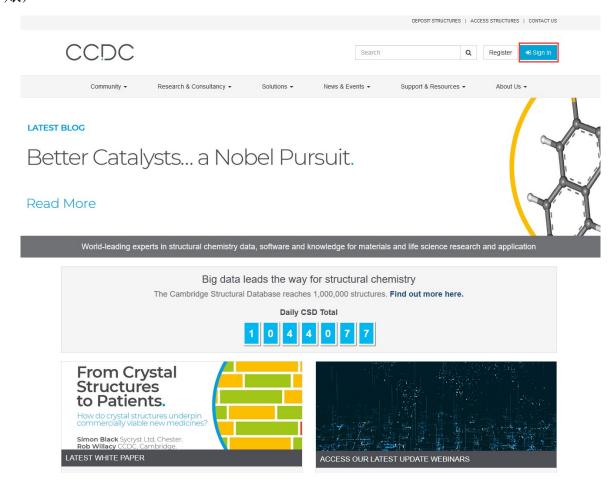
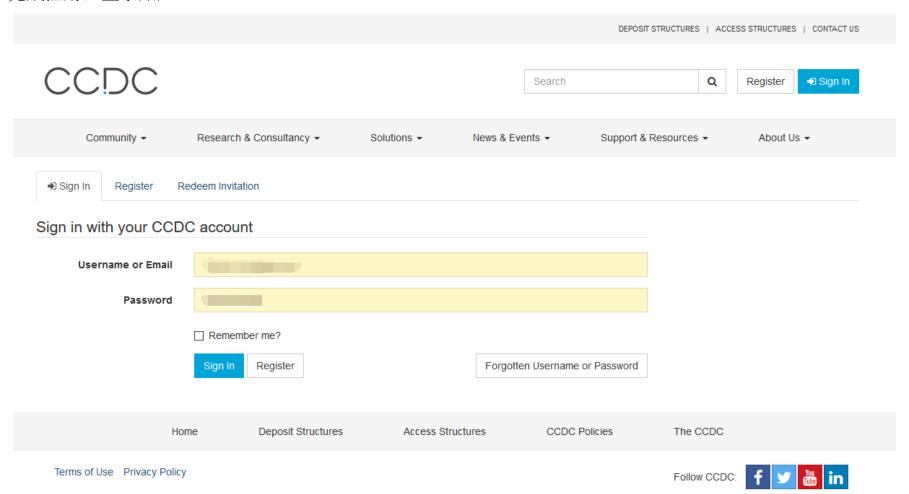
- 1.打开 CCDC 官网: https://www.ccdc.cam.ac.uk/
- 2.注册并登录 CCDC 账户



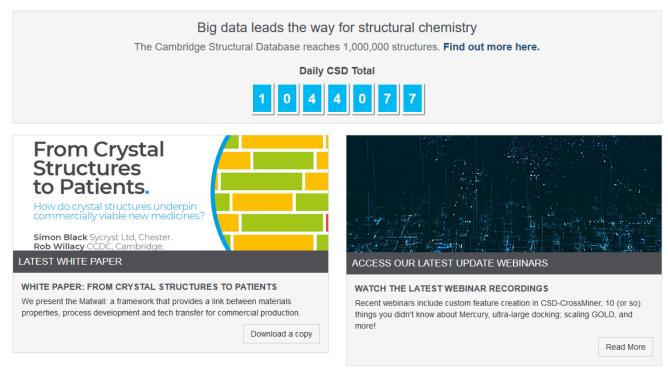




3. 完成注册, 登录账户



4. 登录成功,下载 CSD 客户端软件





Deposit Structures

Upload your data for inclusion in the Cambridge Structural Database or the Inorganic Crystal Structure Database



Access Structures

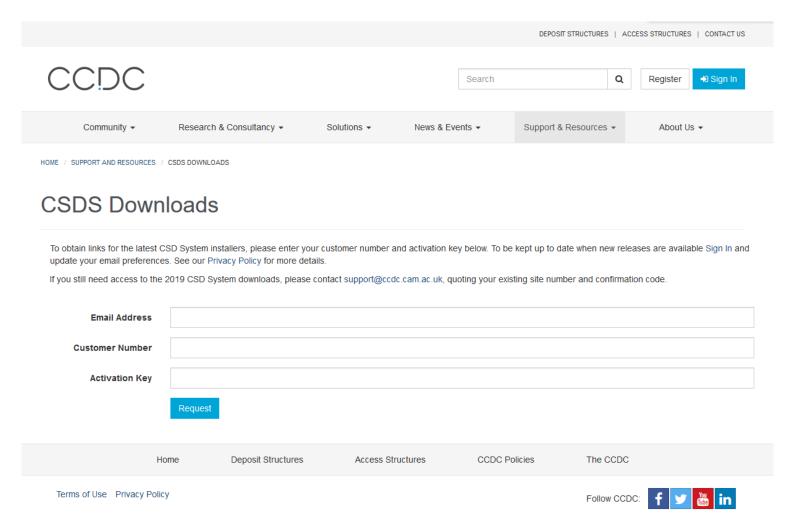
View and retrieve structures in the Cambridge Structural Database



CSD 2020.0

Available Now. The world's repository for small-molecule crystal structures. **Download CSD 2020.0**. Find out more about the latest data updates here.

5. 输入注册账户的邮箱以及 Customer Number & Activation Key(即为 licences)



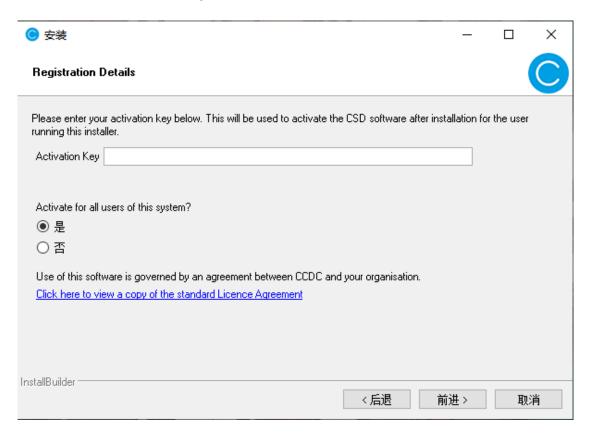
6. 注册邮箱会收到下载链接,点击所需的版本完成下载(链接只有24小时有效,请及时下载)

Pipeline Pilot Component Collection Installation Instructions

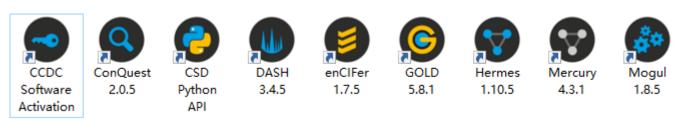
```
Pipeline Pilot Component Collection
Python 3.7 CSD Python API KNIME module 3.1.0 Windows 64-bit conda installer
Python 3.7 CSD Python API KNIME module 3.1.0 Linux 64-bit conda installer
Python 3.7 CSD Python API KNIME module 3.1.0 MacOS 64-bit conda installer
CSDS 2024.1.0 Release & Installation Notes
CSD Portfolio 2024.1.0 Windows Online Installer (recommended, 25 MB)
CSD Portfolio 2024.1.0 Linux Online Installer (recommended, 25 MB)
CSD Portfolio 2024.1.0 MacOS Online Installer (recommended, 25 MB)
CSD Portfolio Download sha256 Validation Checksums
Python 3.7 CSD Python API 3.1.0 Windows 64-bit conda installer
Python 3.7 CSD Python API 3.1.0 Windows 64-bit pip installer
Python 3.7 CSD Python API 3.1.0 Linux 64-bit conda installer
Python 3.7 CSD Python API 3.1.0 Linux 64-bit pip installer
Python 3.7 CSD Python API 3.1.0 MacOS 64-bit conda installer
Python 3.7 CSD Python API 3.1.0 MacOS 64-bit pip installer
CSD Python API example scripts
CSD Python API utilities
IsoStar Server (linux only)
Python 3.9 CSD Python API 3.1.0 Windows 64-bit conda installer
Python 3.9 CSD Python API 3.1.0 Windows 64-bit pip installer
Python 3.9 CSD Python API 3.1.0 Linux 64-bit conda installer
Python 3.9 CSD Python API 3.1.0 Linux 64-bit pip installer
Python 3.9 CSD Python API 3.1.0 MacOS 64-bit conda installer
Python 3.9 CSD Python API 3.1.0 MacOS 64-bit pip installer
Python 3.9 CSD Python API KNIME module 3.1.0 Windows 64-bit conda installer
Python 3.9 CSD Python API KNIME module 3.1.0 Linux 64-bit conda installer
Python 3.9 CSD Python API KNIME module 3.1.0 MacOS 64-bit conda installer
Python API 3.1.0 Documentation
Python API 3.1.0 Tests
CSD Portfolio 2024.1.0 Linux Offline Installer (18 GB)
CSD Portfolio 2024.1.0 MacOS Offline Installer (18 GB)
CSD Portfolio 2024.1.0 Windows Offline Installer (20 GB)
```

7. 完成下载, 大约 9. 5GB

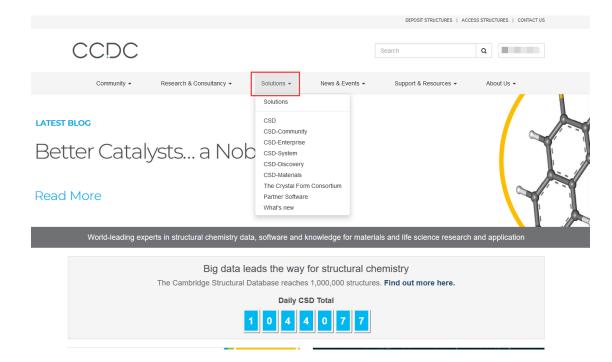
8. 开始安装, 在此处再次输入 Activation Key, 并完成安装



9. 根据需求,选择对应模块,开始使用

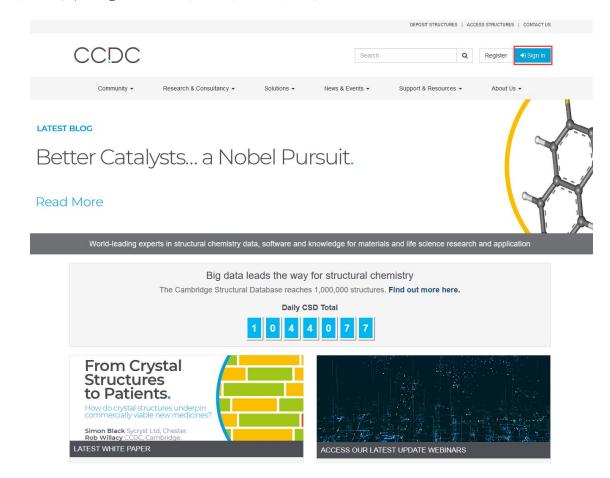


10. 更多问题,请点击首页的 solutions 查询

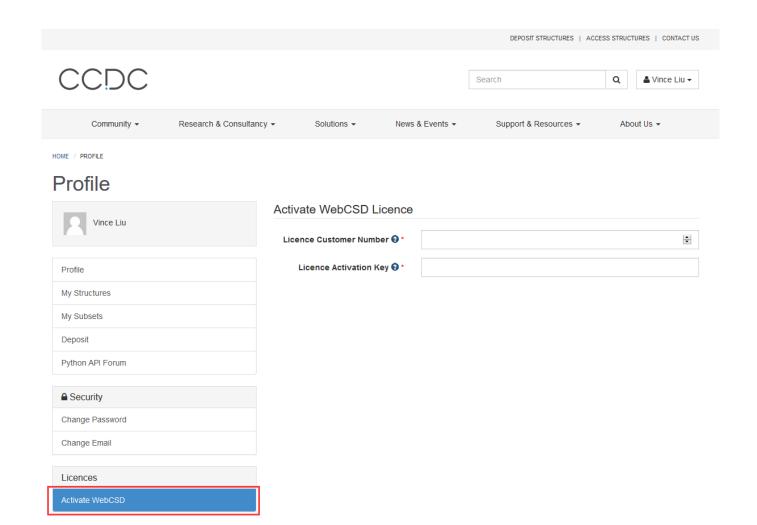


获得 WebCSD 进阶功能,需要进行对 CCDC 账号授予权限

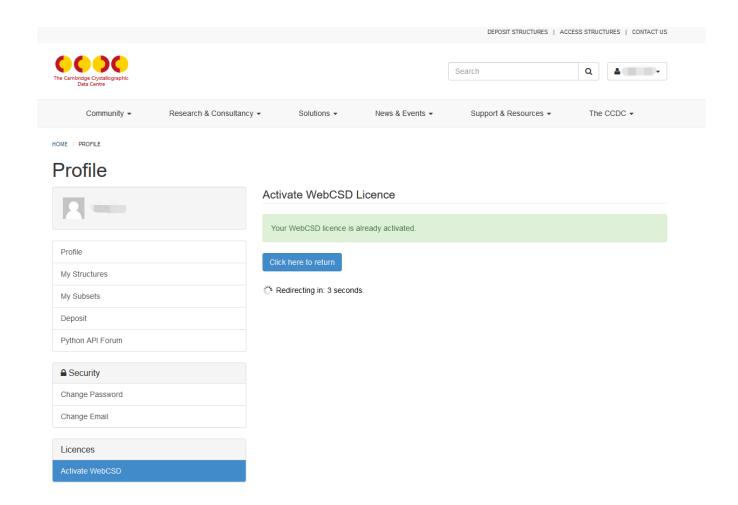
进入 CCDC 官网,点击右上角 log in,登录您的 CCDC 账号



登陆后进入个人详情页,点击左侧下方的 Activate WebCSD, 在页面输入相关信息对您的账号进行机构权限的授权



激活成功



点击 https://www.ccdc.cam.ac.uk/structures/ 即可进行 WebCSD 进阶功能的使用,也可进行 ICSD 的结构查询





WebCSD

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Welcome to WebCSD. This service now includes the ability to search for inorganic structures through the CCDC's and FIZ Karlsruhe's joint Access Service using the Simple Search tab. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. More information and search help		
Identifier(s)	CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s)	0
Compound name	e.g. sulfadiazine	8
DOI	A single publication DOI, CSD DOI or ICSD DOI	0
Authors	e.g. F.H.Allen	0
Journal	e.g. Journal of the American Chemical Society	0
Publication details	Year ♥ Volume Page	0
Database to search	● Entire published collection ○ CSD ○ ICSD ○ Teaching subset	
	+ Add New Search Field V	
	Search	Clear

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