OSCARS

Open Science Clusters' Action for Research & Society

Funded Project

AI-SCOPE: AI-Driven Enhancement of Surface Scattering Data for Open Science Platforms Across Europe

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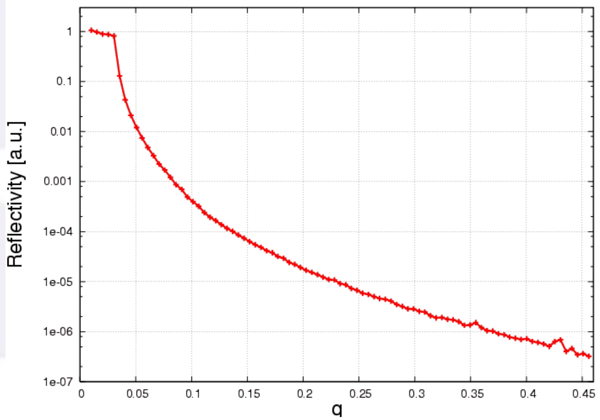
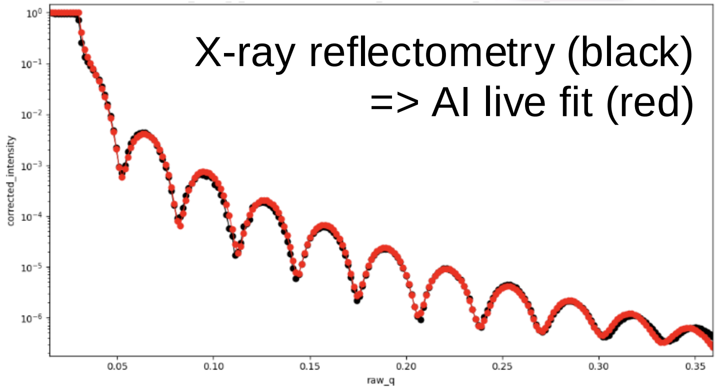
What problems are we going to solve?

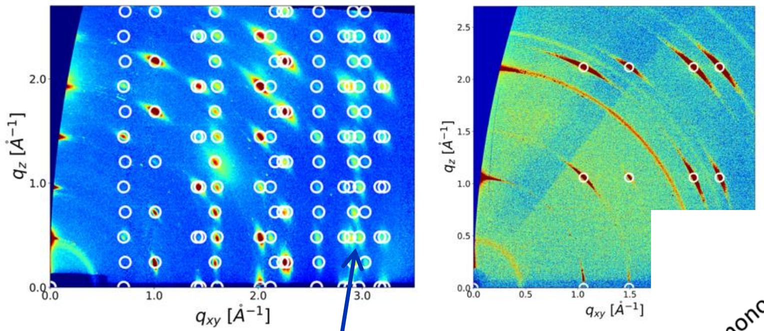
- X-ray data overwhelms users
  → experimental mistakes, sub-optimal planning, selective data analysis
- Limited metadata (electronic lab book, sample description)
- Low submission rates to FAIR and open databases



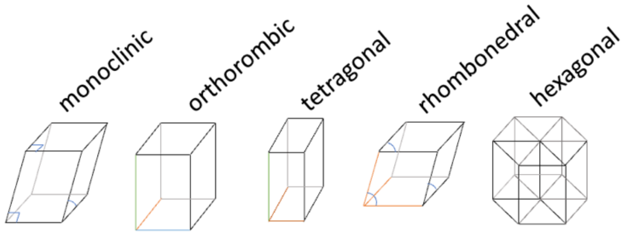
What are we planning to do to solve the problem?

- AI Copilot: Development of an AI-tool for rapid analysis of X-ray scattering data
- Use this AI for live annotation of datasets to create FAIR and open data
  → “Raw data” includes structural models (Orsopy: “.ort”, Crystals “.cif”)
- Establishing a curated database of surface scattering data



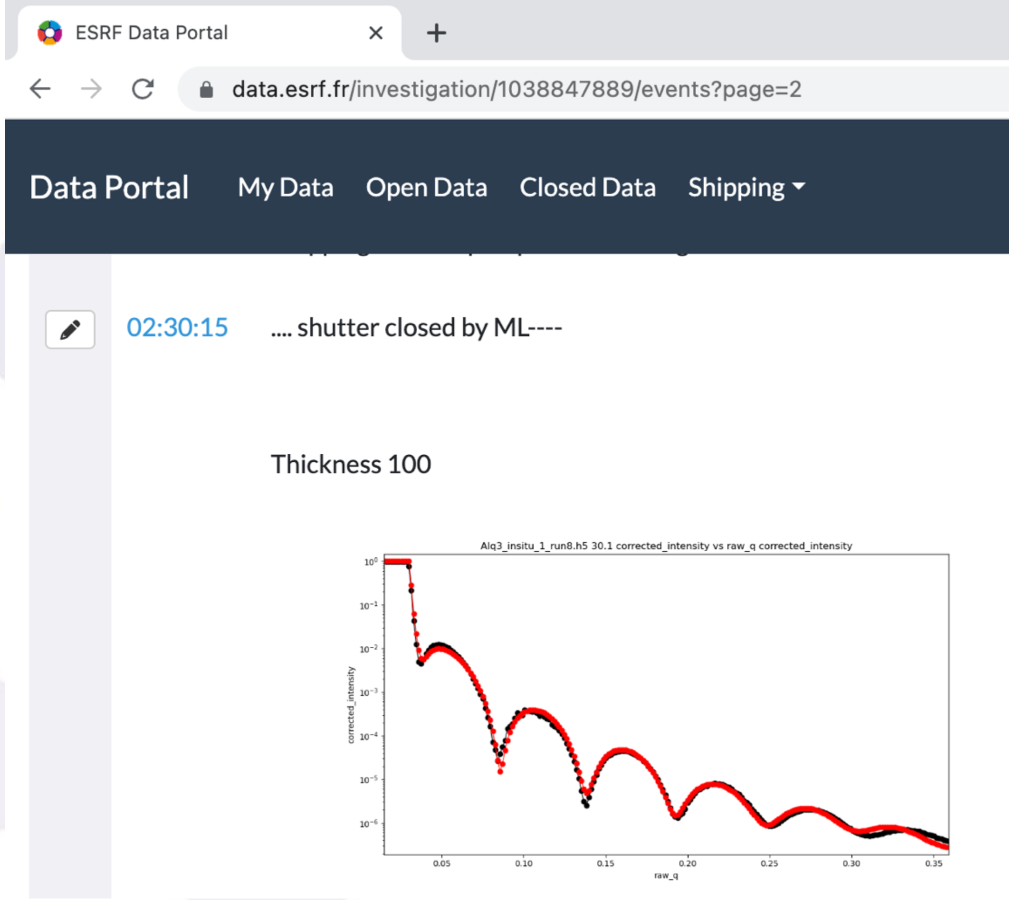


AI analyses Bragg reflections
=> crystal structure



What will be the results and how do we plan to make them available to the broader community?

- Automated live AI analysis tools deployed at large-scale facilities
- Live annotation
  → rich metadata in ESRF data portal ...
- Less work needed for FAIR and open data
  → enhanced database submissions
- Best practice examples



What risks could limit the success of the project, and how can they be mitigated

- **What if the AI does not work for my specific samples?**

⟹ Tailor AI for most important use cases

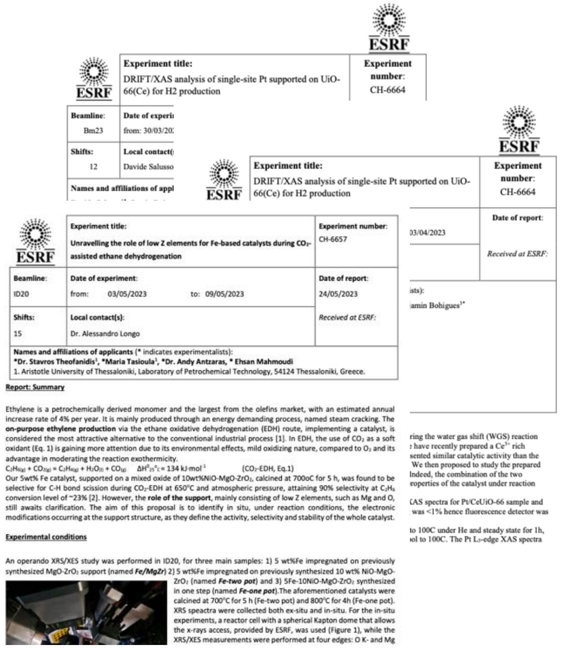
⟹ LLM analysis of 13,000 experimental reports of ESRF

⟹ Enable wide range of materials, easy training

- **AI analysis and annotation seems complicated to use**

⟹ Readily trained models available

⟹ Integration into workflow (e.g. ESRF Ewoks):
experiment control, data treatment, peak finding etc.



TEAM

OSCARS

200 × 235

Who is doing it?

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