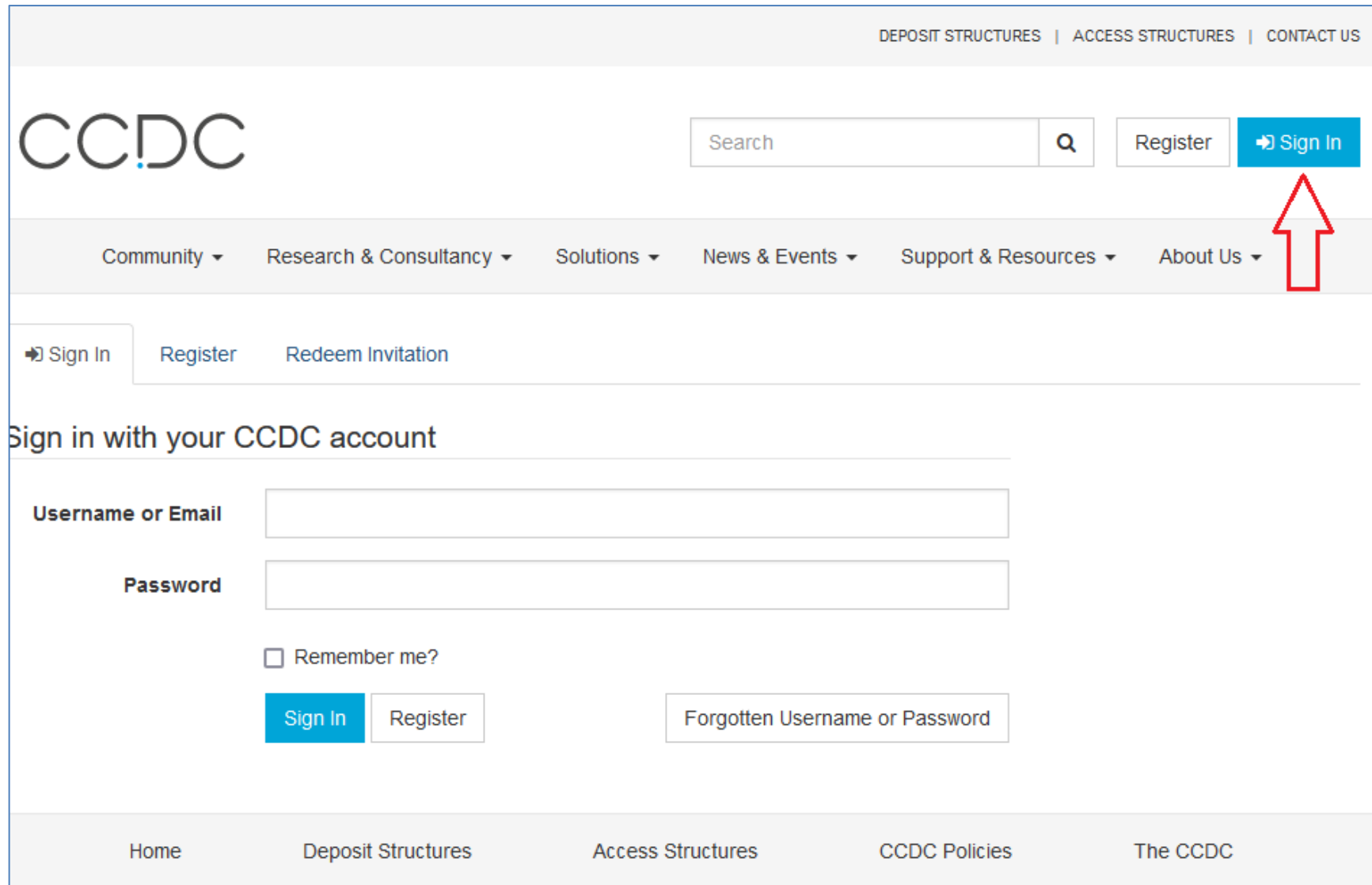


1. Access CCDC website: <https://www.ccdc.cam.ac.uk/>

2. Register and sign in CCDC Account



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By registering on the CCDC website you can set your email preferences and add posts to CCDC forums. By registering, depositors can deposit data more easily and access and share their data. CSD subscribers can access our advanced web services such as WebCSD. Your email address will be used in order to set up and verify your account. For more information see our [Privacy Policy](#).

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I'm not a robot



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3. Complete the Register then sign in

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4. Download CSD client

Join the thousands of scientists using the CSD data and CCDC software to **discover new drugs, improve material stability, and advance structural science.**

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Current structures in the Cambridge Structural Database:

1 1 5 5 2 6 5

WHITEPAPER
Ultra-large GOLD docking using cloud resources.

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LATEST WHITE PAPER

ULTRA LARGE GOLD DOCKING WHITEPAPER

This whitepaper details how GOLD, a comprehensively validated and widely used docking software, was used to perform a virtual screen on cloud resources.

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WATCH THE LATEST WEBINAR RECORDINGS

Recent webinars include custom feature creation in CSD-CrossMiner, 10 (or so) things you didn't know about Mercury, ultra-large docking; scaling GOLD, and more!


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 **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 2021.3**

Available Now. The world's repository for small-molecule crystal structures. [Download CSD 2021.3](#). Find out more about the latest data updates here.



5. Type your email address, Customer Number (5545), Activation Key (0ED5F1-D15019-4503B0-03045C-B37BA3-970825)

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CSDS Downloads

To obtain links for the latest CSD Suite installers, please enter your customer number and activation key below. To be kept up to date when new releases are available [Sign In](#) and update your email preferences. See our [Privacy Policy](#) for more details.

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6. You will get the download link by email, the download link will be available in 24 hours

 Thu 1/6/2022 10:33 AM
Sales Operations <admin@ccdc.cam.ac.uk>
CCDC Download Request

收件人
抄送 Yubin Gu

Dear CSD System 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 -

The majority of CSD-Portfolio functionality, such as the data, ConQuest, Mercury and GOLD, is contained in the CSDS download - we would recommend

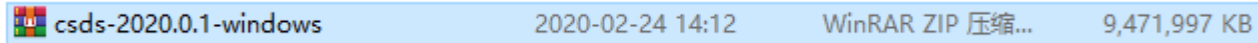
The Python API package links provided below are for advanced users to install into their own Python; the CSD-Portfolio installers include their own Python

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

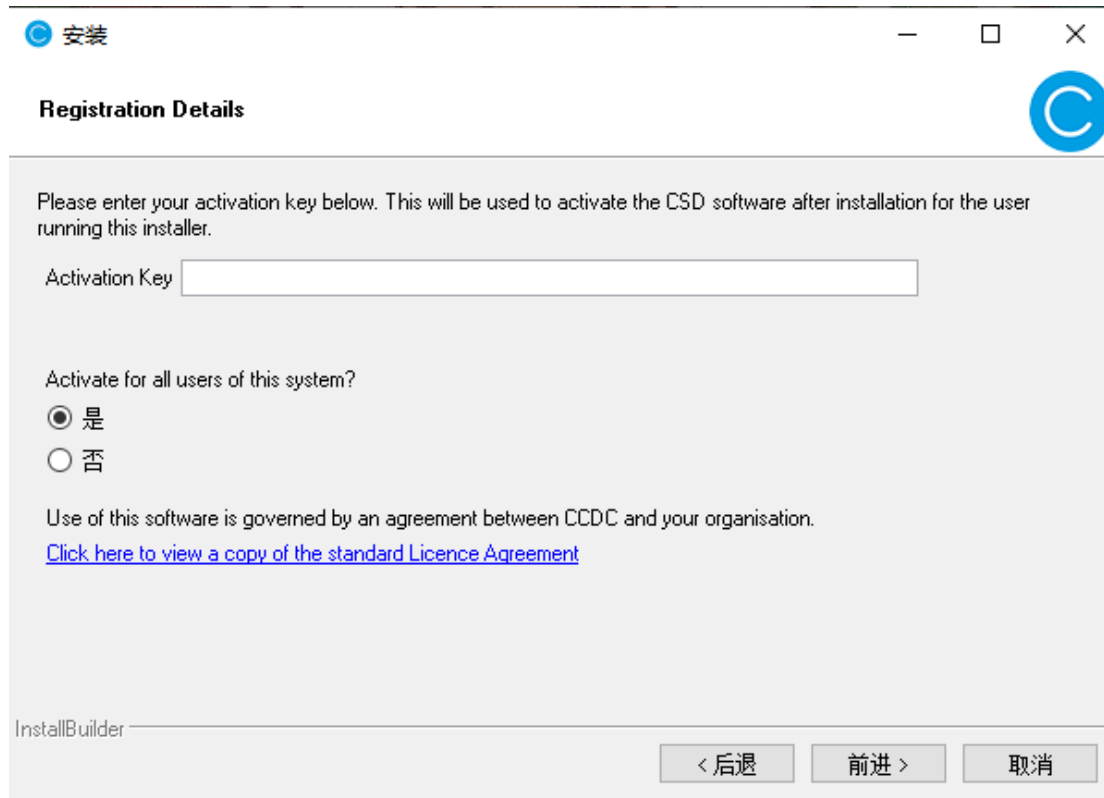
The IsoStar server is only required to install a local IsoStar server - access is otherwise available from our public server at <http://isostar.ccdc.cam.ac.uk>

[Pipeline Pilot Component Collection Installation Instructions](#)
[Pipeline Pilot Component Collection](#)
[Python 3.7 CSD Python API KNIME module 3.0.9 Windows 64-bit conda installer](#)
[Python 3.7 CSD Python API KNIME module 3.0.9 Linux 64-bit conda installer](#)
[Python 3.7 CSD Python API KNIME module 3.0.9 MacOS 64-bit conda installer](#)
[CSDS 2021.3 Release & Installation Notes](#)
[CSDS 2021.3 Windows](#)
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[Python 3.7 CSD Python API 3.0.9 Windows 64-bit conda installer](#)
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[Python 3.7 CSD Python API 3.0.9 MacOS 64-bit pip installer](#)
[CSD Python API example scripts](#)
[CSD Python API utilities](#)
[IsoStar Server \(linux only\)](#)

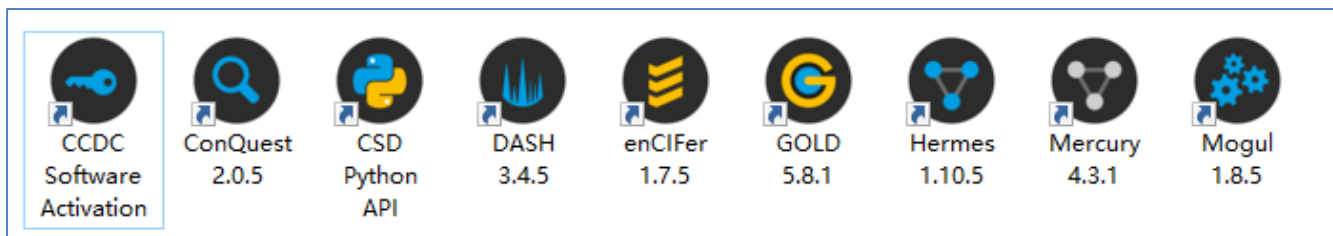
7. Complete download, about 10.2GB



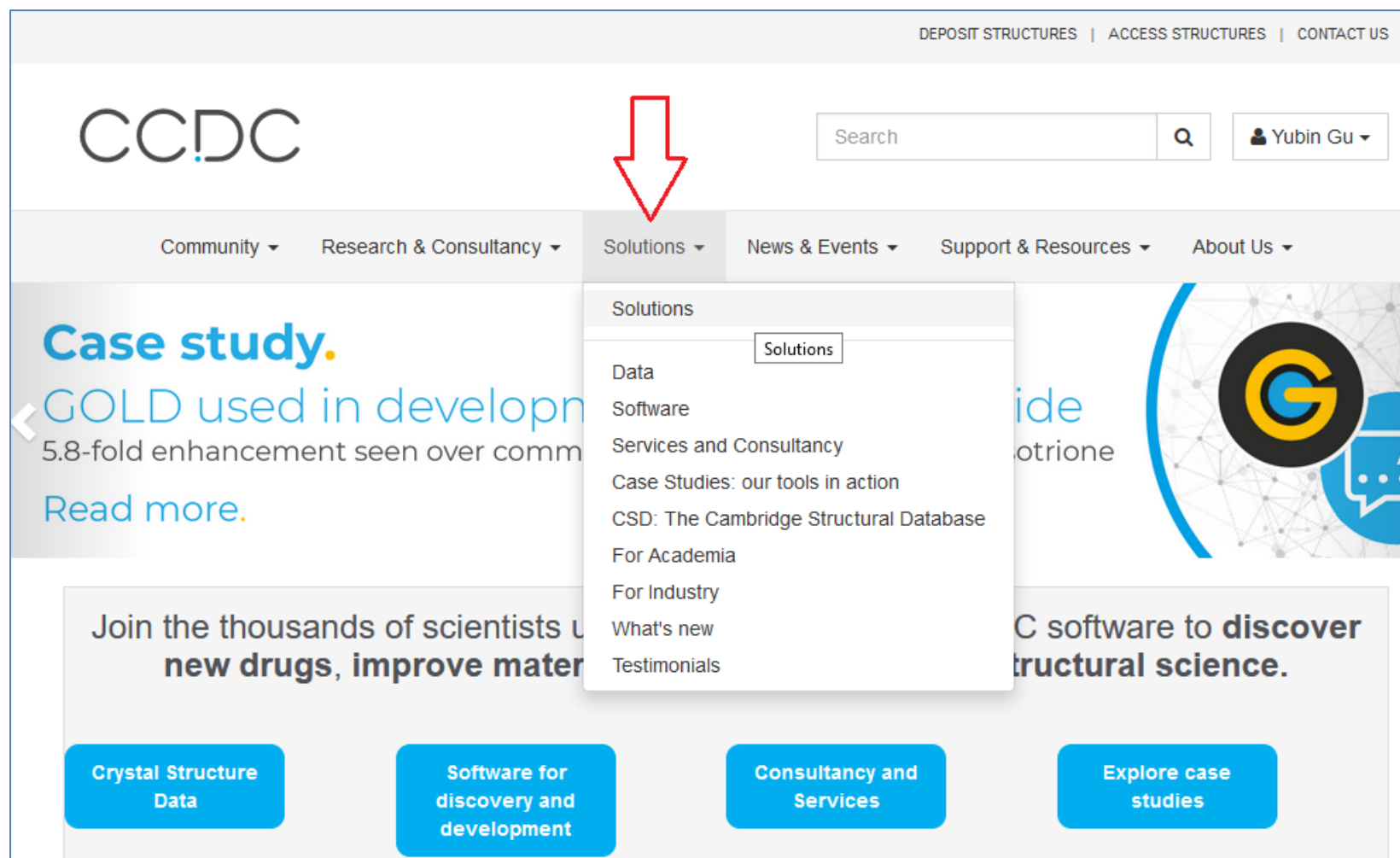
8. Start installation, activate with Activation Key (0ED5F1-D15019-4503B0-03045C-B37BA3-970825)



9. Select relevant module then start to use

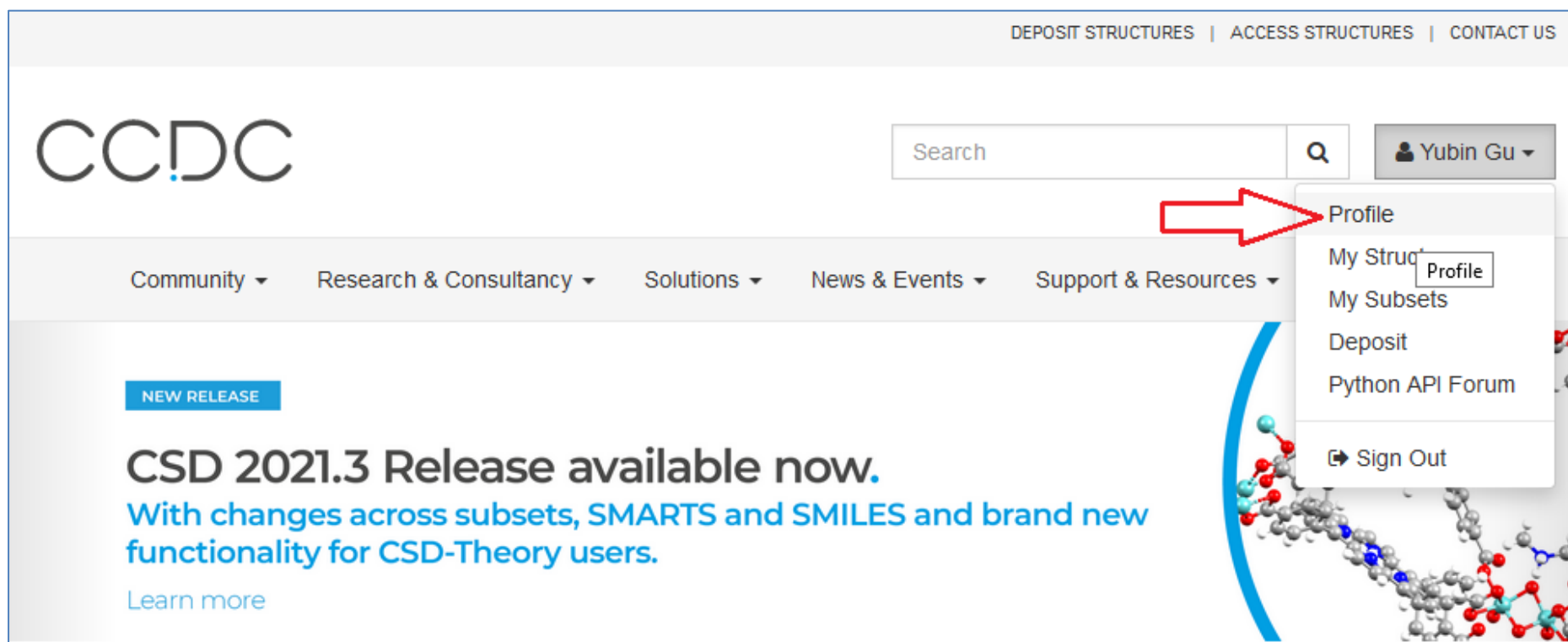


10. For more problems, you can refer to “Solutions” on CCDC website



For WebCSD access, you need to do authorization first.

You need to sign in first, then click "Profile"



The screenshot shows the CCDC website interface. At the top right, there are links for "DEPOSIT STRUCTURES", "ACCESS STRUCTURES", and "CONTACT US". The CCDC logo is on the left. A search bar is in the center, and a user profile dropdown is on the right, showing the name "Yubin Gu". A red arrow points to the "Profile" option in the dropdown menu. The dropdown menu also includes "My Structures", "My Subsets", "Deposit", "Python API Forum", and "Sign Out". Below the navigation bar, there is a "NEW RELEASE" banner for "CSD 2021.3 Release available now." with a "Learn more" link. The background features a molecular structure visualization.

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NEW RELEASE

CSD 2021.3 Release available now.
With changes across subsets, SMARTS and SMILES and brand new functionality for CSD-Theory users.
[Learn more](#)


Click "Activate WebCSD" , then type Customer Number (5545), Activation Key (0ED5F1-D15019-4503B0-03045C-B37BA3-970825)

The screenshot shows a web browser window with the URL <https://www.ccdc.cam.ac.uk/profile/activatewebcscd>. The page header includes the CCDC logo, a search bar, and a user profile dropdown for 'Yubin Gu'. The main navigation menu contains links for Community, Research & Consultancy, Solutions, News & Events, Support & Resources, and About Us. The breadcrumb trail indicates the user is on the 'PROFILE' page.

The left sidebar contains a 'Profile' section with links to 'Yubin Gu', 'Profile', 'My Structures', 'My Subsets', 'Deposit', and 'Python API Forum'. Below this is a 'Security' section with links for 'Change Password' and 'Change Email'. At the bottom of the sidebar is a 'Licences' section with a link to 'Activate WebCSD', which is highlighted with a red arrow.

The main content area is titled 'Activate WebCSD Licence' and contains two input fields: 'Licence Customer Number' and 'Licence Activation Key'. Below these fields is a reCAPTCHA widget with the text 'I'm not a robot' and a blue 'Activate' button.


Activate successfully

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- Profile
- My Structures
- My Subsets
- Deposit
- Python API Forum

Security

- Change Password
- Change Email

Licences

- Activate WebCSD



Activate WebCSD Licence

Your WebCSD licence is already activated.

[Click here to return](#)

🌀 Redirecting in: 2 seconds.

Now you can access WebCSD via <https://www.ccdc.cam.ac.uk/structures/>



WebCSD

Yubin Gu ▾

Licensed to: Xi'an Jiaotong-Liverpool University

Simple Search | Structure Search | Unit Cell Search | Formula Search

Simple text and numeric searching

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) ?

Compound name ?

DOI ?

Authors ?

Journal ?

Publication details ? ? ?

Database to search Entire published collection CSD ICSD Teaching subset

▾

Search

Clear