

Processing and analysis of catalysis data

Experimental Data Capture



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PHYSICAL SCIENCES
DATA INFRASTRUCTURE

Pathfinder



Goal:

- Accelerate Processing

Problem:

- Interactive tools do not facilitate processing large datasets.

Proposal:

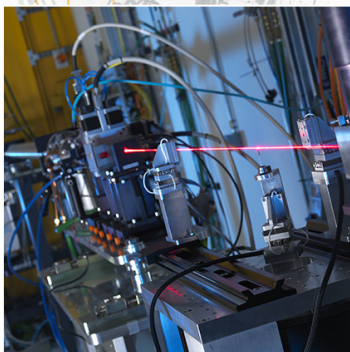
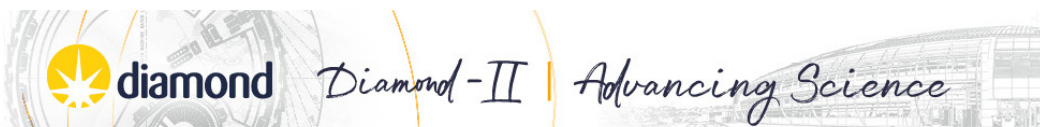
- Create/adopt tools which automate part or the whole workflow



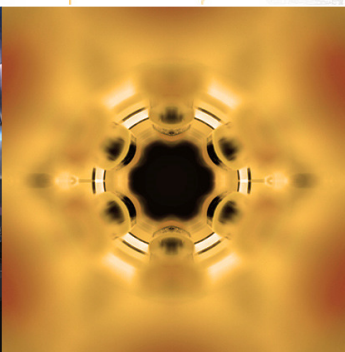
XAS analyses

[1971] In one trip to the synchrotron we collected more and better data in three days than in the previous ten years. I shut down all three X-ray spectrometers in the Boeing laboratory. A new era had arrived! (Lytle 1999)

- XAS analyses are important tools for catalysis research
- New developments will produce larger quantities of data increasing the time and resources for processing and analysis

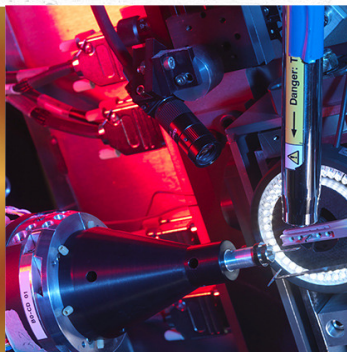


Brighter



More coherent

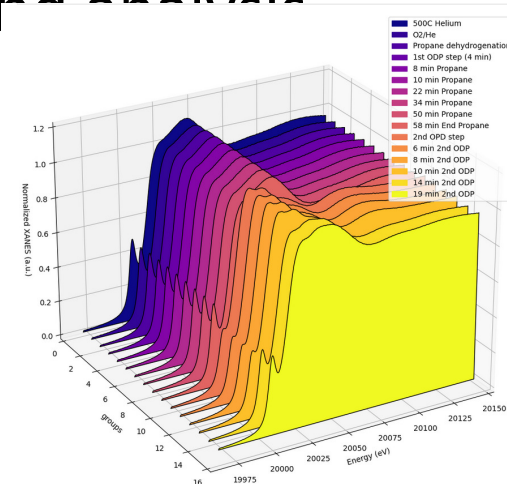
06/09/2023



Faster



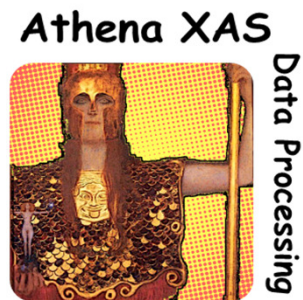
Higher throughput



More data to process and analyse

DAWN, Artemis, Athena, Larch

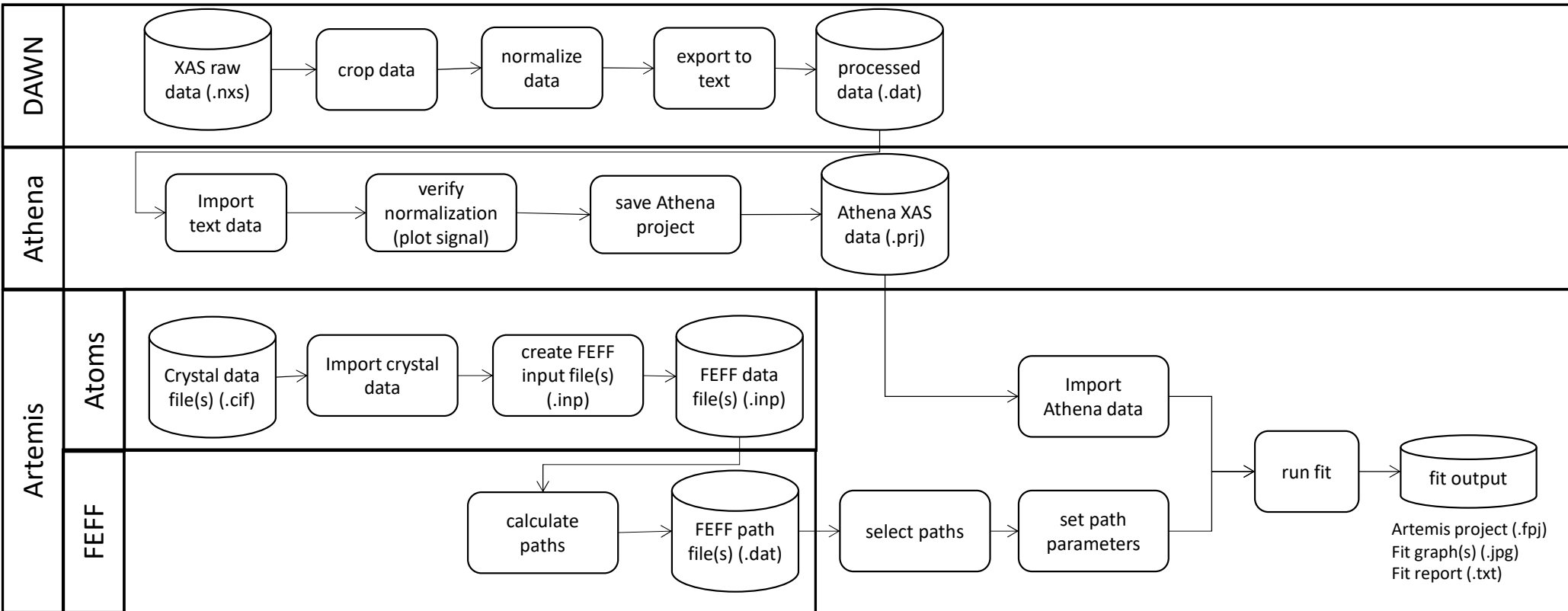
- XAS processing and analysis tools
- Very good interface
- Cater to all the needs of the researcher
- Well documented: Tutorials and training materials available
- Hides or reduces much of the complexity of processing and analysing data
- Perl based scripting required for automation
- Need to create the methods to collect and save metadata



Larch

Data Analysis Tools for X-ray Spectroscopy

Initial example: EXAFS Workflow





Athena XAS



Data Processing

Artemis: EXAFS



Data Analysis

3,790 XAS readings



Novice: ~63 Days

Expert: ~26 Days

Read Raw Data



Process, Normalise,
Re-bin, Data



FEFF fit of Crystal Paths
to EXAFS Data

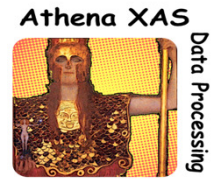
3,790 XAS readings



Novice: ~63 Days



Expert: ~26 Days



Demeter Script:

~23 Hours



Perl



Larch Script:

~103 Hours



python



Nextflow Workflow:

~7 Hours



GALAXY Workflows



Larch

Data Analysis Tools for X-ray Spectroscopy

Scientific Computing
Department STFC

- Python, X-Ray Larch, Galaxy
- Web Based
- No setup required
- Medium-Large scale spectra analyses (e.g. data generated from in-situ or operando experiments)



Faster EXAFS: ~7 Hours



EXAFS Galaxy Workflow

A screenshot of the Galaxy web interface. The main panel shows the 'Larch Athena generate Athena projects from XAFS data' tool configuration. Under 'Merge inputs', the 'No' radio button is selected. The 'XAFS data file' dropdown is set to '1: 262875_PtSn_OCO_Abu_1.nxs'. The 'Edge energy (eV)' dropdown is also set to '1: 262875_PtSn_OCO_Abu_1.nxs'. The 'History' panel on the right shows a sequence of steps: 1: 262875_PtSn_OCO_Abu_1.nxs, 2: Athena project of data 1, 3: Edge fitting of data 1, 4: Flattened plot of data 1, and 5: Derivative plot of data 1. The left sidebar lists various XAS-related tools like 'Larch Artemis generate Artemis projects from XAFS data' and 'Larch FEFF generate FEFF paths from XAFS data'.

3,790 XAS readings

~7 Hours



Started adding tools to allow more processing options

- XANES analysis
- Linear Combination Fitting
- EXAFS analysis
- Stop conditions long running workflow
- Find the best path combination for fitting

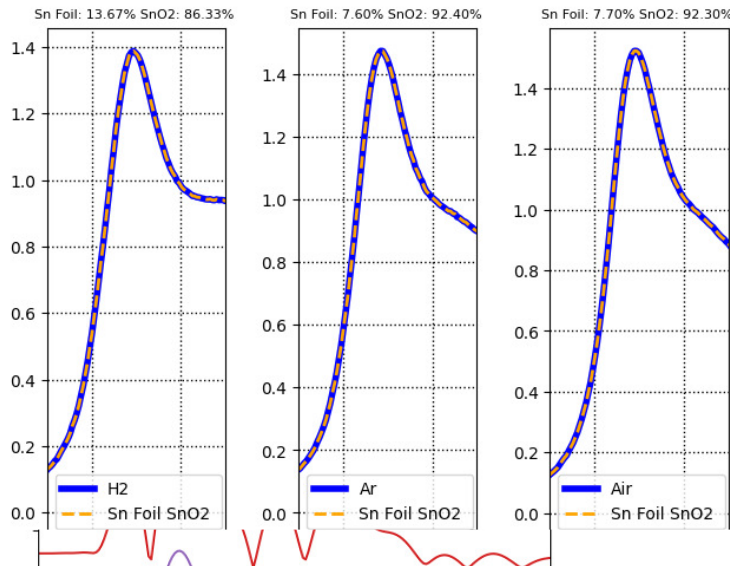


Linear combination fitting (LCF)

Lineal combination fitting with defaults for the H2, Ar and Air readings (Shown on Fig. 4 B)

```
In [6]: 1 # import custom plot functions (replicate plots in paper)
        2 import paper01_plots as c_plots

In [7]: 1 lcf_components = [merged_results["Sn Foil"],merged_results["SnO2"]] # List of groups to use as components
        2
        3 r_H2 = athenamgr.lcf_group(merged_results["H2"], lcf_components)
        4 r_Ar = athenamgr.lcf_group(merged_results["Ar"], lcf_components)
        5 r_Air = athenamgr.lcf_group(merged_results["Air"], lcf_components)
        6
        7 c_plots.compare_lcf_plot([merged_results["H2"],r_H2], [merged_results["Ar"],r_Ar], [merged_results["Air"],r_Air])
        8 plt.show()
        9
        10 print(r_H2.arrayname)
```



Normal plot of aligned samples

Compare fit components

3D plot of different samples

Plot with inset zoom

Formation of components in time

Highlight regions in a catalytic surface

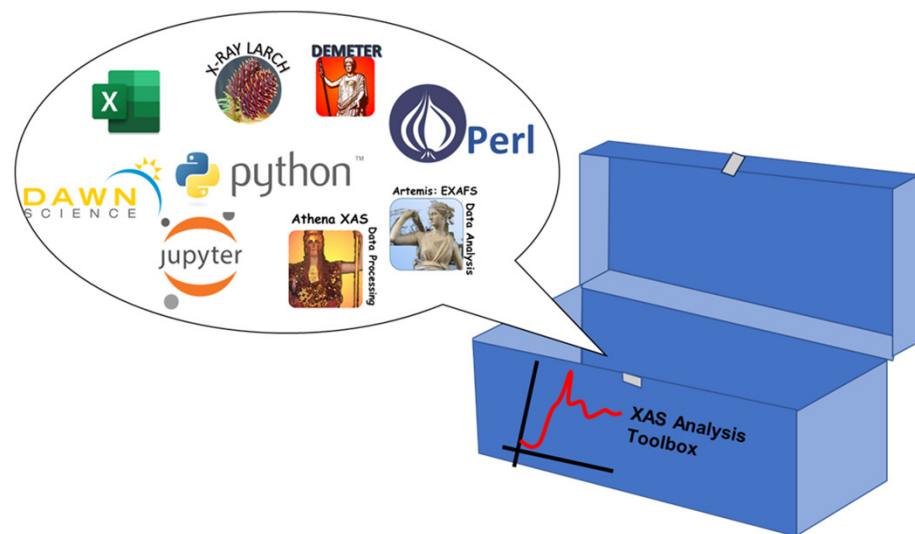
Compare standard to samples

Sample behaviour in time

Linear Combination Fit of different samples

Galaxy workflows for XAS analysis

- Provide XAS analysis and processing tool in an online platform
- No need to install specialised software
- Support common processing and analysis tasks
- Accessible to novice and expert users
- Support processing of large data sets

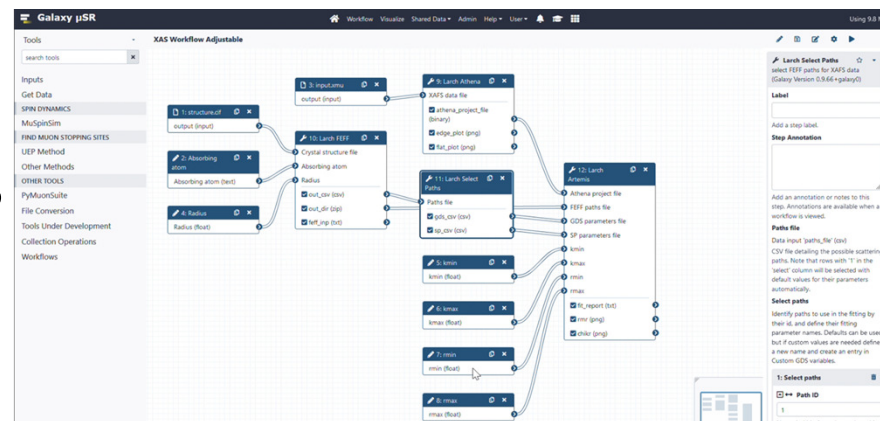


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Galaxy
PROJECT

CatalysisHub

Share and customise workflows



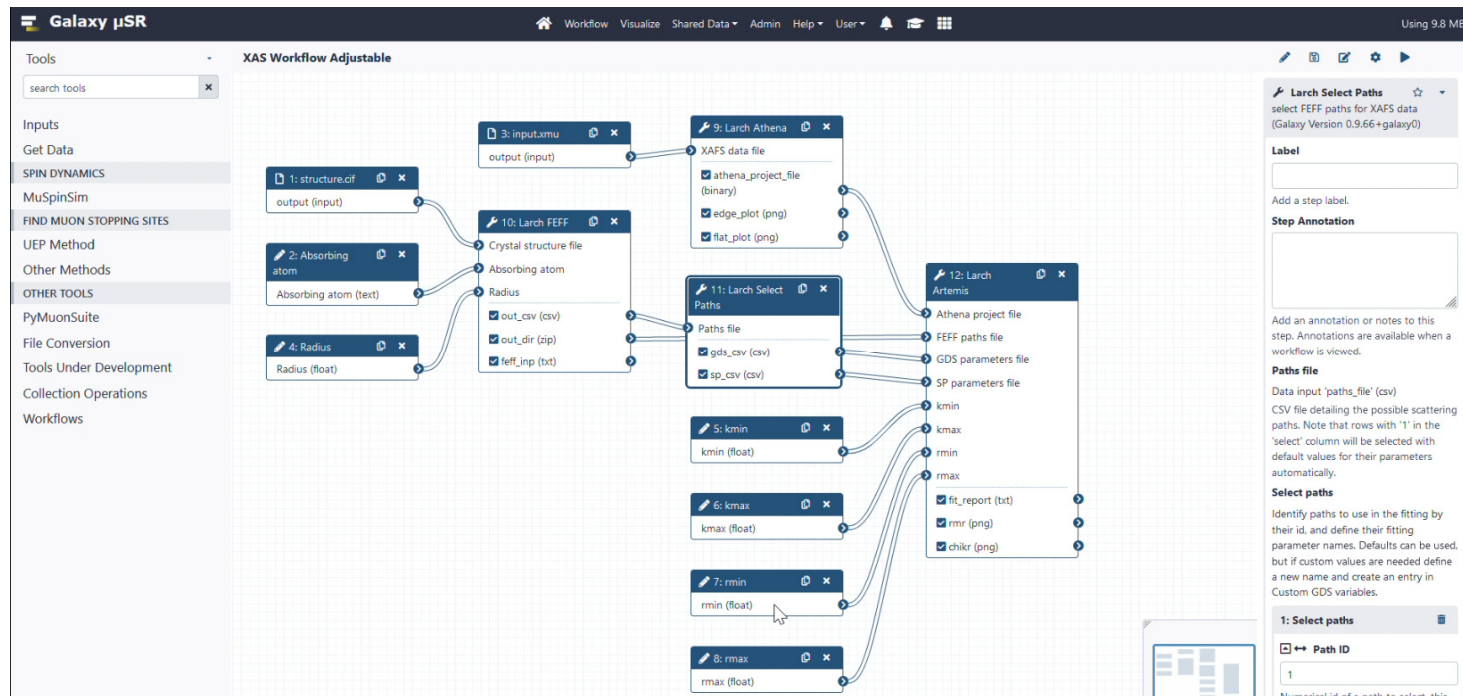
Export workflows for other platforms (CWL)



Package the entire workflow execution as a FAIR DO



Linking of tools into workflows



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Deployment and Support



Block Allocation Group
(BAG) Beamline Access

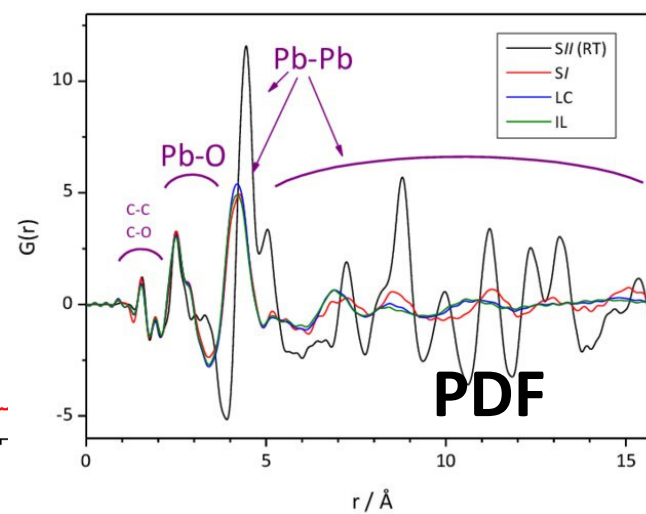
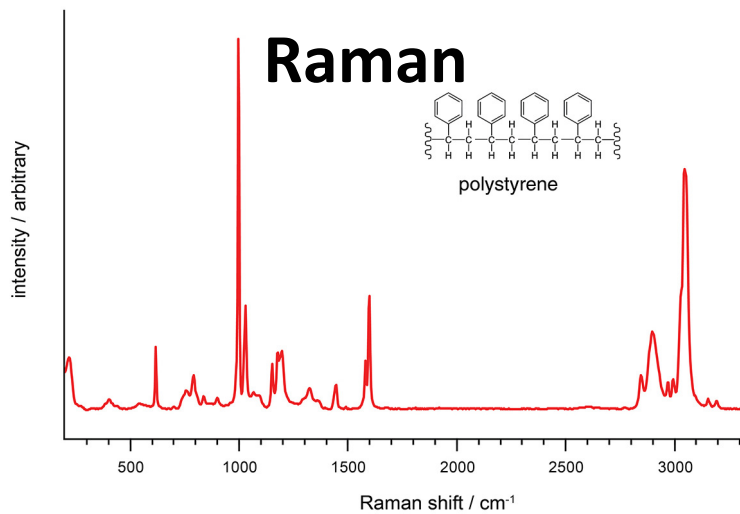
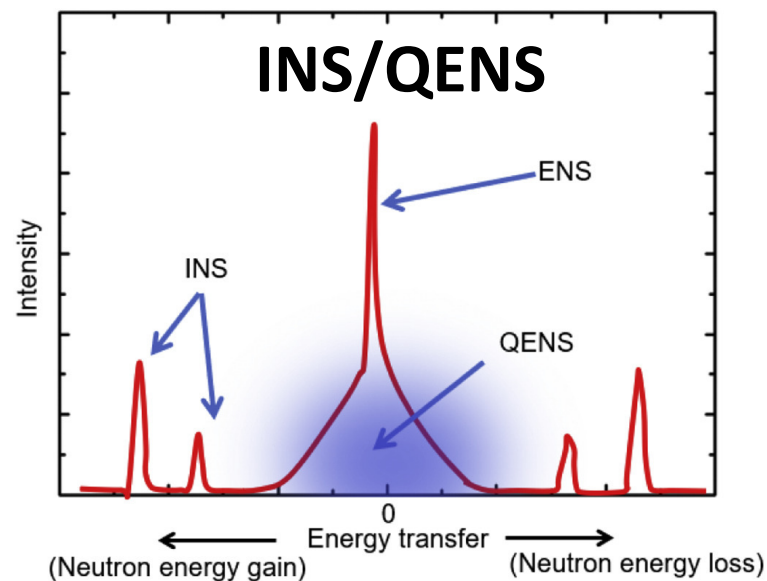


Six examples from Manchester

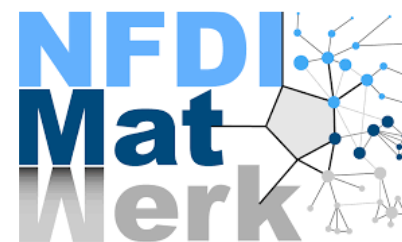
Beyond XAS analysis



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Opportunities for collaboration





Extended call for abstracts to the 7th of November

T16 Data as a Key Resource in Digital Catalysis

Organising committee

Annette Trunschke
Fritz Haber Institute

Pedro Mendes
University of Lisbon

Stephan Schunk
BASF

The Galaxy Platform: Applications to Catalysis Workflows and Interactions with Computer Clusters

Theoretical and Computational
Physics Group - SCD

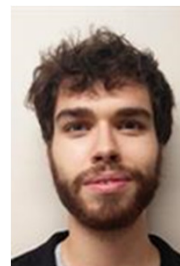


LIBORIO

Data & Software Engineering Group
SCD



GONZALEZ-
BELTRAN



AUSTIN

UK Catalysis Hub



NIEVA DE LA HIDALGA



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PROJECT

al.c
ada lovelace centre



Software
Sustainability
Institute

eosc

EuroScienceGateway

CatalysisHub

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