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

CHAPTER

ONE

FEATURES OF EASYINTERFACE

Boom!

CHAPTER

TWO

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

CHAPTER

THREE

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 cryspy 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 a 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 crysolagraphic unit cell parameters

classmethod default()
Default constructor for a crystolographic unit cell

Return type *Cell*

Returns Default crystolographic unit cell container

classmethod fromPars(*length_a*, *length_b*, *length_c*, *angle_alpha*, *angle_beta*, *angle_gamma*)
Constructor of a crystolographic 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*, *spacegroup*, *cell*, *atoms*, *sites*)
Container for crysolographic 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_numb*, *origin_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*, *calculated_pattern*, *limits*)
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*, *intensity*)

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*, *wavelength*, *offset*, *phase*, *background*, *resolution*, *measured_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*, *measured_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_pha*

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=No*, *sy_obs_down=N*

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

CHAPTER

FOUR

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