The following is the documentation of CrysX-3D Viewer version 1.9.2.

Introduction

The crystal or molecule visualizer tool, *CrysX – 3D Viewer*, is available for *Windows*, *Linux*, *MacOS* and *Android* devices. The visualizer enables the users to open popular *CIF, VASP files such as POSCAR, CONTCAR, TURBOMOLE's coord files and extended XYZ* format files, to visualize the *crystal structures* of any compound. Even *molecular structures* and *isosurfaces* depicting densities and orbitals can be visualized by opening popular *.xyz/.mol/.tmol* and *.cub/.cube* format files, respectively. The visualizer is built using a gaming engine (*Unity3d*) ensuring *stellar, never-before seen graphics* on any other molecule/crystal visualizer. This makes the app really useful for researchers to *prepare illustrations* and figures for their research papers, thesis and dissertation. The app lets the users visualize *lattice planes*, and draw *vectors* to indicate electric/magnetic fields. Users can model *supercells*, *monolayers (currently disabled due to a bug)* (thin film/quantum well) or *quantum dots.* One can also edit the structures to create a *vacancy* or introduce an *impurity*. There is also a feature that lets you draw your own *custom 3D molecule/nanocluster*. Structures can also be analyzed by measuring the bond angles and lengths. Although, the app is quite straight-forward to use, high quality YouTube tutorials and documentation will get you up to speed in no time.

Application Details

Download and Installation:

CrysX – 3D Viewer is available as a .apk file for the Android platform and a zip package for the Windows platform. The .apk file can be downloaded from here or installed directly from the Google Play Store. The advantage of installing it from the Google Play Store is that the app will get updated automatically. However, if you do download it from the former link, then you might have to enable a setting to 'Allow apps from external sources' in your Android settings, to be able to install it successfully. Similarly, for Windows the updates would have to be checked manually.

Features:

The app version 1.9.2 contains the following features:

1. Can read and visualize `.CIF, .XYZ, .CUB, POSCAR, CONTCAR, .VASP, .TMOL, .COORD` and `.MOL` files.
2. Can model supercells, defects, vacancies, quantum dots, custom 3d molecules, etc.
3. Can visualize lattice planes via Miller indices.
4. Can visualize vector arrows using Cartesian coordinates.
5. Can calculate COM of selected atoms, measure bond-lengths and -angles.
6. Export structures as `.XYZ, .CIF, .TMOL,` and `.VASP` for use in other popular packages.
7. Export .STL for 3D printing.
8. Can visualize isosurfaces depicting the density or orbitals from the Gaussian cube format file (`.cub` or `.cube`)

Report a Bug:

You can report a bug by either leaving a review on the Google Play Store, or leaving a comment here, or reaching out to the developer via email: feedback@bragitoff.com

Request a Feature:

You can request a feature by either leaving a review on the Google Play Store, or leaving a comment here, or reaching out to the developer via email: feedback@bragitoff.com

Usage Instructions, Tips and Examples

The following YouTube videos demonstrate how to use the different features of CrysX-3D Viewer:

Open Source Libraries

The app uses the following open source libraries, and the developer thanks the awesome community:

1. Unity Simple File Browser by yasirkula | License: MIT
2. pb_Stl by karl | License: MIT
3. HSV Color Picker Unity by judah4 | License: MIT
4. mXParser by Mariusz Gromada | License: Simplified BSD Licens
5. Unity Native Toolkit by Ryan Webb | License: MIT
6. MarchingCubesBurst by Nezix (XavierM) | License: MIT

Special Notes

It should be noted, that due to the large variety of `.CIF` formats out there, CrysX may not yet support all of them as the application is still in the budding stage. However, if you ever encounter a file that fails to be parsed, let me know and mail the file to me. I will try to add the compatibility for the various formats. Similarly while file conversion, for some complicated systems the converted CIF may not be what you expected. Please let me know if you encounter a problem.

Legal Disclaimer

While I try to make everything as accurate as possible, with honesty, the following disclaimer applies to all the softwares I create:

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Users are advised to make sure and confirm that the results obtained through CrysX-3D Viewer are correct or not on their own and I cannot be held responsible for faulty results. Users are responsible for their results, not me.

There is absolutely no WARRANTY associated or provided with the use of this software.

License

CrysX-3D Viewer is currently copyrighted with its source code not open to the public; we wish to control the development and future of CrysX-3D Viewer by ourselves. This software is distributed free of charge for academic, scientific, educational, and commercial users. Permission to use this software is hereby granted under the following conditions:

1. Results or structures or calculations done/ produced by CrysX-3D Viewer may be used in any publications (original and review articles) provided that its use is explicitly acknowledged. A suitable reference for CrysX-3D Viewer is:

M. Sharma and D. Mishra, Journal of Applied Crystallography 52, (2019).

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CrysX – 3D Viewer FAQ (Frequently Asked Question)

How to cite this product?

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Is it free?

Yup! It's completely free to use.

Will it get updates?

CrysX is always in development and will get regular updates. I still have a lot of features planned that I have to add. So updates are gonna be frequent.

Where can I download the supported .xyz or .cif files from?

CrysX works best with .cif files downloaded from AMCSD database as well as materialsproject.org.
For .xyz files, you can download the mol files from PubChem, ChemSpider or CACTUS and then convert it to .xyz format using Open Babel or this tool.

When will CrysX come to iOS?

Soon. The application packages are almost ready. But I cannot afford to buy an Apple device right now for testing. So basically as soon as I can borrow one or buy one, I will test it and publish to Apple store.

Can I visualize DNA or biomolecules?

Technically yes, BUT only if they are in the supported file formats which are `.xyz, .mol, .cif, .tmol, .coord, POSCAR, CONTCAR, .vasp` or `.cub`.

Can I visualize Turbomole Coord files with CrysX-3D Viewer?

Yes, CrysX-3D Viewer supports the TURBOMOLE's `coord` file format, since the version 1.9.1.
It can visualize a molecular structure as well as a periodic structure if `$cell` or `$lattice` keywords are present in the coord file.

One should ensure that

1. The file has a `.tmol` or `.coord` extension (example: `water.coord` or `water.tmol`).
2. Atomic positions are in atomic units (bohrs).
3. For periodic structures the coord file should contain the `$cell` or `$lattice` keywords.
4. Only 3D periodic structures are supported so either the three lattice vectors should be provided or the six lattice constants: `a, b, c, alpha, beta, gamma`.

Can CrysX-3D Viewer visualize VASP formats such as POSCAR/CONTCAR?

Yes, CryX-3D Viewer supports visualizing `POSCAR` or `CONTCAR` files, since the version 1.9.1. One has to make sure that the files have either the `.vasp` extension or the names contain `POSCAR` or `CONTCAR` in them.