

PWscf + XCrySDen: Advanced I/O handling

(part-I)

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Basic scheme ...

prepare by **PWgui**



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



analyze by **XCrySDen**

XCrySDen → **PWgui** → **PWscf**

About XCrySDen

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

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

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

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

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.

Install XCRYSDEN yourself

– download from:

<http://www.xcrysdn.org/Download.html>

– unpack (`tar zxvf *.tar.gz`)

– `cd XCrySDen-B1.0bin-static/`

– `./xcConfigure`

– for **Bash**: `source ~/.bashrc`

– for **Csh**: `source ~/.cshrc; rehash`

– `xcrysdn`

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

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.xcrysdn.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

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`

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)

Advanced feature : scripting

- select menu: File->Save Current State and Structure
- save the file (`CO_lumo.xcrysden`) and exit from XCRYSDEN
- execute: `xcrysden -s CO_lumo.xcrysden`
- copy the file: `cp CO_lumo.xcrysden test.xcrysden`
- edit the file `test.xcrysden` and replace the “STRUCTURE-PART” of the script with the following:

```
::scripting::open --xsf $env(XCRYSDEN_TOPDIR)/examples/XSF_Files/CO_homo.xsf
```
- then execute: `xcrysden -s test.xcrysden`

Advanced feature : scripting

- try other scripting examples located in `$XCRYSDEN_TOPDIR/examples/Scripting/` directory. For example:

```
xcrystden -s colorplane_animation.tcl
```

- **Note:** to exit from fullscreen mode double-click the left mouse button

*****END*****