

OSCARS

Open Science Clusters' Action
for Research & Society

Funded Project

Open-Data for Computational Chemistry and Materials Science: ioChem-BD

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Implemented by



ICIQ ^R Institut Català
d'Investigació Química

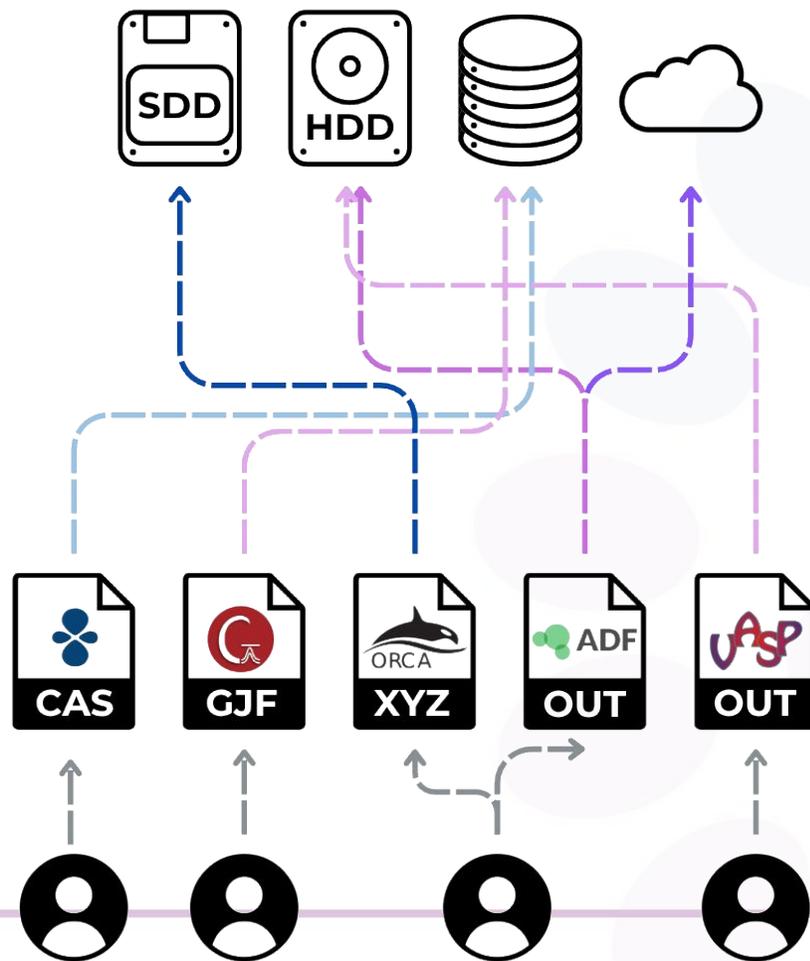


ioChem-BD



Funded by
the European Union

Managing computational chemistry and materials science data at scale



Scientific Challenges:

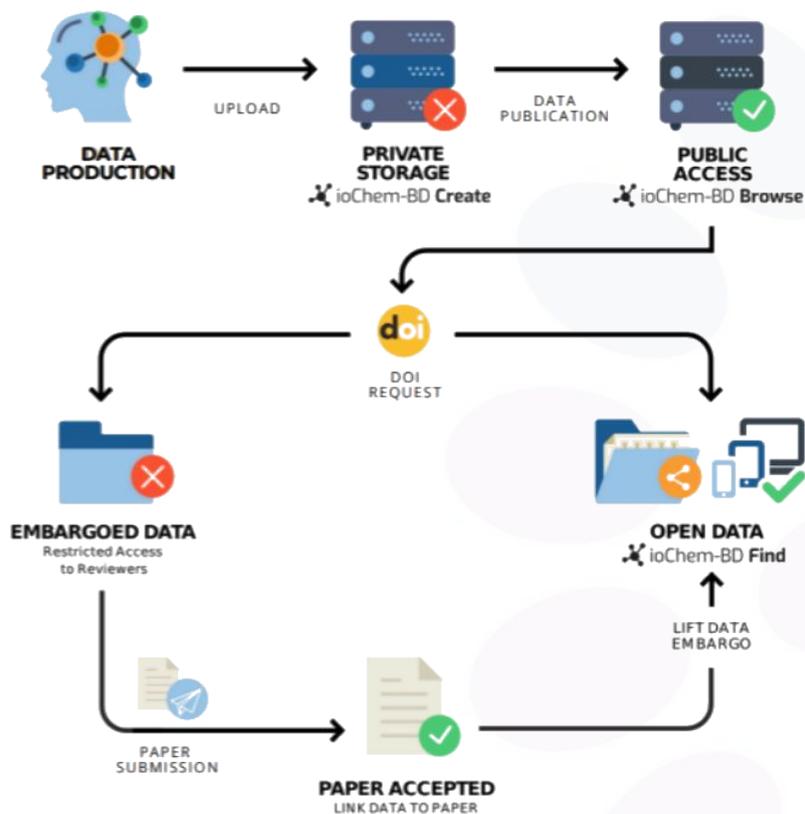
- Unstructured post processing (affect since the data analysis until the documentation) (F,A)
- Multiple data formats and storage media - (I)
- Lack of adapted repositories

Cultural & Structural Challenges:

- Reusability and reproducibility (R) - SD
- Difficulty implementing FAIR open data
- Fragmented workflows
- Sustainability beyond project funding

Infrastructure and community-driven strategies

ioChem-BD DATA PIPELINE



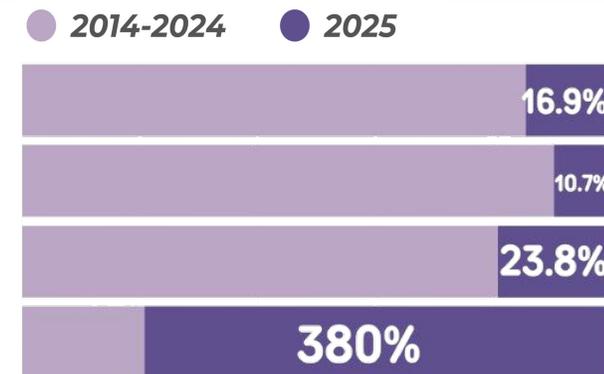
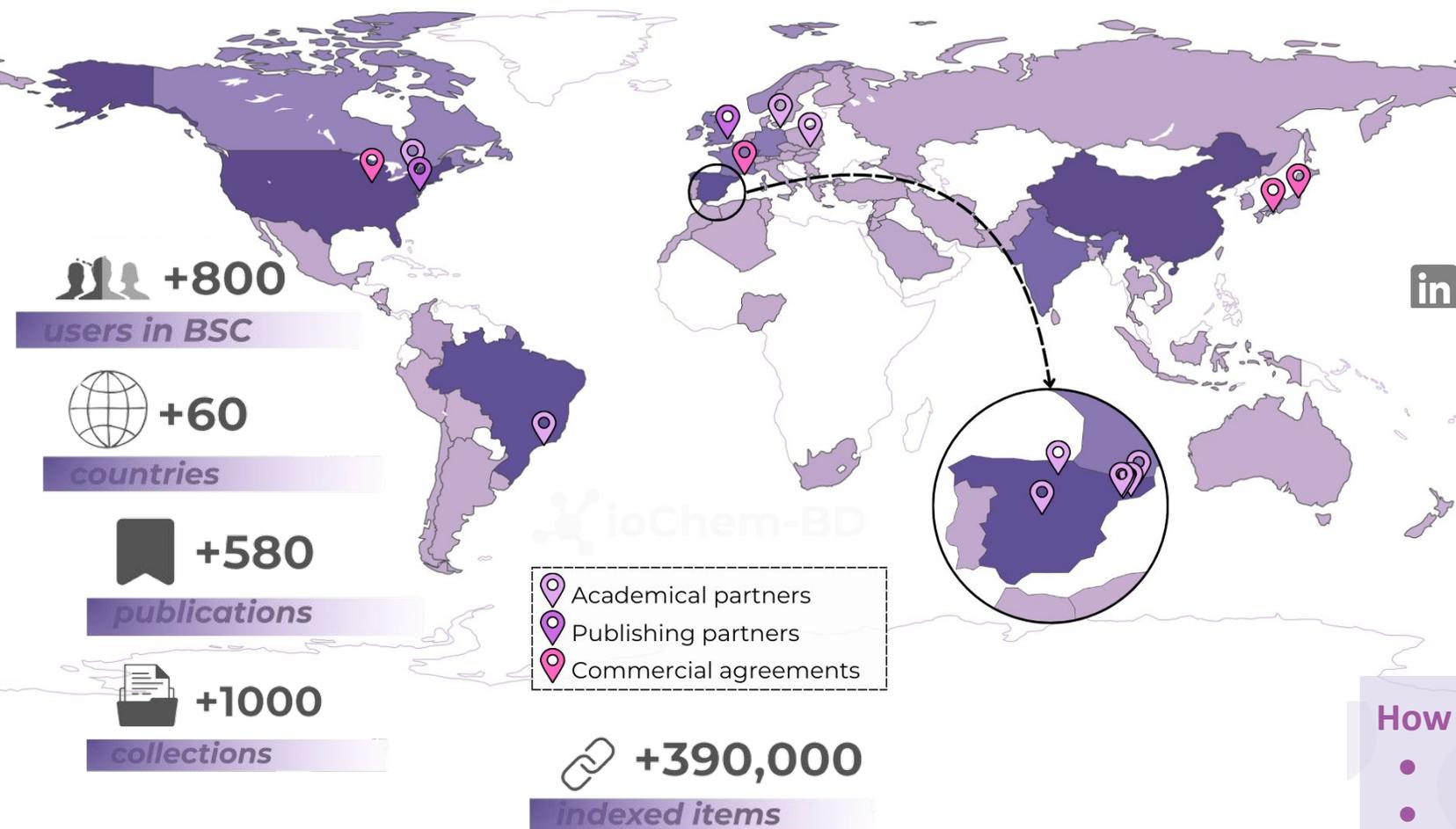
Technical & organizational solutions

- Data curation (using CML format)
- FAIR-by-design repository for CompChem
- Programmatic access via Shell Client/ REST APIs
- Open, public and free access (BSC node)

Community & collaboration

- Standardized SI and data analysis
- Establish a global community
- Receive industry feedback through commercial agreements

RESULTS - *our reach*



Key results

- FAIR open datasets for computational chemistry
- Reproducible and reusable research outputs
- A shared, trusted data infrastructure

How results are made available

- Open access via the ioChem-BD platform
- Programmatic reuse through REST APIs
- Integration with scientific publications
- Global access through the public BSC node

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“ioChem-BD: Open your research to the world”