

# User Manual for CSD Materials Suite– Installation Guide & User Manual

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INSTALLATION GUIDE – USER MANUAL

S.D. LIBRARY, IIT (BHU) VARANASI

RESEARCH SUPPORT TOOL

CSD Materials Suite

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## 1. Introduction: Cambridge Structural Database (CSD) Materials Suite

The Cambridge Structural Database (CSD) Materials Suite is a powerful toolset for researchers in materials science, enabling the exploration, visualization, and analysis of crystal structures from the CSD, which contains over 1.25 million small-molecule organic and metal-organic structures as of April 2025. The suite includes specialized tools like Mercury, CSD-CrossMiner, and components of the CSD Python API, tailored for applications such as crystal packing analysis, stability assessment, and materials design.

It provides tools for:

- **Database searching** (CSD database)
- **Structure visualization & analysis** (Mercury)
- **Conformational analysis** (ConQuest)
- **Molecular docking & interaction analysis** (Mogul, IsoStar)

This guide provides step-by-step instructions for installing the CSD-Materials Suite and an introductory manual for its core functionalities.

## 2. System Requirements

Before installing, ensure your system meets the following minimum requirements:

- **Operating System:** Windows 10/11, macOS 11 (Big Sur) or later, or a supported Linux distribution (e.g., Ubuntu 20.04+ or CentOS 7+).
- **RAM:** Minimum 8 GB (16 GB recommended for large datasets).
- **Disk Space:** Approximately 50 GB free during installation; ~40 GB post-installation.
- **Internet Connection:** Required for downloading installers and updates.
- **Graphics:** OpenGL-compatible graphics card for 3D visualization.

### 3. Step-by-Step Installation Guide

#### Step 1: Register for an Account

- Submit your request for getting the software through email to the Deputy Librarian at [deputylibrarian@iitbhu.ac.in](mailto:deputylibrarian@iitbhu.ac.in)

#### Step 2: Install the Software

##### i. Access the Download Options:

- You will receive an email to download the software and activation key(which will be used during installation). The mail contains links to download the correct version of the software package based on the type of operating system installed in the computer.

Dear CSD-Portfolio User,

Please find below all of the CSD-Portfolio downloads available to you, together with related documentation. These links will remain active for 24 hours - after this time you can request a new set of download links to obtain access.

The majority of CSD-Portfolio functionality, such as the data, ConQuest, Mercury and GOLD, is contained in the CSD-Portfolio download - we would recommend you start with this download.

The Python API package links provided below are for advanced users to install into their own Python; the CSD-Portfolio installers include their own Python with the API pre-installed, so for standard use the separate API pip and conda packages should not be necessary.

The Pipeline Pilot and KNIME downloads are only required for integration with these systems.

The IsoStar server is only required to install a local IsoStar server - access is otherwise available from our public server at <https://isostar.ccdc.cam.ac.uk>

[Python 3.11 CSD Python API KNIME module 3.3.1 Windows 64-bit conda installer](#)

[Python 3.11 CSD Python API KNIME module 3.3.1 Linux 64-bit conda installer](#)

[Python 3.11 CSD Python API KNIME module 3.3.1 MacOS 64-bit conda installer](#)

[CSD Portfolio 2024.3.0 Release & Installation Notes](#)

[CSD Portfolio 2024.3.0 Windows Online Installer \(recommended\\_small download\)](#)

[CSD Portfolio 2024.3.0 Linux Online Installer \(recommended\\_small download\)](#)

[CSD Portfolio 2024.3.0 MacOS Online Installer \(recommended\\_small download\)](#)

[CSD Portfolio Download sha256 Validation Checksums](#)

[Python 3.11 CSD Python API 3.3.1 Windows 64-bit conda installer](#)

[Python 3.11 CSD Python API 3.3.1 Windows 64-bit pip installer](#)

[Python 3.11 CSD Python API 3.3.1 Linux 64-bit conda installer](#)

[Python 3.11 CSD Python API 3.3.1 Linux 64-bit pip installer](#)

[Python 3.11 CSD Python API 3.3.1 MacOS 64-bit conda installer](#)

[Python 3.11 CSD Python API 3.3.1 MacOS 64-bit pip installer](#)

[Python API 3.3.1 example scripts](#)

[Python API 3.3.1 utilities](#)

[IsoStar Server \(linux only\)](#)

[Python 3.9 CSD Python API 3.3.1 Windows 64-bit conda installer](#)

[Python 3.9 CSD Python API 3.3.1 Windows 64-bit pip installer](#)

[Python 3.9 CSD Python API 3.3.1 Linux 64-bit conda installer](#)

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[Python 3.9 CSD Python API KNIME module 3.3.1 MacOS 64-bit conda installer](#)

[Python API 3.3.1 Documentation](#)

[Python API 3.3.1 Tests](#)

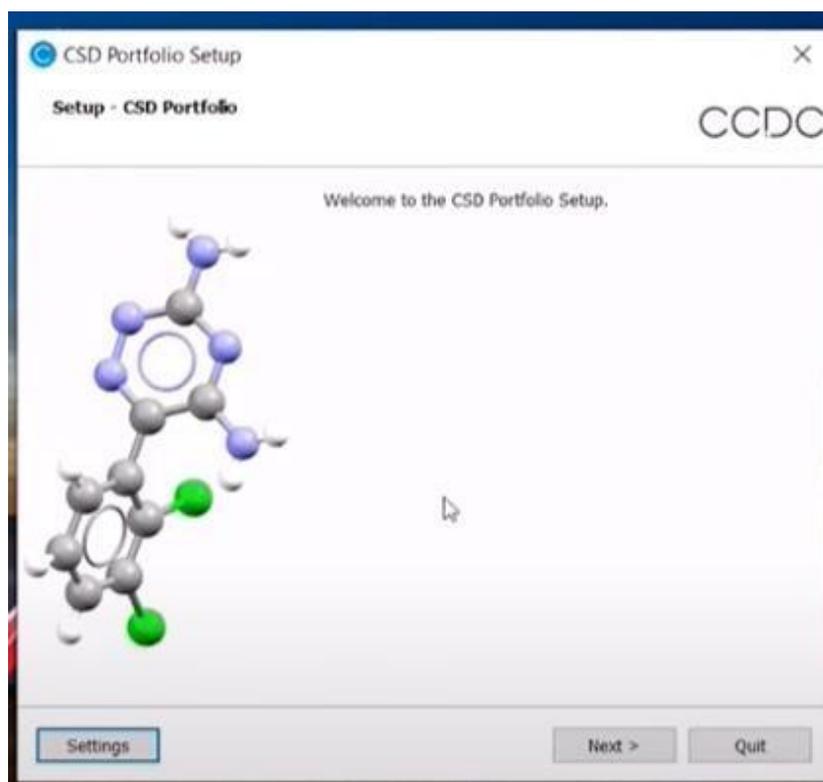
[CSD Portfolio 2024.3.0 Linux Offline Installer \(large download\)](#)

[CSD Portfolio 2024.3.0 MacOS Offline Installer \(large download\)](#)

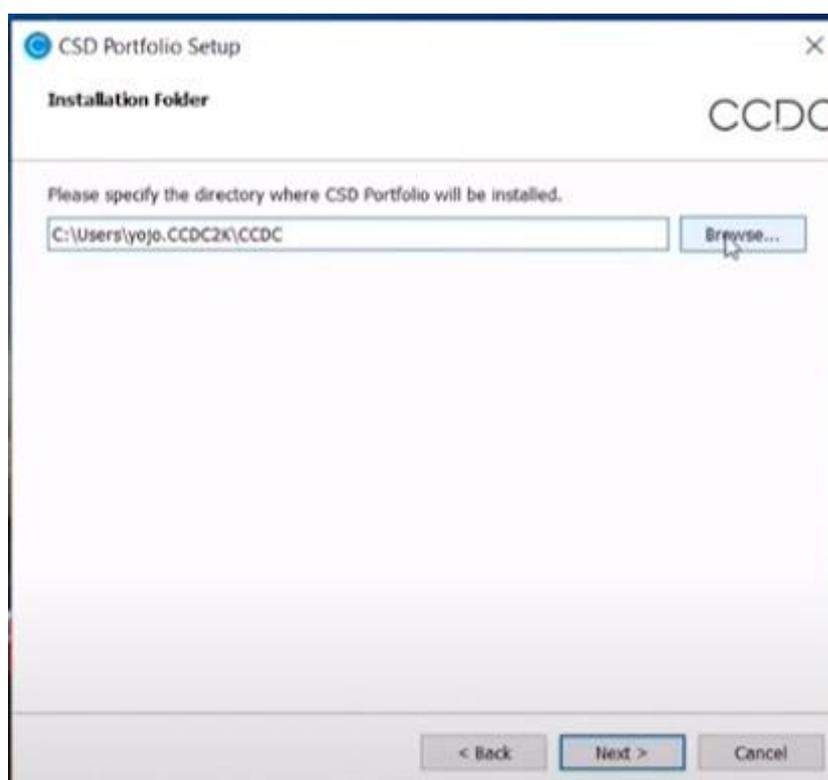
[CSD Portfolio 2024.3.0 Windows Offline Installer \(large download\)](#)

##### ii. Select appropriate Version:

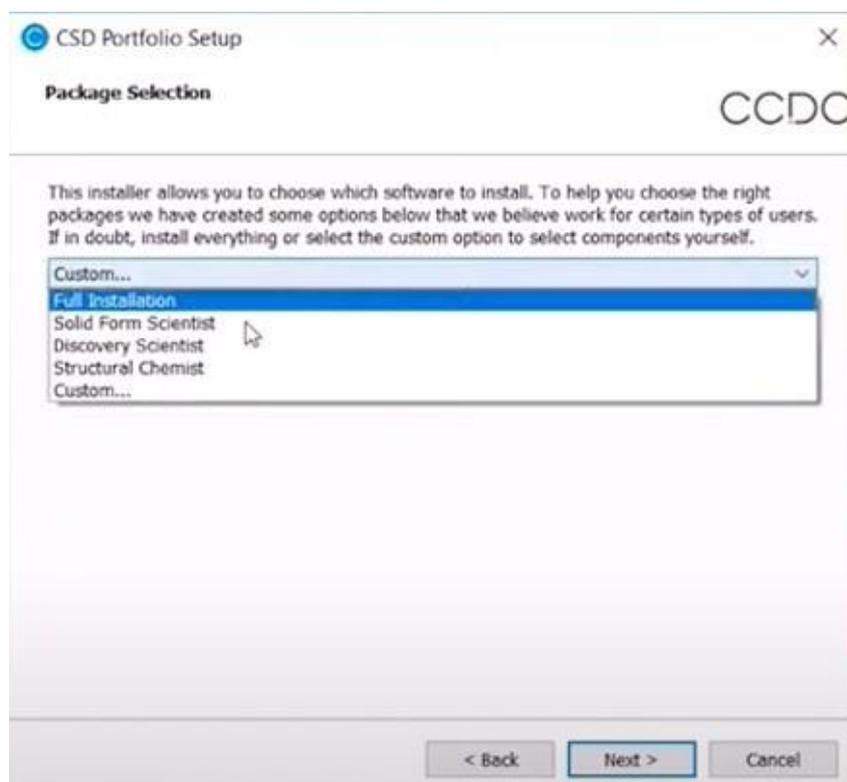
- If using a Windows-based operating system, click on the Windows Online Installer to download a file named CSDInstallerOnline.exe
- Open the downloaded file by double clicking it and click next.



- In the next window, select the directory (location) where the file must be installed (Full package installation requires around 22GB of storage space; please make sure that sufficient space is available).



- In the next windows, the type of products to be installed is shown. Select appropriate option and proceed further.



### iii. Copy the Activation Code:

- In the next window, enter the Activation key which was provided in the mail.

CSD Portfolio Setup

Activate licence

CCDC

Please choose how you would like to activate your CSD licensed features.

I want to activate my licence using an activation key

Please enter your licence key

I want to activate my licence using a local licence server I have previously set up

Licence Server  Port

I want to activate my licence after the installation

< Back Next > Cancel

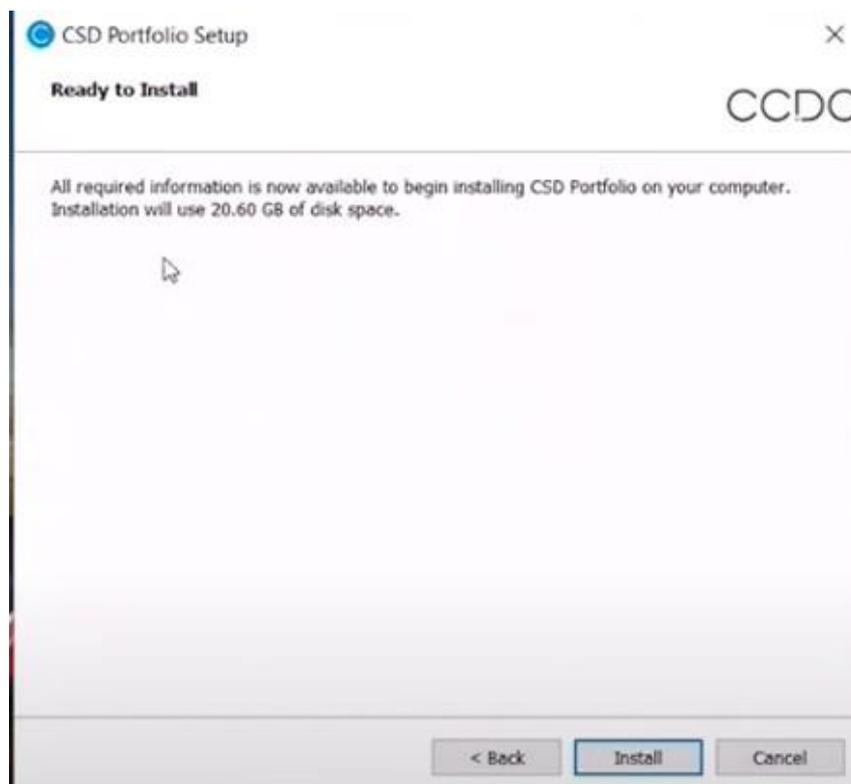
- Based on the use, select the softwares that are to be installed and click on Next.
- Click on the checkbox to accept the license terms and click Next.



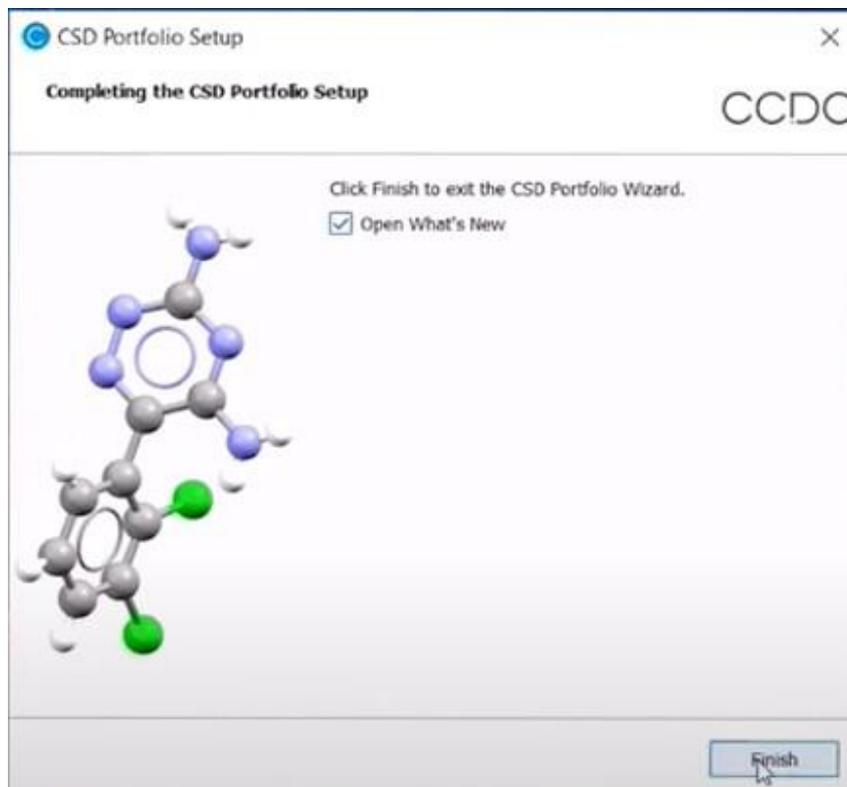
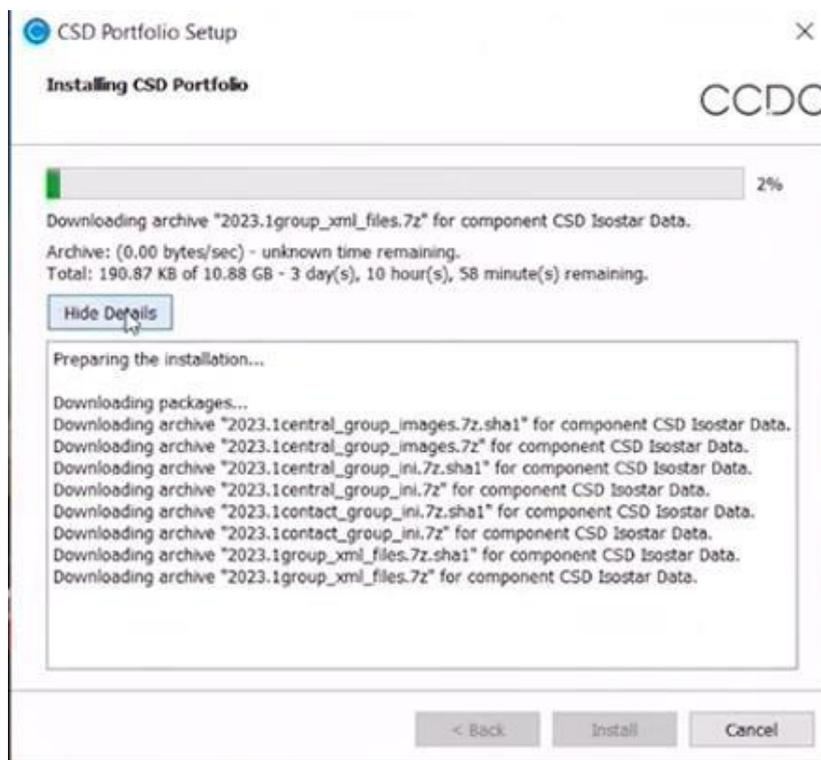
- ➔ Select appropriate option based on requirement for enabling/disabling telemetry for the software installed.



- ➔ Then click the Install button



- ➔ Wait till downloading and installation completes and then click finish. The installation is complete and the software is ready to use.



## 4. User Manual – Getting Started

### Accessing Installed Tools

After installation, the CSD Materials Suite will include tools such as:

- **Mercury** – for visualizing and exploring crystal structures.
- **ConQuest** – for database searches.
- **CSD Python API** – for programmatic access to structural data.
- **Hermes, Gold**, etc. – if installed, for structure modelling and docking.

### Running the Applications

- Locate the installed tools via:
  - **Start Menu (Windows):** Look for “CCDC Software”.
  - Or use search bar with terms like “Mercury”, “ConQuest”, etc.

## 5. Troubleshooting Common Issues

- **Email Not Received:** Check your spam/junk folder.
- **License not recognized:** Check internet connection, re-enter key, or contact the library staff, if it fails.
- **Installation Fails:** Ensure you have admin rights on your computer. Try running the installer as an administrator (right-click > “Run as Administrator” on Windows).
- **Slow rendering in Mercury:** Update GPU drivers, reduce structure complexity.
- **Database connection error:** Verify network settings, reinstall if needed.
- **Further Help:** Contact library staff or mail your queries at [libraryservices@iitbhu.ac.in](mailto:libraryservices@iitbhu.ac.in)

## 6. Support and Contact Information

- **CCDC Support:** [support@ccdc.cam.ac.uk](mailto:support@ccdc.cam.ac.uk)
- **Documentation:** <https://www.ccdc.cam.ac.uk/support/>
- **Institutional Contact:** Reach out to the library for subscription-specific assistance.
- **Current Date:** This guide is accurate as of April 23, 2025. Check for updates if installing later.

Congratulations! You've successfully installed CSD Materials Suite using your institutional subscription. Start creating professional chemical diagrams and advancing your research today!

## 7. Basic queries:

➤ All in One/Discovery/Remote access/ OPAC:

<https://iitbhu.lsdiscovery.in/home/dashboard>

➤ Please give your feedback: [Click here](#)

➤ Request for call back: [Click here](#)

➤ Ask the Librarian: [Click here](#)

➤ For more details, visit the Library website: <https://www.iitbhu.ac.in/cf/lib>

➤ Feel free to contact us with any queries, email [libraryservices@iitbhu.ac.in](mailto:libraryservices@iitbhu.ac.in) or visit the library.

*Please don't share your user ID and password with anyone.*

**Thank You**