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/scripts:
    $XCRYSDEN_TOPDIR/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 xcrysden.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

- Compile application with make command:
  $ make all

- 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