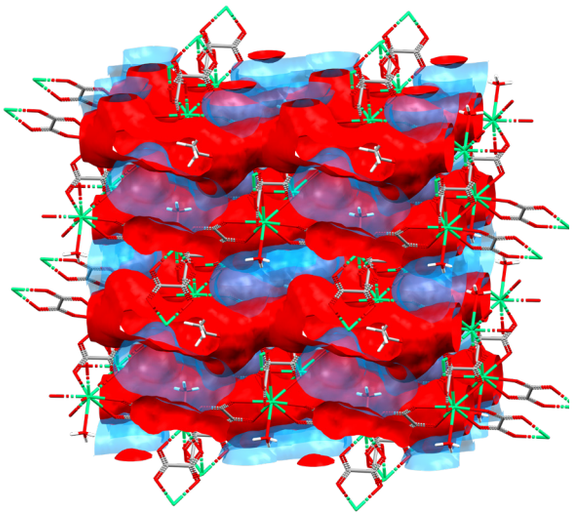
CCDC
advancing structural science

Design Porous Materials

CSD-Frameworks

For structural scientists to:

- Accelerate MOF and other porous materials research.
- Optimize materials design.
- Get deep insights into porous materials.
- Use trusted experimental data to analyse and assess your porous materials.



An Erbium Oxalate MOF structure (CSD entry WEMBUN) with solvents visualized using CSD-Frameworks.

Water molecule surfaces (blue) and ethanol solvate surfaces (red) are visualized.

CSD-Frameworks Capabilities:

- 3D display and manipulation of structures.
- High resolution graphics and movie generation.
- 3D printing file output.
- Simulate powder diffraction patterns and compare with reference patterns.
- Predict preferred orientations.
- Generate molecules from sketches or SMILES.
- Advanced structure editing.
- Calculate void and pore volumes and properties.
- Energy calculations.
- Calculate volume for guests such as solvates.
- Advanced search across the whole Cambridge Structural Database (CSD).
- Access to the whole CSD including 128k+ MOFs for commercial use.
- Python API for programmatic access.

CSD-Frameworks: Design Porous Materials

CSD-Frameworks is used to accelerate MOF and other porous materials research, optimize materials design, and gain deeper insights into porous materials–all using trusted experimental and curated data from the Cambridge Structural Database (CSD).

Giving access to a full crystal structure visualization and analysis software package, CSD-Frameworks enables pore and void characterization, solvate and guest molecule analysis, and chemical and structural searches.

CSD-Frameworks provides access to the entire CSD, including a curated collection of 128,000+ MOF structures.

Key Features

Access to the CSD including a curated and enhanced MOF subset

Work with high-quality, curated data that is ready for computational analysis. Access the full 1.3M+ structures, including 128,000+ experimentally determined MOF structures.

Advanced visualization and analysis

Explore crystal structures, including void space, pore dimensionality, guest analysis, and framework dimensionality. Easily modify symmetry. Easily analyse structural properties.

Efficient data mining and search

Identify structures based on chemical connectivity, ligands, structural features, or unit cell parameters. Find similar frameworks to guide new material design using the structure similarity tool.

Integrated Powder Diffraction Capabilities

Simulate and compare powder diffraction patterns from single-crystal structures. Validate experimental data efficiently.

Customizable solvent and guest molecule analysis

Define and analyse guest molecules within porous structures. Calculate solvent-accessible volumes for adsoroption studies.

Includes the software:

Web-CSD

Fast online searching for known structures by keywords, sketch, or DOI.

Mercury

Detailed analysis and custom visualizations to explore proprietary and public crystal structures on your desktop.

ConQuest

Perform searches of known structural data, to deeply understand the landscape.

CSD Python API

Perform data mining, search, and analyses programmatically for repeatable, automated results.