recreate the project dictionary.

Parameters **save_dir** (str) – Directory to where the project cif files should be saved.

Returns None

setExperiment (*experiment*)

Set phases (sample model tab in GUI)

setExperimentDefinition (*exp_path*)

Parse the relevant phases file and update the corresponding model

setExperiments (*experiments=None*)

Set experiments (Experimental data tab in GUI)

setPhase (*phase*)

Set phases (sample model tab in GUI)

setPhaseDefinition (*phase_path*)

Parse a phases cif file and replace existing crystal phases

Parameters **phase_path** (str) – Path to new phase definition file (*.cif*)

Example:

```
interface = CalculatorInterface(calculator)
phase_path = '~/Experiments/phases.cif'
interface.setPhaseDefinition(phase_path)
```

setPhases (*phases=None*)

Set phases (sample model tab in GUI)

setProjectFromCalculator ()

Sets the project dictionary from the calculator given on initialisation. Calling this function will regenerate the project dictionary and changes may be lost.

updatePhases ()

Synchronise the phases in project dictionary by queering the calculator object.

Returns None

writeExpCif (*save_dir*)

Write the *experiments.cif* where all experiments in the project dictionary are saved to file. This includes the instrumental parameters and which phases are in the experiment/s

Parameters **save_dir** (str) – Directory to where the experiment cif file should be saved.

Returns None

writeMainCif (*save_dir*)

Write the *main.cif* where links to the experiments and phases are stored and other generalised project information.

Parameters **save_dir** (str) – Directory to where the main cif file should be saved.

Returns None

writePhaseCif (*save_dir*)

Write the *phases.cif* where all phases in the project dictionary are saved to file. This cif file should be compatible with other crystallographic software.

Parameters `save_dir` (`str`) – Directory to where the phases cif file should be saved.

Returns `None`

easyInterfaces Project Dictionary

```
class easyInterface.Diffraction.Interface.ProjectDict (interface, app, calculator,  
                                                    info, phases, experiments,  
                                                    calculations)
```

This class deals with the creation and modification of the main project dictionary.

```
classmethod default ()
```

Create a default and empty project dictionary

Return type `ProjectDict`

Returns Default project dictionary with undo/redo functionality

```
classmethod fromPars (experiments, phases, calculations)
```

Create a main project dictionary from phases and experiments.

Parameters

- **experiments** (`Union[Experiments, Experiment, List[Experiment]]`) – A collection of experiments to be compared to calculations
- **phases** (`Union[Phases, Phase, List[Phase]]`) – A Collection of crystallographic phases to be calculated

Return type `ProjectDict`

Returns Project dictionary with undo/redo

easyInterface Cryspy Calculator

```
class easyInterface.Diffraction.Calculators.CryspyCalculator (main_rcif_path=None)
```

```
asCifDict ()
```

...

Return type `dict`

```
getPhases ()
```

Set phases (sample model tab in GUI)

Return type `Phases`

```
refine ()
```

refinement ...

```
setExperiments (experiments)
```

Set experiments (Experimental data tab in GUI)

```
setObjFromProjectDicts (phases, experiments)
```

Set all the cryspy parameters from project dictionary

```
setPhases (phases)
```

Set phases (sample model tab in GUI)

3.3.4 Container Classes

Phase Classes

```
class easyInterface.Diffraction.DataClasses.PhaseObj.Atom.ADP (u_11, u_22,  
u_33, u_12, u_13,  
u_23)
```

Data store for Atom site anisotropic displacement parameters

```
class easyInterface.Diffraction.DataClasses.PhaseObj.Atom.Atom (atom_site_label,  
type_symbol,  
scat_length_neutron,  
fract_x, fract_y,  
fract_z, occupancy,  
adp_type,  
U_iso_or_equiv,  
ADp, MSp)
```

Storage for details about an atom

```
classmethod default (atom_site_label)
```

Default constructor for an atom given a unique name in the phase

Parameters **atom_site_label** (*str*) – The atoms unique name in the phase

Return type *Atom*

Returns Default atom with a given name

```
classmethod fromPars (atom_site_label, type_symbol, scat_length_neutron, fract_x, fract_y,  
fract_z, occupancy, adp_type, U_iso_or_equiv, ADp=None, MSp=None)
```

Atom constructor from parameters

Parameters

- **atom_site_label** (*str*) – The unique name of the atom in the phase
- **type_symbol** (*str*) – The type of atom
- **scat_length_neutron** (*float*) – Neutron scattering length
- **fract_x** (*float*) – X position
- **fract_y** (*float*) – Y position
- **fract_z** (*float*) – Z position
- **occupancy** (*float*) – Site occupancy
- **adp_type** (*str*) – ADP type code
- **U_iso_or_equiv** (*float*) – Isotropic atomic displacement parameter

Return type *Atom*

Returns Fully formed atom data store

```
classmethod fromXYZ (atom_site_label, type_symbol, x, y, z)
```

Construct an atom from name, type and position

Parameters

- **atom_site_label** (*str*) – The atoms unique name in the phase
- **type_symbol** (*str*) – The type of atom

- **x** (float) – X position
- **y** (float) – Y position
- **z** (float) – Z position

Return type *Atom*

Returns Atom with name type and position filled in

class easyInterface.Diffraction.DataClasses.PhaseObj.Atom.**Atoms** (*atoms*)
Container for multiple atoms

class easyInterface.Diffraction.DataClasses.PhaseObj.Atom.**MSP** (*MSPTYPE*, *chi_11*,
chi_22, *chi_33*,
chi_12, *chi_13*,
chi_23)
Data store for Atom site magnetic susceptibility parameters

class easyInterface.Diffraction.DataClasses.PhaseObj.Cell.**Cell** (*length_a*,
length_b,
length_c, *angle_alpha*,
angle_beta,
angle_gamma)
Container for crystallographic unit cell parameters

classmethod default ()
Default constructor for a crystallographic unit cell

Return type *Cell*

Returns Default crystallographic unit cell container

classmethod fromPars (*length_a*, *length_b*, *length_c*, *angle_alpha*, *angle_beta*, *angle_gamma*)
Constructor of a crystallographic unit cell when parameters are known

Parameters

- **length_a** (float) – Unit cell length a
- **length_b** (float) – Unit cell length b
- **length_c** (float) – Unit cell length c
- **angle_alpha** (float) – Unit cell angle alpha
- **angle_beta** (float) – Unit cell angle beta
- **angle_gamma** (float) – Unit cell angle gamma

Return type *Cell*

Returns

class easyInterface.Diffraction.DataClasses.PhaseObj.Phase.**Phase** (*name*, *space-group*, *cell*,
atoms, *sites*)
Container for crystallographic phase information

classmethod default (*name*)
Default constructor for a crystallographic phase with a given name

Return type *Phase*

Returns Default empty phase with a name

class easyInterface.Diffraction.DataClasses.PhaseObj.Phase.**Phases** (*phases*)
 Container for multiple phases

renamePhase (*old_phase_name*, *new_phase_name*)
 Easy method of renaming a phase

Parameters

- **old_phase_name** (*str*) – phase name to be changed
- **new_phase_name** (*str*) – new phase name

Return type NoReturn

class easyInterface.Diffraction.DataClasses.PhaseObj.SpaceGroup.**SpaceGroup** (*crystal_system*,
space_group_name_H
space_group_IT_num
ori-
gin_choice)

Data Classes

class easyInterface.Diffraction.DataClasses.DataObj.Calculation.**BraggPeaks** (*bragg_peaks*)
 Container for multiple calculations

class easyInterface.Diffraction.DataClasses.DataObj.Calculation.**CalculatedPattern** (*x*,
y_calc,
y_diff_lower
y_diff_upper)

Storage container for a calculated pattern

class easyInterface.Diffraction.DataClasses.DataObj.Calculation.**Calculation** (*name*,
bragg_peaks,
cal-
cu-
lated_pattern,
lim-
its)

Storage container for calculations

class easyInterface.Diffraction.DataClasses.DataObj.Calculation.**Calculations** (*calculations*)
 Container for multiple calculations

class easyInterface.Diffraction.DataClasses.DataObj.Calculation.**CrystalBraggPeaks** (*name*,
h,
k,
l,
ttheta)

Generator for HKL reflections and corresponding two theta.

class easyInterface.Diffraction.DataClasses.DataObj.Calculation.**Limits** (*y_obs_lower=-*
inf,
y_obs_upper=inf,
y_diff_upper=inf,
y_diff_lower=-
inf,
x_calc=None,
y_calc=None)

Generator for limits of a dataset

```
class easyInterface.Diffraction.DataClasses.DataObj.Experiment.Background (ttheta,  
                                                                    in-  
                                                                    ten-  
                                                                    sity)  
  
Data store for the background data parameters  
  
classmethod default ()  
    Default constructor for a background point  
  
    Return type Background  
  
    Returns Default background data object  
  
classmethod fromPars (ttheta, intensity)  
    Constructor for background when two theta and intensity are known  
  
    Parameters  
        • ttheta (float) – Two Theta angle in degrees  
        • intensity (float) – Value for intensity  
  
    Return type Background  
  
    Returns Background data dict  
  
class easyInterface.Diffraction.DataClasses.DataObj.Experiment.Backgrounds (backgrounds)  
    Store for a collection of background points  
  
class easyInterface.Diffraction.DataClasses.DataObj.Experiment.Experiment (name,  
                                                                    wave-  
                                                                    length,  
                                                                    off-  
                                                                    set,  
                                                                    phase,  
                                                                    back-  
                                                                    ground,  
                                                                    res-  
                                                                    o-  
                                                                    lu-  
                                                                    tion,  
                                                                    mea-  
                                                                    sured_pattern)  
  
Experimental details data container  
  
classmethod default (name)  
    Default constructor for an Experiment  
  
    Parameters name (str) – What the experiment should be called  
  
    Return type Experiment  
  
    Returns Default empty experiment  
  
classmethod fromPars (name, wavelength, offset, scale, background, resolution, mea-  
                                                                    sured_pattern)  
    Constructor of experiment from parameters  
  
    Parameters  
        • name (str) – What the experiment should be called  
        • wavelength (float) – Experimental wavelength
```

- **offset** (float) – Experimental offset
- **scale** (float) – Scale parameter
- **background** (*Backgrounds*) – Background model
- **resolution** (*Resolution*) – Resolution model
- **measured_pattern** (*MeasuredPattern*) – The Measured data

Return type *Experiment*

Returns Experiment from parameters

class easyInterface.Diffraction.DataClasses.DataObj.Experiment.**ExperimentPhase** (*name*, *scale*)

Storage container for the Experimental Phase details

classmethod default (*name*)

Default experimental phase data container

Return type *ExperimentPhase*

Returns Default experimental phase data container

classmethod fromPars (*name*, *scale*)

Parameter initialised experimental phase data container

Return type *ExperimentPhase*

Returns Set experimental phase data container

class easyInterface.Diffraction.DataClasses.DataObj.Experiment.**ExperimentPhases** (*experiment_phases*)

Storage of multiple phase markers associated with experiments

class easyInterface.Diffraction.DataClasses.DataObj.Experiment.**Experiments** (*experiments*)

Container for multiple experiments

class easyInterface.Diffraction.DataClasses.DataObj.Experiment.**MeasuredPattern** (*x*, *y_obs*, *sy_obs*, *y_obs_up=None*, *sy_obs_up=None*, *y_obs_down=None*, *sy_obs_down=None*)

Storage container for measured patterns

classmethod default (*polarised=False*)

Default constructor for measured data container.

Parameters **polarised** (bool) – Should the container be initialised as a polarised data container?

Returns Empty data container

property isPolarised

Is the measured data of a polarised type?

Return type bool

Returns True if it is from a polarised measurement, false otherwise

property y_obs_lower

Lower data confidence bound.

Return type list

Returns value of lower confidence bound

property y_obs_upper

Upper data confidence bound.

Return type list

Returns value of upper confidence bound

```
class easyInterface.Diffraction.DataClasses.DataObj.Experiment.Resolution(u,  
                                                                           v,  
                                                                           w,  
                                                                           x,  
                                                                           y)
```

Data store for the resolution parameters

classmethod default()

Default constructor for the resolution dict

Return type *Resolution*

Returns Default resolution dict

classmethod fromPars(u, v, w, x, y)

Constructor when resolution parameters are known

Parameters

- **u** (float) – resolution parameter u
- **v** (float) – resolution parameter v
- **w** (float) – resolution parameter w
- **x** (float) – resolution parameter x
- **y** (float) – resolution parameter y

Return type *Resolution*

Returns Resolution dictionary with values set

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