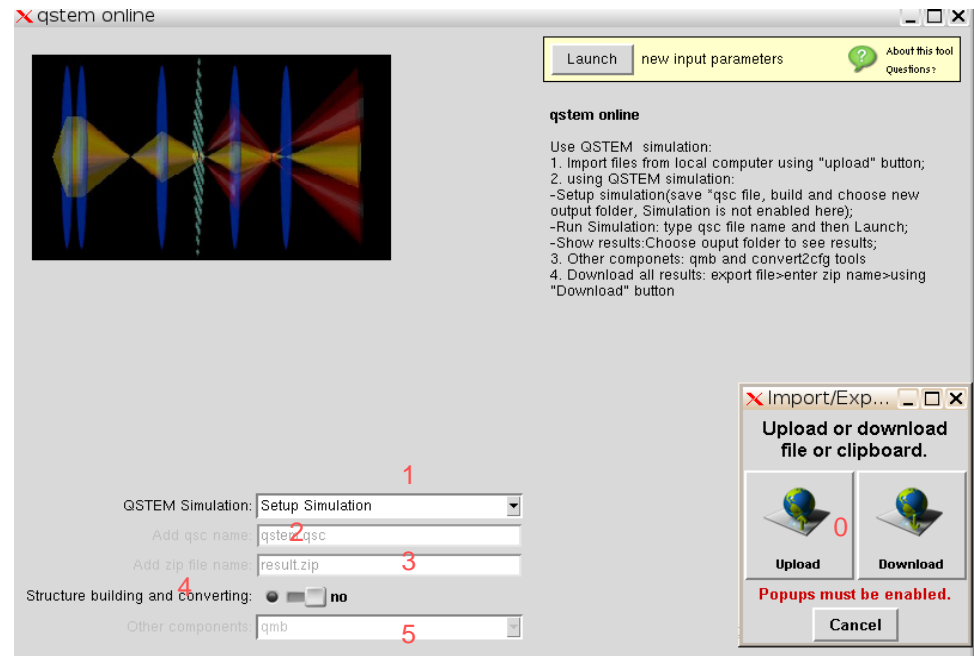


# QSTEM online user Manual

By Mingxuan Lu, Chang Wan Han

## Network for Computational Nanotechnology (NCN)

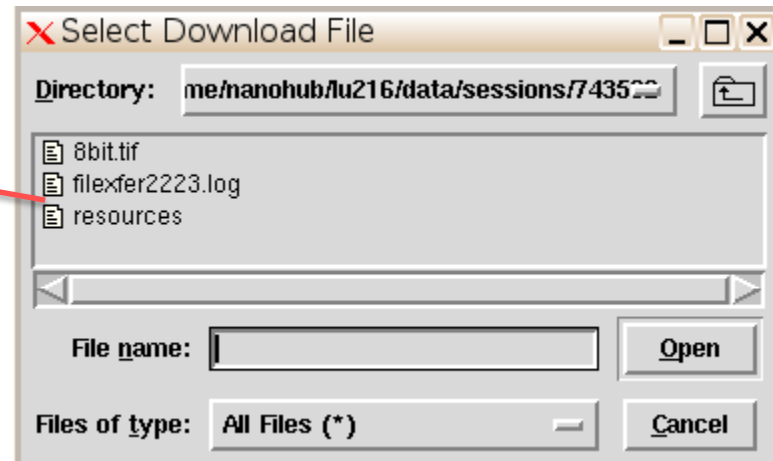
0. Loader: upload/download file from/to local computer;
1. QSTEM simulation, including: Setup simulation, Run simulation, Show results, focal series reconstruction, export results;
2. Enter qsc configuration file name you saved when setting up simulation;
3. Enter zip file name you want to save as;
4. Choose to use Structure building and converting tools;
5. Other components, including: qmb model builder and convert2cfg;



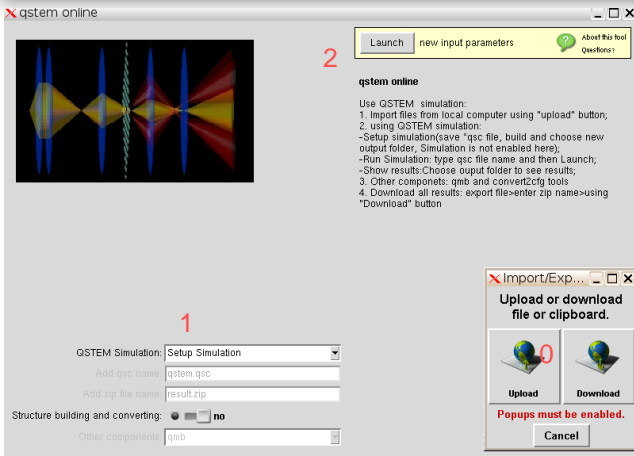
## Network for Computational Nanotechnology (NCN)

Upload: upload files from local computer

Download: Download files to local computer

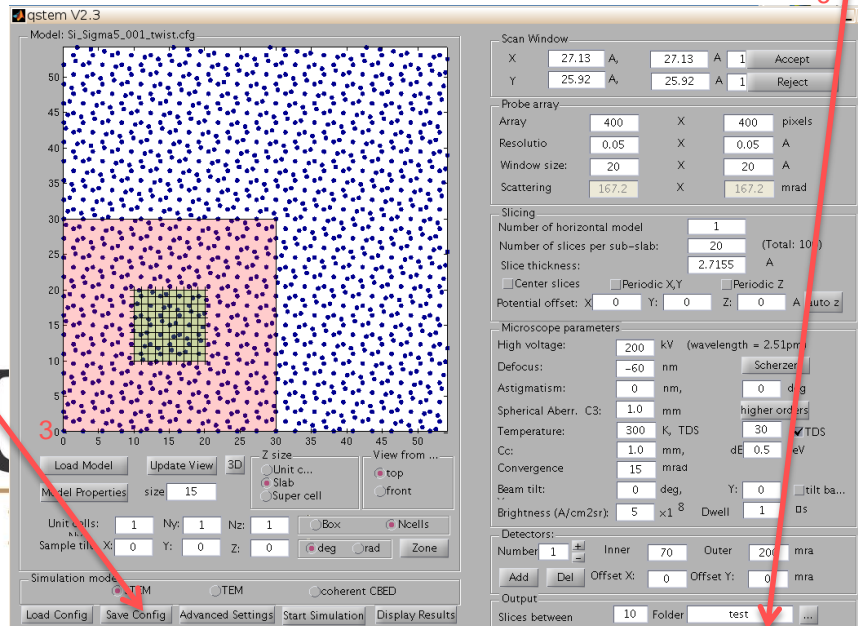
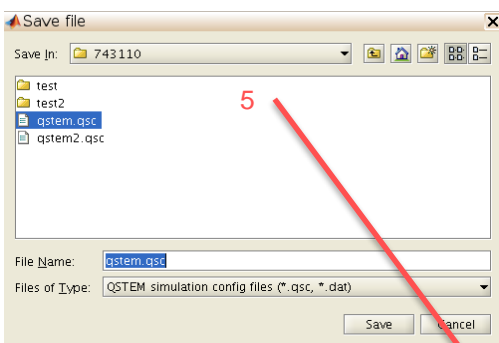
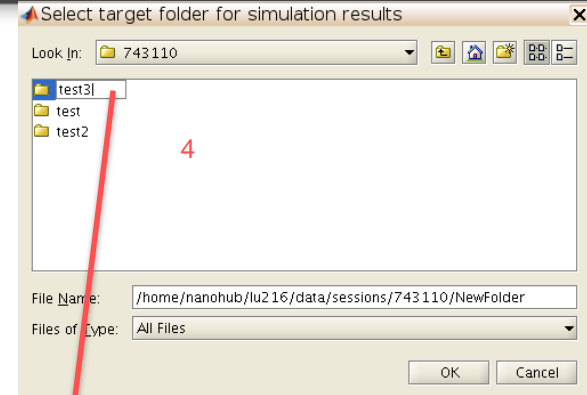


## Network for Computational Nanotechnology (NCN)



Steps for setting up simulation:

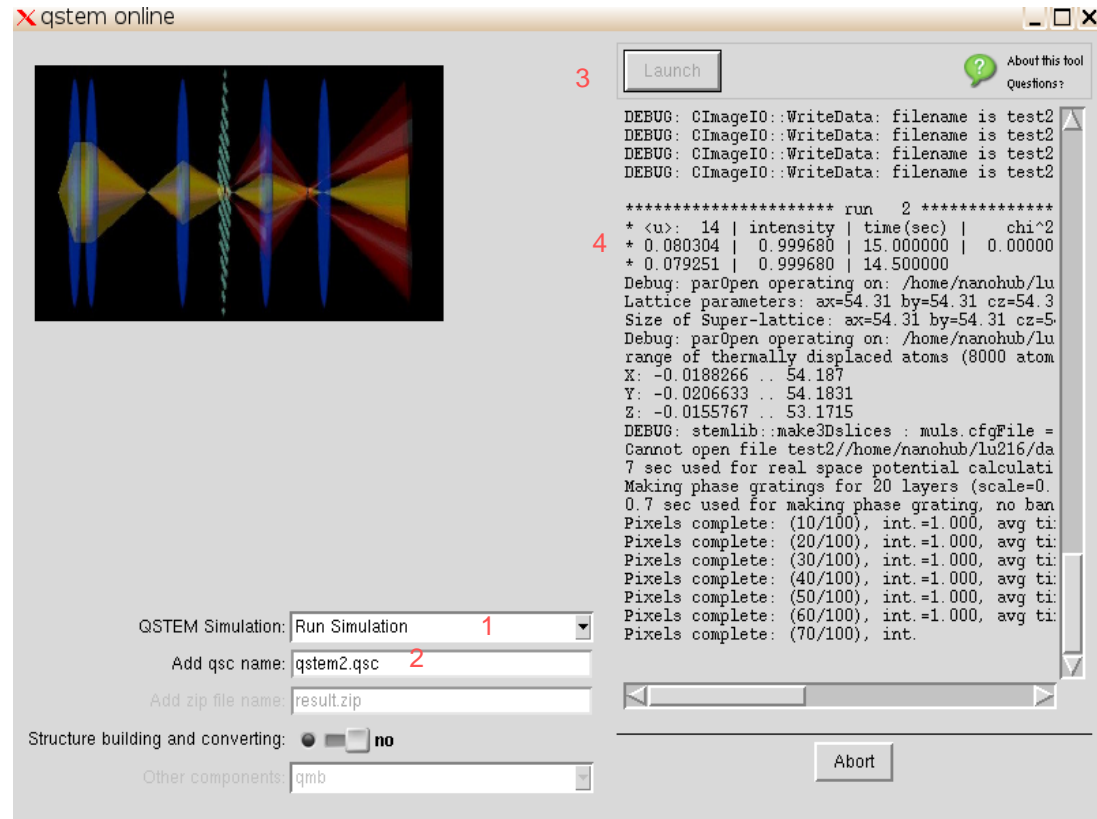
0. upload cfg file from local computer;
1. Choose setup simulation;
2. Press Launch;
3. Load cfg model



4. Create and select a new folder for results for each simulation;
5. Save a new qsc file for each simulation;
6. Close this page(simulation is not enabled through this page).

## Network for Computational Nanotechnology (NCN)

1. Choose Run simulation;
2. Enter qsc config file name you saved when setting up simulation;
3. Press Launch;
4. Simulation Processing;



Launch

3

4

```

DEBUG: CImageIO::WriteData: filename is test2
DEBUG: CImageIO::WriteData: filename is test2
DEBUG: CImageIO::WriteData: filename is test2
DEBUG: CImageIO::WriteData: filename is test2

***** run 2 *****
* <u>: 14 | intensity | time(sec) | chi^2
* 0.080304 | 0.999680 | 15.000000 | 0.00000
* 0.079251 | 0.999680 | 14.500000

Debug: parOpen operating on: /home/nanohub/lu
Lattice parameters: ax=54.31 by=54.31 cz=54.3
Size of Super-lattice: ax=54.31 by=54.31 cz=5
Debug: parOpen operating on: /home/nanohub/lu
range of thermally displaced atoms (8000 atom
X: -0.0188266 .. 54.187
Y: -0.0206633 .. 54.1831
Z: -0.0155767 .. 53.1715
DEBUG: stemlib::make3Dslices : muls.cfgFile =
Cannot open file test2//home/nanohub/lu216/da
7 sec used for real space potential calculati
Making phase gratings for 20 layers (scale=0.
0.7 sec used for making phase grating, no ban
Pixels complete: (10/100), int.=1.000, avg ti:
Pixels complete: (20/100), int.=1.000, avg ti:
Pixels complete: (30/100), int.=1.000, avg ti:
Pixels complete: (40/100), int.=1.000, avg ti:
Pixels complete: (50/100), int.=1.000, avg ti:
Pixels complete: (60/100), int.=1.000, avg ti:
Pixels complete: (70/100), int.

QSTEM Simulation: Run Simulation 1
Add qsc name: qstem2.qsc 2
Add zip file name: result.zip

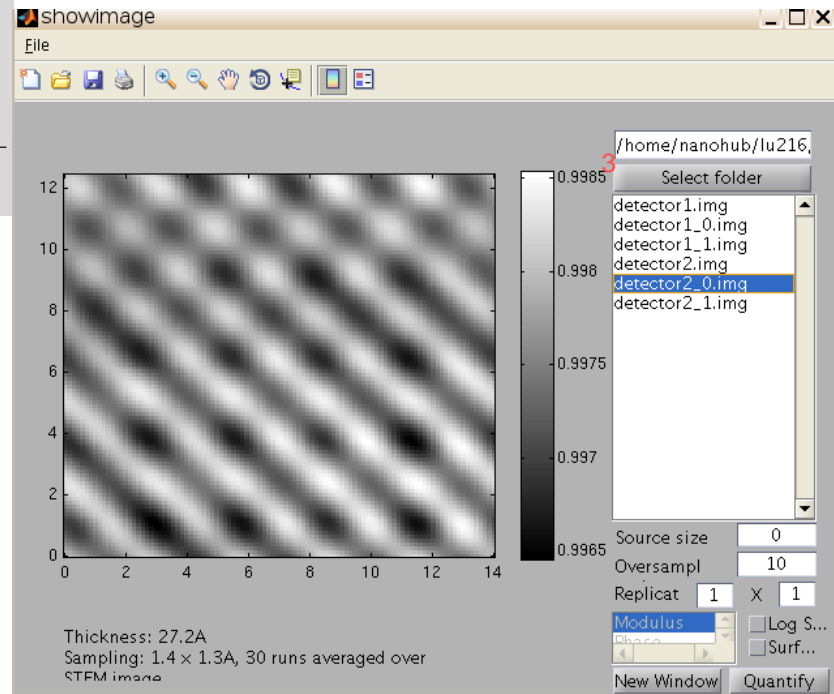
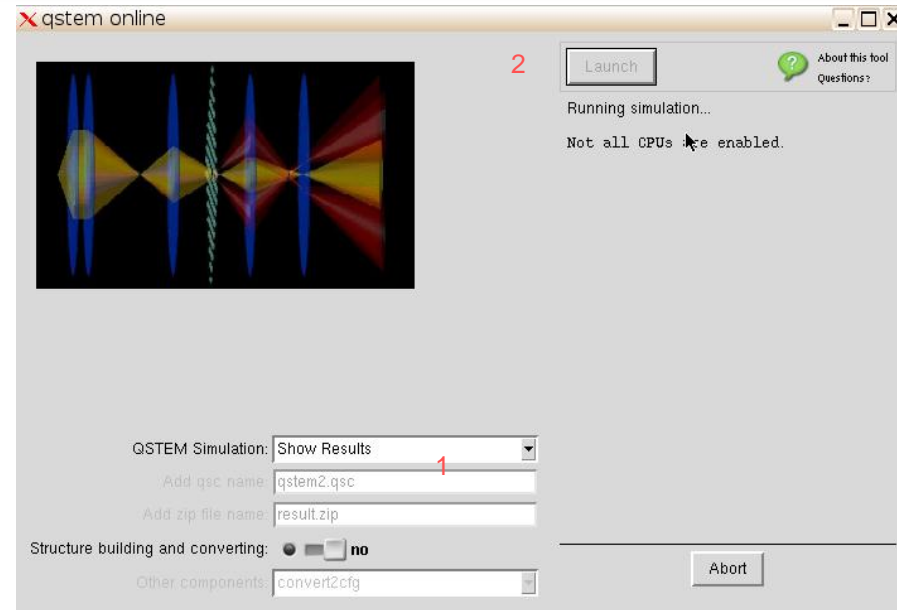
Structure building and converting:   no
Other components: qmb
  
```

Abort

## Network for Computational Nanotechnology (NCN)

Steps for showing results(similar procedure for focal series reconstruction):

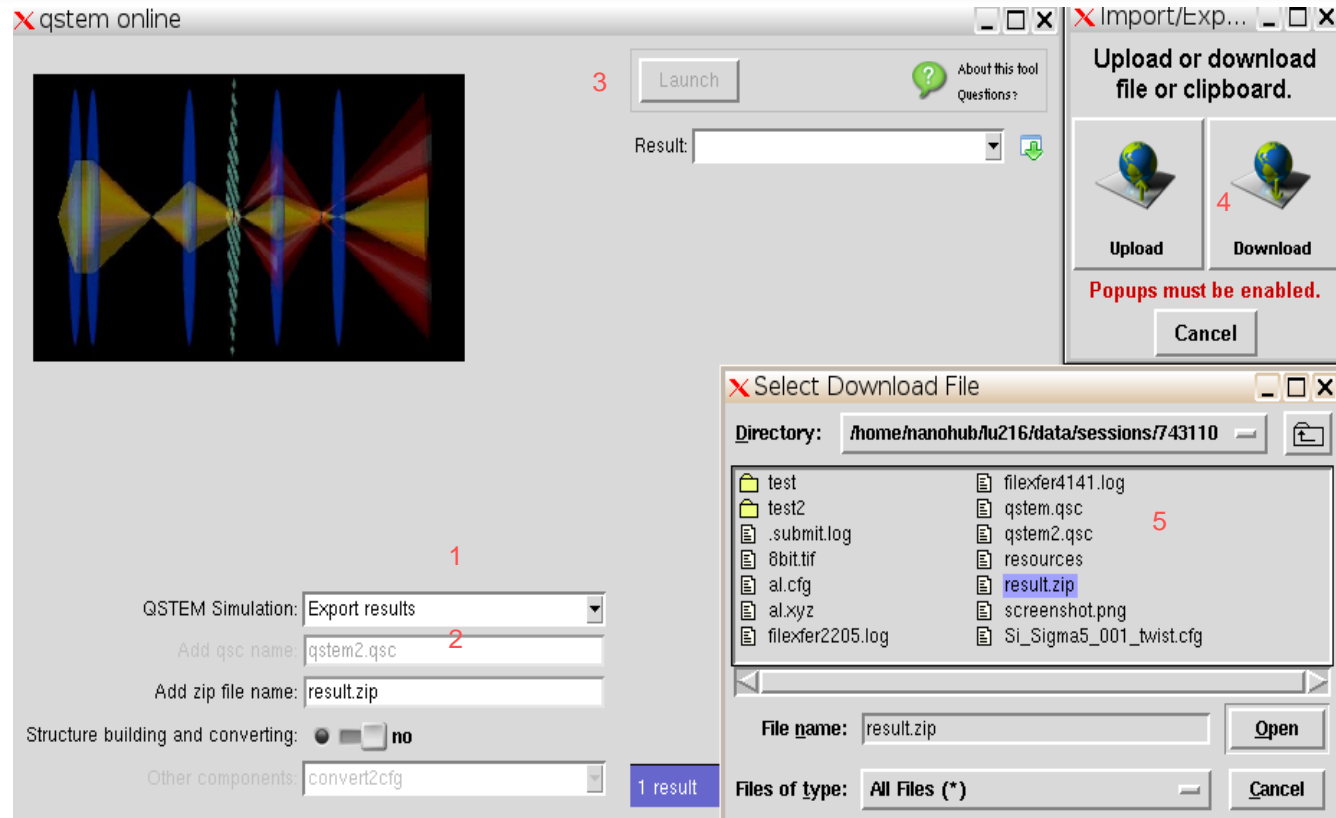
1. Choose Show results;
2. Press Launch;
3. Select folder and img file.



## Network for Computational Nanotechnology (NCN)

Steps for exporting results:

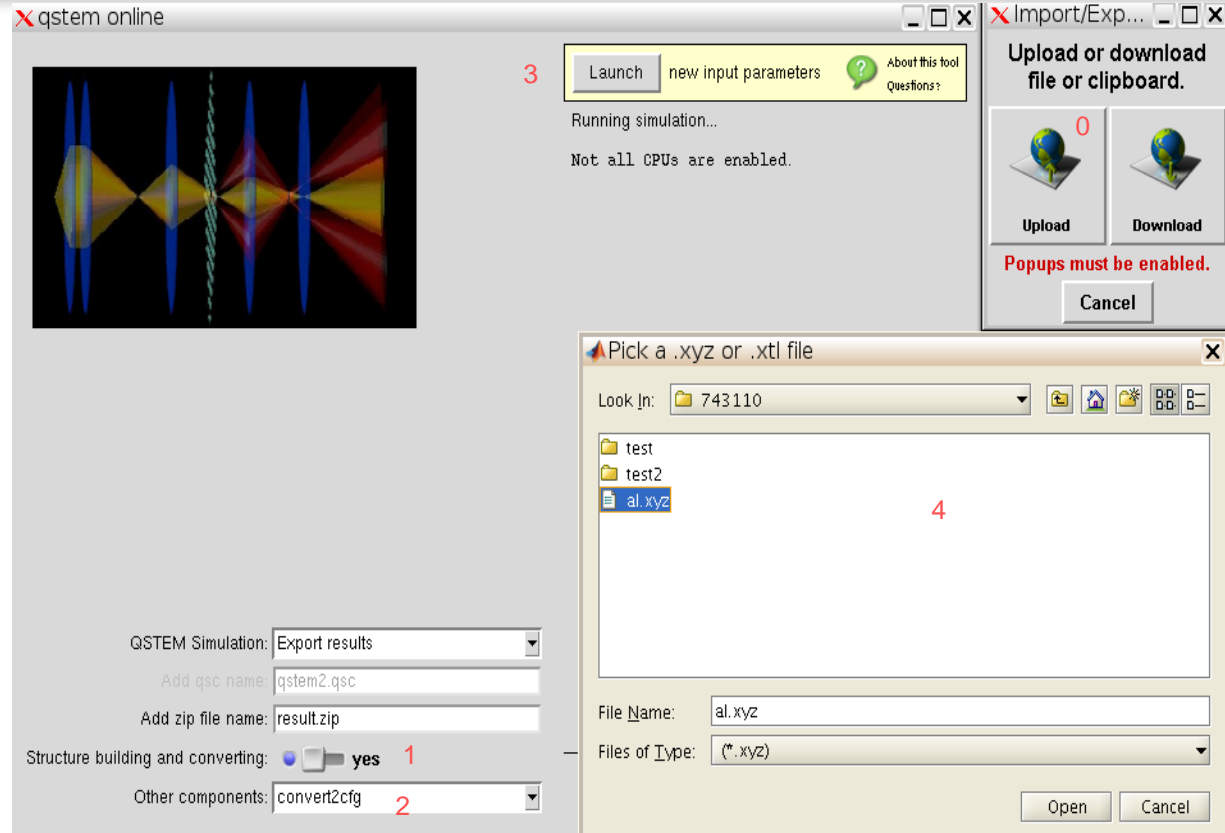
1. Choose Export results;
2. Enter zip file name you want to save as;
3. Press launch;
4. Press “Download” ;
5. Find the zip file you saved and export to local. (zip file contains all the files including cfg file, folders, img files and other config files)



## Network for Computational Nanotechnology (NCN)

Steps for using file converting:

0. Upload xyz or xtl file using loader
1. Choose “yes” for “Structure building and converting”;
2. Choose “convert2cfg”
3. Press Launch;
4. Choose file you want to convert.



The screenshot shows the 'qstem online' web interface. On the left, there is a 3D visualization of a simulation. On the right, a status bar shows '3 Launch new input parameters' and 'Running simulation... Not all CPUs are enabled.' Below this, there are controls for 'Structure building and converting' (set to 'yes' with a red '1') and 'Other components' (set to 'convert2cfg' with a red '2'). A 'Launch' button is visible. In the bottom right, a file selection dialog titled 'Pick a .xyz or .xtl file' is open, showing a file named 'al.xyz' selected in a directory. A red '4' is overlaid on the dialog. To the right of the main interface, there is a panel for 'Upload or download file or clipboard' with 'Upload' and 'Download' buttons and a note 'Popups must be enabled.' with a 'Cancel' button.

QMB model builder is not fully functional in this version! We are trying to make it functional in later version.



- More resources:

QSTEM software introduction: <http://qstem.org/>

QSTEM group mailing list: <https://groups.google.com/forum/#!forum/qstem>

QSTEM software at Ulm University: [http://elim.physik.uni-ulm.de/?page\\_id=834](http://elim.physik.uni-ulm.de/?page_id=834)

QSTEM source code is hosted on [github.com](https://github.com).

- Reference

Christoph Koch, “Determination of Core Structure Periodicity and Density Along Dislocations,” PhD dissertation, Arizona State University (2002)