

Useful information

- Check the [Youtube videos](#) from Edwin if you want.
- Make sure to have the script: pos2xyz.pl in your local bin folder. If not, copy it from Federico Dattila's tekla home bin folder (home/fdattila/bin).
- Make sure to have atomic blender enabled. Otherwise go to: Edit (top left) -> Preferences -> search for atomic blender -> enable the tick.
- Keyboard shortcut:
 - N (to see the transform panel where you can modify atom size, camera position, etc),
 - 7, 4 (or 1), 0 respectively for getting top view, sides view and camera view.
 - Select the camera with the mouse and click G to move it with your mouse; same to move the light.
 - Render engine: cycles; Render 4 (for tests), 32 (for final image); Film -> transparent (for transparent background).
 - Enable denoising and use 2 px as radius.

Steps:

- Enter each clean surface folder;
- run the script pos2xyz.pl CONTCAR from your local PC (tun1, tun2 before);
- copy your CONTCAR.xyz to your shared folder keeping the xyz extension.