



**EUROPEAN  
SPALLATION  
SOURCE**



# EasyReflectometry

User-friendly specular neutron reflectometry analysis

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# Overview

EasyReflectometry is a user-friendly analysis package for **specular** reflectometry

- EasyReflectometry is part of the EasyScience project
- Currently EasyReflectometry has development effort from European Spallation Source and Diamond Light Source
- We are in the process of engaging with other collaborations

The screenshot shows the homepage of the EasyReflectometry website. At the top left is the logo 'easyreflectometry' with a blue square icon containing a white stylized 'e'. To the right of the logo are navigation links for 'Home', 'Features', and 'Contact', followed by a dark moon icon for a dark mode toggle. The main heading is 'Making reflectometry data analysis and modelling easy', where 'reflectometry' and 'easy' are in blue. Below the heading is a paragraph: 'An intuitive and user-friendly application which integrates multiple popular reflectometry data analysis libraries such as [refnx](#) and [refl1d](#). Allowing for the simulation of reflectometry profiles based on layered structures and refinement against experimental data.' At the bottom left of the page, it says 'Version 0.0.4-beta (2 May 2022)'.

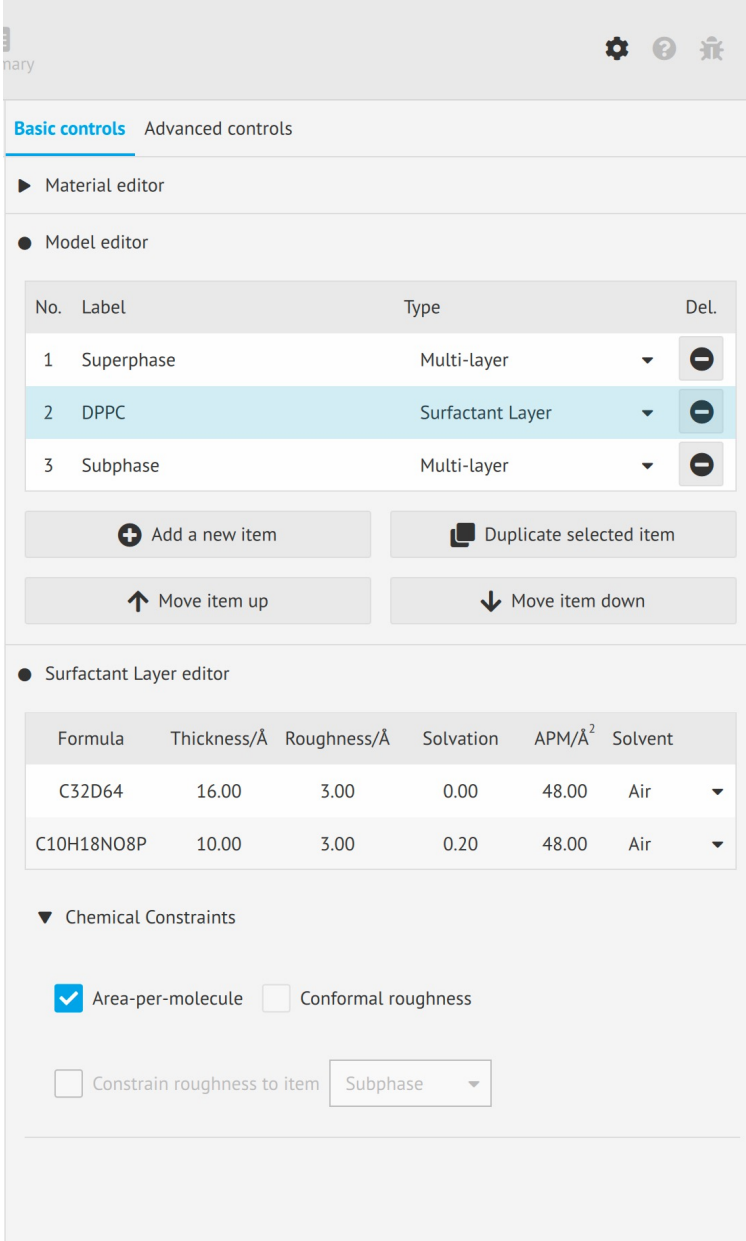
# Aims/Design

The principle aim of EasyReflectometry is to be **easy-to-use**, enabling new users of reflectometry to analyse their data successfully **and** accurately

- Designed around an *item-type* model construction
- These *item-types* facilitate chemical and physical constraints

EasyReflectometry consists of an application and a Python library

- User can use either based on preference



The screenshot displays the software interface with the following components:

- Basic controls / Advanced controls** tabs at the top.
- Material editor** section.
- Model editor** section containing a table:

No.	Label	Type	Del.
1	Superphase	Multi-layer	⊖
2	DPPC	Surfactant Layer	⊖
3	Subphase	Multi-layer	⊖

Below the table are buttons for:

- + Add a new item
- 📄 Duplicate selected item
- ↑ Move item up
- ↓ Move item down

- Surfactant Layer editor** section containing a table:

Formula	Thickness/Å	Roughness/Å	Solvation	APM/Å <sup>2</sup>	Solvent
C32D64	16.00	3.00	0.00	48.00	Air
C10H18NO8P	10.00	3.00	0.20	48.00	Air

Below the table are **Chemical Constraints** with checkboxes:

- Area-per-molecule
- Conformal roughness
- Constrain roughness to item (Subphase)





# Demonstration

# The role of EasyReflectometry

As mentioned in the previous reflectometry STAP report:

- New/inexperienced users will be supported to use the EasyReflectometry application, with the potential to “graduate” to the Python interface (with support) if necessary
- Users with complex analysis requirements (e.g. kinetic measurements) will be supported to use the Python interface to impose the potentially complex constraints (common use cases will be promoted to the application)
- Experienced reflectometry users are welcome to use their preferred analysis package, and the IS/IDS will support them in-kind (if necessary)
- Users that want to co-refinement specular/off-specular/GISANS will be supported to use the BornAgain Python interface





# Plans for EasyReflectometry

EasyReflectometry has been in development for nearly one year, it is **not** yet full featured; in the coming years the following is included in the development plans:

- Support for multi-contrasts in the GUI
- A rich *item-type* library
- Support for magnetic specular reflectometry analysis
- Support for other calculators
- Bayesian sampling methods

Throughout this process we will engage with users to develop a community



# Links

- The EasyReflectometry homepage: [easyreflectometry.org](https://easyreflectometry.org)
- EasyReflectometry Python docs: [easyscience.github.io/EasyReflectometryLib](https://easyscience.github.io/EasyReflectometryLib)
- Github repositories:
  - [github.com/easyScience/EasyReflectometryApp](https://github.com/easyScience/EasyReflectometryApp)
  - [github.com/easyScience/EasyReflectometryLib](https://github.com/easyScience/EasyReflectometryLib)

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# Finish presentation