

XCRYSDEN

– a short tutorial –

Cagliari, September 2005

Guido Fratesi

(mostly based on Anton Kokalj's work)

Copy me ...

- this tutorial can be downloaded from:

[http://\[ESPRESSO-TUTORIAL-SITE\]/tutorial_xcrysden.pdf](http://[ESPRESSO-TUTORIAL-SITE]/tutorial_xcrysden.pdf)

Basic scheme ...

prepare by **PWgui**



pw.x < **stdin** > **stdout**



analyze by **XCRYSDEN**

- perform SCF calculation:

PWgui

pw.x < **stdin** > stdout

output: *prefix.**

analyze by **XCrySDen**

- calculate property:

PWgui

pp.x < **stdin** > stdout

output: *filplot*

- filter (transform) the data:

PWgui

pp.x < **stdin** > stdout

output: *fileout*

analyze by **XCrySDen**

About XCrySDen

XCrySDen is a **crystalline** and **molecular structure**
visualisation program

XCrySDen = (**X**-window) **Cry**stalline **S**tructures and
Densities

- ✓ is free software (GNU General Public License)
- ✓ WEB page: <http://www.xcrysden.org/>

XCRYSDEN Installation

- Download latest **XCRYSDEN**'s version to **local-scratch** area as:
 - `cd /scratch/$USER/**** (**** == your directory)`
 - `wget http://www.xcrysdn.org/download/xc-latest-linuxPC-static.tar.gz`
 - (or open web page <http://www.xcrysdn.org>)
 - `tar zxvf xc-latest-linuxPC-static.tar.gz`

XCrySDen Installation

Minimal installation (*binary package*):

- **define:** `XCRYSDEN_TOPDIR` and `XCRYSDEN_SCRATCH`
environmental variables
- **create:** `XCRYSDEN_SCRATCH` directory.
- **execute:** `xcrysdn`

But use instead: `./xcConfigure` script

BEWARE: set `XCRYSDEN_SCRATCH` to something like:

`/scratch/$USER/xcrys_tmp`

What `xcConfigure` does?

- (1) **defines:** `XCRYSDEN_TOPDIR` and `XCRYSDEN_SCRATCH` environmental variables (writes either into `~/.bashrc`, `~/.profile` or `~/.cshrc`)
- (2) **creates:** `XCRYSDEN_SCRATCH` directory.
- (3) **creates:** `$HOME/.xcrysdn` directory.
`$HOME/.xcrysdn/custom-definitions` file.
`$HOME/.xcrysdn/Xcrysdn_defaults` file.
- (4) **asks** several questions and writes answers in `$HOME/.xcrysdn/custom-definitions` file.

XCrySDen Installation

- Do the following:
- `cd XCrySDen-*bin-static/`
- `./xcConfigure`
(set `XCRYSDEN_SCRATCH` to `/scratch/$USER/xcrystmp`)
- for Csh: `source ~/.cshrc; rehash`
 - (for **Bash:** `source ~/.bashrc`)
- then execute with: `xcrystden`

XCRYSDEN as a molecular viewer

- select menu: **File->XCrySDen Examples ...->XSF Files**
- open file: **2.xsf**
- learn how to:
 - rotate, zoom, change display mode, ...
 - measure distances, angles, dihedrals, ...
 - modify various display parameters ...
- learn the menus:
 - **Display** menu: toggles displays (on/off)
 - **Modify** menu: changes the appearance of displayed items

How to print (to file)

- select menu: **File->Print**
- in the “Print to File” windows specify the name of the file. The format is selected by a given extension. For example:
 - *file.png* – will save PNG file
 - *file.gif* – will save GIF file
 - *file.eps* – will save EPS file
 - etc.
- XCRYSDEN's print is a screen-dump therefore before printing (to file):
 - maximize XCRYSDEN's main window
 - zoom the structure as much as possible
 - increase the tessellation factor (Modify->Tessellation Factor) to approx. 40 to 50

Lighting On/Off display-mode

- **VERY IMPORTANT !!!**
 - two levels of display modes:
 - **Lighting-Off** mode:
 - very fast, but can display **only atoms and bonds !!!**
 - **Lighting-On** mode:
 - more fancy display with shades, not so fast, but displays **all possible items !!!**

- Message:

!!!for isosurfaces and alike use **Lighting-On** mode !!!

XCRYSDEN as a crystal-structure viewer

- select menu: **File->XCrySDen Examples ...->XSF Files**
- open file: **ZnS.xsf**
- learn how to:
 - modify number of displayed cells (**Modify->Number of Units Drawn**)
 - change the unit of repetition (**Display->Unit of Repetition ...->**)
 - display Wigner-Seitz cell (**Display->Wigner-Seitz Cells**)
 - display Brillouin zone (**Tools->k-path Selection**)
- remember!!!
 - **Display** menu: toggles displays (on/off)
 - **Modify** menu: changes the appearance of displayed items
- open file: **fcc-410-1x1.xsf**
 - display at least 4×4 unit cells (**Modify->Number of Units Drawn**)
 - try: **Tools->Color Scheme**; select: **slab colors**

Generic use of XCRYSDEN

- **Q:** *I want to visualize the structure from **xxx** formatted file with XCRYSDEN?*
- **A:** Write an **xxx2xsf** filter and convert your file to XSF format:
 - **xxx2xsf < file.xxx > file.xsf**
 - **xcrysdn --xsf file.xsf**
- **XSF** specification is available on:
<http://www.xcrysden.org/doc/XSF.html>

Animation and Visualization of Forces

- select menu: **File->XCrySDen Examples ...->XSF Files**
- open file: **ANIM.axsf**
- animate forward by pressing: **[>>]** button
- display forces: **Display->Forces**
- modify the display of forces: **Modify->Force Settings**
- try to create a movie: press the **[Animated GIF/MPEG >>]** button
(**Note**: requires the whirlgif and mpeg_encode programs to be defined in ~/.xcrysdn/custom-definitions)

XCRYSDEN & PWscf

- Visualization of structures from PW.X **input** file:
 - **xcrysden --pwi input.file**
- Visualization of structures from PW.X **output** file:
 - **xcrysden --pwo output.file**
- Try PWscf input/output files located in
`$XCRYSDEN_TOPDIR/examples/PWSCF_Files/`
- **Hint:** try **`xcrysden --help`**

XCRYSDEN & PWscf

- **Q:** How to construct a **PWscf's** k-path for band-structure calculation with **XCRYSDEN** ???
- **A:**
 - select menu:
 - **Tools-->k-path Selection**
 - select a k-path by mouse-clicking
 - save the file with **.pwscf** extension
(**BEWARE: .pwscf** extension is mandatory to get the pw.x formatted k-list)

Isosurfaces and Contours

- select menu: **File->XCrySDen Examples ...->XSF Files**
- open file: **CO_lumo.axsf.gz** (Note: *xcrysdn* can open compressed files)
- select menu: **Tools->Data Grid**
- then:
 - + press **[OK]**
 - + specify isovalue = 0.1
 - + select: **Render +/- isosurface**
 - + press: **[Submit]**
- two isosurfaces are drawn; isovalue: **-0.01** and **+0.01**
- **Q:** what is the unit of the isovalue?
- **A:** XCRYSDEN does not assume any unit (as specified in file)