
easyInterface

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EXAMPLE GALLERIES

1	Features of easyInterface	3
2	Projects using easyInterface	5
3	Installation	7
3.1	Install via pip	7
3.2	Install as an easyInterface developer	7
3.3	Main Contents	7
4	Indices and tables	23
	Python Module Index	25
	Index	27



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

easyInterface is a way of storing information about crystal structures, providing commonly used functions in an easy to use package. The data structure interfaces to crystallographic libraries, making a common way to calculate observable phenomena regardless of your choice of backend calculator. Currently we support:

- [Cryspy](#) - a crystallographic library for neutron data analysis.

With more interfaces coming.

PROJECTS USING EASYINTERFACE

easyInterface is currently being used in the following projects:

- [easyDiffraction](#) - Scientific software for modelling and analysis of 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

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 `crispy` calculator. Information about the project is then displayed.

```
# import os
#
# from easyInterface.Utils.Helpers import getExamplesDir
# from easyInterface.Diffraction.Calculators import CrispyCalculator
# from easyInterface.Diffraction.QtInterface import QtCalculatorInterface
```

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```
#
# data_dir = getExamplesDir()
# main_rcif = os.path.join(data_dir, '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)

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.Uutils.Helpers import getExamplesDir
from easyInterface.Diffraction.Calculators import CryspyCalculator
from easyInterface.Diffraction.Interface import CalculatorInterface

data_dir = getExamplesDir()
main_rcif = os.path.join(data_dir, '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

Performing a fit

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

```
import os
from easyInterface.Utils.Helpers import getExamplesDir
from easyInterface.Diffraction.Calculators import CrspsyCalculator
from easyInterface.Diffraction.Interface import CalculatorInterface

data_dir = getExamplesDir()
main_rcif = os.path.join(data_dir, 'PbSO4_powder-1d_neutrons-unpol_D1A(ILL)', 'main.
↪cif')

calculator = CrspsyCalculator(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.

addExperiment (*experiment*)

Add an experiment to the list of experiments in both the project dict and the calculator.

Parameters **experiment** (*Experiment*) – Experiment object to be added to the system.

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 phase from an easyInterface phase object to the list of existing crystal phases in the calculator.

Parameters **phase** (*Phase*) – New phase to be added to the phase list.

addPhaseDefinition (*phase_path*)

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

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)
```

addPhaseToExp (*exp_name, phase_name, scale=0.0*)

Link a phase in the project dictionary to an experiment in the project dictionary. Links in the calculator will also be made.

Parameters

- **exp_name** (*str*) – The name of the experiment
- **phase_name** (*str*) – The name of the phase to be associated with the experiment
- **scale** (*float*) – The scale of the crystallographic phase in the experimental system.

Raises **KeyError** – If the *exp_name* or *phase_name* are unknown

asCifDict ()

Converts the project dictionary into a *cif* structure.

Return type *str*

Returns Project dictionary as a string encoded to the cif specification.

asDict ()

Converts the project dictionary info a standard python dictionary. If there is an error then an empty dictionary is returned.

Return type *dict*

Returns Python dictionary of the project dictionary.

canRedo ()

Informs on if the project dictionary can have redo() called. Typically called after an undo function call.

Return type *bool*

Returns Can or Can't redo the project dictionary.

canUndo ()

Informs on if the project dictionary can have undo() called.

Return type *bool*

Returns Can or Can't undo the project dictionary.

clearUndoStack()

Resets the Undo/Redo stack of the project dictionary.

ALL PREVIOUS UNDO/REDO EDITS WILL BE LOST

experimentsCount()

Returns number of experiments in the project dictionary.

Return type `int`

experimentsIds()

Returns labels of the experiments in the project dictionary.

Return type `List[str]`

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

getCalculation(*calculation_name*)

Returns a specified calculation from the project dictionary.

Parameters **calculation_name** (`str`) – Name of the calculation to be returned.

Raises **KeyError** – If the calculation_name is not known.

Return type `Calculation`

Returns Calculation requested.

getCalculations()

Returns all calculations in the project dictionary. Calculations will be updated if members of the phases or experiments section of the project dictionary has been modified.

Return type `Calculations`

Returns Calculations object containing all calculations.

getDictByPath(*keys*)

Returns an object in the project dictionary by the path to the object.

Parameters **keys** (`List[str]`) – Path to the object in the project dictionary

Raises **KeyError** – The supplied keys do not return an object in the project dictionary

Return type `Any`

Returns Object from the project dictionary.

getExperiment(*experiment_name*)

Returns a experiment from the project dictionary by name if one is supplied. If the experiment name is None then all experiments are returned. If the experiment name does not exist KeyError is thrown.

Parameters **experiment_name** (`Optional[str]`) – Name of the experiment to be returned or None for all experiments

Return type `Experiment`

Returns Copy of the project dictionaries phase object with name experiment_name

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

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

name ()

Returns the name of the current project.

Return type `str`

Returns Name of the current project

phasesCount ()

Returns number of phases in the project dictionary.

Return type `int`

phasesIds ()

Returns labels of the phases in the project dictionary.

Return type `List[str]`

redo ()

Perform an redo operation on the project dictionary.

refine ()

Perform a refinement on parameters which are marked in the project dictionary. If the refinement fails then only the “refinement_message” will be returned in the results dictionary with an explanation of the error.

Return type `dict`

Returns Refinement results of the following fields: “num_refined_parameters”, “refinement_message”, “nfev”, “nit”, “njev”, “final_chi_sq”

removeExperiment (*experiment_name*)

Remove a experiment from both the project dictionary and the calculator.

Parameters **experiment_name** (`str`) – Name of the experiment to be removed.

removePhase (*phase_name*)

Remove a phase of a given name from the dictionary and the calculator object.

Parameters **phase_name** (`str`) – name of the phase to be removed.

removePhaseFromExp (*exp_name*, *phase_name*)

Remove the link between an experiment and a crystallographic phase. Links in the calculator will also be removed.

Parameters

- **exp_name** (`str`) – The name of the experiment.
- **phase_name** (`str`) – The name of the phase to be removed.

Raises **KeyError** – If the *exp_name* or *phase_name* are unknown

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.

setCalculatorFromProject ()

Resets the project phases and experiments fields of the project dictionary from the calculator.

Return type *None*

setDictByPath (*keys*, *value*)

Set an object in the project dictionary by a key path.

Parameters

- **keys** (*List[str]*) – Path to the object to be modified/created
- **value** (*Any*) – Value to be set at the key path

Return type *None*

setExperiment (*experiment*)

Set phases (sample model tab in GUI)

setExperimentDefinition (*exp_path*)

Set an experiment/s 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*)

setExperiments (*experiments*)

Set experiments (Experimental data tab in GUI)

setPhase (*phase*)

Modify a phase in the calculator. The phase will be added if it does not currently exist.

Parameters **phase** (*Union[Phase, dict]*) – easyInterface phase object to be added.

Raises **TypeError** – If the phase object is not a easyInterface phase object or dictionary object.

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 the phases in the calculator to an easyInterface phases object. If a phase in the supplied phases exists then the phase will be modified, if not, it will be added.

Parameters **phases** (*Union[Phase, Phases, None]*) – phases to be added to the calculator.

Raises **TypeError** – If the phase object is not a easyInterface phase/phases object or dictionary object.

setProjectFromCalculator ()

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

undo ()

Perform an undo operation on the project dictionary.

updateCalculations ()

Calculate all experiments and populate the calculations field in the project dictionary. Note that this will only occur if a member of the phases or experiments section of the project dictionary has been modified since the last call to *updateCalculations*.

updateExperiments ()

Synchronise the experiments portion of the project dictionary from the calculator.

updatePhases ()

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

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.

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.

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.

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 LoggedUndoableDict

Returns Default project dictionary with undo/redo functionality

classmethod fromPars (experiments, phases, calculations={})

Create a main project dictionary from phases and experiments.

Parameters

- **calculations** (Union[*Calculations*, *Calculation*, List[*Calculation*], None]) –
- **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 LoggedUndoableDict

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_Hi, space_group_IT_number, 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,  
                                                                    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

INDICES AND TABLES

- `genindex`
- `modindex`
- `search`

PYTHON MODULE INDEX

e

`easyInterface.Diffraction.DataClasses.DataObj.Calculation,`
17
`easyInterface.Diffraction.DataClasses.DataObj.Experiment,`
18
`easyInterface.Diffraction.DataClasses.PhaseObj.Atom,`
15
`easyInterface.Diffraction.DataClasses.PhaseObj.Cell,`
16
`easyInterface.Diffraction.DataClasses.PhaseObj.Phase,`
17
`easyInterface.Diffraction.DataClasses.PhaseObj.SpaceGroup,`
17

INDEX

A

addExperiment () (easyInterface.Diffraction.Interface.CalculatorInterface method), 9

addExperimentDefinition () (easyInterface.Diffraction.Interface.CalculatorInterface method), 9

addPhase () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

addPhaseDefinition () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

addPhaseToExp () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

ADP (class in easyInterface.Diffraction.DataClasses.PhaseObj.Atom), 15

asCifDict () (easyInterface.Diffraction.Calculators.CrspyCalculator method), 15

asCifDict () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

asDict () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

Atom (class in easyInterface.Diffraction.DataClasses.PhaseObj.Atom), 15

Atoms (class in easyInterface.Diffraction.DataClasses.PhaseObj.Atom), 16

B

Background (class in easyInterface.Diffraction.DataClasses.DataObj.Experiment), 18

Backgrounds (class in easyInterface.Diffraction.DataClasses.DataObj.Experiment), 18

BraggPeaks (class in easyInterface.Diffraction.DataClasses.DataObj.Calculation), 17

C

CalculatedPattern (class in easyInterface.Diffraction.DataClasses.DataObj.Calculation), 17

Calculation (class in easyInterface.Diffraction.DataClasses.DataObj.Calculation), 17

Calculations (class in easyInterface.Diffraction.DataClasses.DataObj.Calculation), 18

CalculatorInterface (class in easyInterface.Diffraction.Interface), 9

canRedo () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

canUndo () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

Cell (class in easyInterface.Diffraction.DataClasses.PhaseObj.Cell), 16

clearUndoStack () (easyInterface.Diffraction.Interface.CalculatorInterface method), 10

CrspyCalculator (class in easyInterface.Diffraction.Calculators), 15

CrystalBraggPeaks (class in easyInterface.Diffraction.DataClasses.DataObj.Calculation), 18

D

default () (easyInterface.Diffraction.DataClasses.DataObj.Experiment.Background class method), 18

default () (easyInterface.Diffraction.DataClasses.DataObj.Experiment.Experiment class method), 19

default () (easyInter- **F**
 face.Diffraction.DataClasses.DataObj.ExperimentExperimentPhase
 class method), 19 final_chi_square () (easyInter-
 default () (easyInter- face.Diffraction.Interface.CalculatorInterface
 face.Diffraction.DataClasses.DataObj.ExperimentMeasuredPattern property), 11
 class method), 20 fromPars () (easyInter-
 default () (easyInter- face.Diffraction.DataClasses.DataObj.Experiment.Background
 face.Diffraction.DataClasses.DataObj.ExperimentResolution class method), 18
 class method), 20 fromPars () (easyInter-
 default () (easyInter- face.Diffraction.DataClasses.DataObj.Experiment.Experiment
 face.Diffraction.DataClasses.PhaseObj.Atom.Atom fromPars () (easyInter-
 class method), 15 class method), 19
 default () (easyInter- face.Diffraction.DataClasses.DataObj.Experiment.ExperimentPh
 face.Diffraction.DataClasses.PhaseObj.Cell.Cell fromPars () (easyInter-
 class method), 16 class method), 19
 default () (easyInter- face.Diffraction.DataClasses.DataObj.Experiment.Resolution
 face.Diffraction.DataClasses.PhaseObj.Phase.Phase fromPars () (easyInter-
 class method), 17 class method), 20
 default () (easyInter- face.Diffraction.DataClasses.PhaseObj.Atom.Atom
 face.Diffraction.Interface.ProjectDict class fromPars () (easyInter-
 method), 14 class method), 15
 class method), 16
E fromPars () (easyInter-
 easyInterface.Diffraction.DataClasses.DataObj.CalcDiffraction face.Diffraction.Interface.ProjectDict class
 (module), 17 method), 14
 easyInterface.Diffraction.DataClasses.DataObj.Experiment (easyInter-
 (module), 18 face.Diffraction.DataClasses.PhaseObj.Atom.Atom
 easyInterface.Diffraction.DataClasses.PhaseObj.Atom class method), 16
 (module), 15
 easyInterface.Diffraction.DataClasses.PhaseObj.Cell **G**
 (module), 16 getCalculation () (easyInter-
 easyInterface.Diffraction.DataClasses.PhaseObj.Phase face.Diffraction.Interface.CalculatorInterface
 (module), 17 method), 11
 easyInterface.Diffraction.DataClasses.PhaseObj.SpaceGroup (easyInter-
 (module), 17 getCalculations () (easyInter-
 Experiment (class in easyInter- face.Diffraction.Interface.CalculatorInterface
 face.Diffraction.DataClasses.DataObj.Experiment) method), 11
 18 getDictByPath () (easyInter-
 ExperimentPhase (class in easyInter- face.Diffraction.Interface.CalculatorInterface
 face.Diffraction.DataClasses.DataObj.Experiment) method), 11
 19 getExperiment () (easyInter-
 ExperimentPhases (class in easyInter- face.Diffraction.Interface.CalculatorInterface
 face.Diffraction.DataClasses.DataObj.Experiment) method), 11
 20 getPhase () (easyInter-
 Experiments (class in easyInter- face.Diffraction.Interface.CalculatorInterface
 face.Diffraction.DataClasses.DataObj.Experiment) method), 11
 20 getPhases () (easyInter-
 experimentsCount () (easyInter- face.Diffraction.Calculators.CrspyCalculator
 face.Diffraction.Interface.CalculatorInterface method), 15
 method), 11
 experimentsIds () (easyInter- **I**
 face.Diffraction.Interface.CalculatorInterface isPolarised () (easyInter-
 method), 11 face.Diffraction.DataClasses.DataObj.Experiment.MeasuredPatt
 property), 20

L

Limits (class in easyInterface.Diffraction.DataClasses.DataObj.Calculation), 18

M

MeasuredPattern (class in easyInterface.Diffraction.DataClasses.DataObj.Experiment), 20

MSP (class in easyInterface.Diffraction.DataClasses.PhaseObj.Atom), 16

N

name () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

P

Phase (class in easyInterface.Diffraction.DataClasses.PhaseObj.Phase), 17

Phases (class in easyInterface.Diffraction.DataClasses.PhaseObj.Phase), 17

phasesCount () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

phasesIds () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

ProjectDict (class in easyInterface.Diffraction.Interface), 14

R

redo () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

refine () (easyInterface.Diffraction.Calculators.CrspyCalculator method), 15

refine () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

removeExperiment () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

removePhase () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

removePhaseFromExp () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

renamePhase () (easyInterface.Diffraction.DataClasses.PhaseObj.Phase.Phases method), 17

Resolution (class in easyInterface.Diffraction.DataClasses.DataObj.Experiment), 20

S

saveCifs () (easyInterface.Diffraction.Interface.CalculatorInterface method), 12

setCalculatorFromProject () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setDictByPath () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setExperiment () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setExperimentDefinition () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setExperiments () (easyInterface.Diffraction.Calculators.CrspyCalculator method), 15

setExperiments () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setObjFromProjectDicts () (easyInterface.Diffraction.Calculators.CrspyCalculator method), 15

setPhase () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setPhaseDefinition () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setPhases () (easyInterface.Diffraction.Calculators.CrspyCalculator method), 15

setPhases () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

setProjectFromCalculator () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

SpaceGroup (class in easyInterface.Diffraction.DataClasses.PhaseObj.SpaceGroup), 17

U

undo () (easyInterface.Diffraction.Interface.CalculatorInterface method), 13

updateCalculations () (easyInterface.Diffraction.Interface.CalculatorInterface method), 14

`updateExperiments()` (*easyInterface.Diffraction.Interface.CalculatorInterface*
method), 14

`updatePhases()` (*easyInterface.Diffraction.Interface.CalculatorInterface*
method), 14

W

`writeExpCif()` (*easyInterface.Diffraction.Interface.CalculatorInterface*
method), 14

`writeMainCif()` (*easyInterface.Diffraction.Interface.CalculatorInterface*
method), 14

`writePhaseCif()` (*easyInterface.Diffraction.Interface.CalculatorInterface*
method), 14

Y

`y_obs_lower()` (*easyInterface.Diffraction.DataClasses.DataObj.Experiment.MeasuredPattern*
property), 20

`y_obs_upper()` (*easyInterface.Diffraction.DataClasses.DataObj.Experiment.MeasuredPattern*
property), 20