

## Bring Clarity to Your CSP Landscapes

# CSD-Theory

Search, display and analyse your crystal structure prediction landscapes to spark new insights and advance your solid form design.



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There have been approximately 160 000 Blind Test entries.

CSD-Theory allows you to:

- **See Your Experimental and Predicted Data All in One Place**
  - See your experimental and predicted results side by side, to get the complete picture of your system of interest
  - Automated matching highlights matching predicted and experimental structures.
  - Develop new insights in computer-aided materials design - whether you're an expert or a newcomer
- **View and Understand Your CSP Results via a Web-Based Interface**
  - See and understand CSP results quickly and easily, no matter your technical background
  - Share results with your team through a simple URL, allowing broader awareness and discussion to progress your project faster
- **Easily Analyse Your CSP Data**
  - Plot your CSP landscape on 2D or 3D graphs instantly, right in your web browser, then zoom and pan to examine sections of the graph
- **Generate Reports Automatically**
  - In one click, create a .doc report on your CSP landscape. Including an executive summary, detail on each property, and extensive appendix notes to provide context—ideal to share with your wider project team

### CSD-Theory Web



Display, search and analyse your CSP results in a simple web-based interface.

### CSD-Theory API



Generate, access and search databases from your CSP data programmatically.



## FAQs

### **If I access our in-house structures via the web would they be public or accessible to others?**

No. Our web platform is hosted by a private server behind the firewall of your organisation and no one else can access the data. Anyone within your organisation will be able to access it, to aid data sharing and discussions internally.

In a future update we plan to allow you to control access on a per-database basis, so you can restrict access internally if required.

### **Are you thinking about integration with other CSP platforms (e.g. XtalVision from XtalPi)?**

We had conversations with major CSP vendors (e.g. Avant-garde Materials Simulation AMS, XtalPi) about how we could better serve common customers.

By using our web platform you can:

- Store, search, view and link your experimental and theoretical structures in one place.
- Change provider while keeping the visualisation platform (our system is provider-agnostic).

### **Will my data be compatible?**

Yes - we can help you curate your data from most commonly used CSP data providers - without seeing your proprietary data. See CSD-Theory API.

Maybe - we can help you convert + curate using the CSD Python API - without seeing the proprietary data. See CSD-Theory API

### **How does CSD-Theory Web measure up to FAIR data principles?**

We aim to incorporate FAIR principles into all our products. CSD-Theory Web specifically offers a very Accessible way to search, store and visualise CSP data, and is Interoperable in that it can be used to store results from any CSP provider.

### **How can I chart and analyse my crystal structure prediction data?**

With CSD-Theory Web you can generate 2D or 3D graphs of your CSP landscape, direct in your web browser. You're also able to zoom and pan to examine sections of the graph. Select which properties to plot from a wide range of options including; space group, BFDH habit, hydrogen-bonding, Z', packing coefficient, void volume, void percentage and molecular shape descriptor.

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## Learn More

- Email [hello@ccdc.cam.ac.uk](mailto:hello@ccdc.cam.ac.uk) to ask a question or request an online demo.
- Visit [www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk) for more information.