

XCRYSDEN INSTALLATION

To properly install Xcrysden 1.5 in ubuntu and works with POSCAR files, you must follow next steps:

STEP 1

- Download next tar.gz files from:

<http://www.xcrysden.org/download/xc-1.4.1bin-linuxPC-static.tar.gz>

http://www.xcrysden.org/download/xc-1.5.21-linux_x86_64-semishared.tar.gz

- You must additionally obtain the Poscar2xcrysden.pl script make it for Javier Carrasco.

NOTE: I put a link as soon as possible.

STEP 2

- make /scratch directory and change permissions and group

```
$ mkdir /scratch
$ chgrp users /scratch -R
$ chmod 775 /scratch -R
```

STEP 3

- Use *sudo* or logon as root.
- Go to /opt directory
- Uncompress xc-1.4.1bin-linuxPC-static.tar.gz
- Run .xcConfigure script and follow the instructions.
- Edit the /home/youruser/.bashrc file to make some changes:
 - change

```
XCRYSDEN_TOPDIR=/opt/XCrySDen-1.4.1bin-static
to
XCRYSDEN_TOPDIR_OLD=/opt/XCrySDen-1.4.1bin-static
```
 - change

```
export XCRYSDEN_TOPDIR XCRYSDEN_SCRATCH
to
export XCRYSDEN_TOPDIR_OLD XCRYSDEN_SCRATCH
```
 - change

```
PATH="$XCRYSDEN_TOPDIR:$PATH:$XCRYSDEN_TOPDIR/scripts:
$XCRYSDEN_TOPDIR/util"
to
PATH="$XCRYSDEN_TOPDIR_OLD:$PATH:$XCRYSDEN_TOPDIR_OLD/scripts:
$XCRYSDEN_TOPDIR_OLD/util"
```
- save and exit.
- Edit

```
/opt/XCrySDen-1.4.1bin-static/xcrysden
```

change all strings matches with

```
$XCRYSDEN_TOPDIR  
to  
$XCRYSDEN_TOPDIR_OLD
```

- save and exit.
- Rename file to xcrysdn.old

STEP 4

- Uncompress to /opt directory:
xc-1.5.21-linux_x86_64-semishared.tar.gz
- Change to uncompressed directory:
\$ cd /opt/XCrySDen-1.5.21-bin-semishared
- Configure environment vars and more with:

```
$ ./xcConfigure
```

follow instructions.

Now you have installed two versions of Xcrysden, v1.4 and v1.5.

STEP 5

- Test if both comands works properly:

```
$ xcrysden (for v1.5)  
$ xcrysden.old (for v1.4)
```

NOTE: the v1.4 version is necessary to open files transformed with *Poscar2xcrysden.pl* and will be exported to .xsf format and will be imported for XCrysden v1.5.

Bibliography:

<http://www.google.com>
<http://www.xcrysden.org/XCrySDen.html>