

# Python codes for background subtraction and overlap disentangle of the CdS/CIGS system

About the codes :

To access the scripts please refer to website <https://github.com/AbsoluteNull/pyAPT> or <https://github.com/atomprobempie/pyAPT>. Using the described here scripts you agree with terms and conditions given by the GNU license under which each of the presented script was published. Copyright (C) 2017 Luv Sharma, Anna Koprek, Baptist Gault and Max-Planck-Institut für Eisenforschung GmbH. Use on your own responsibility. See the GNU General Public License for more details.

Installations:

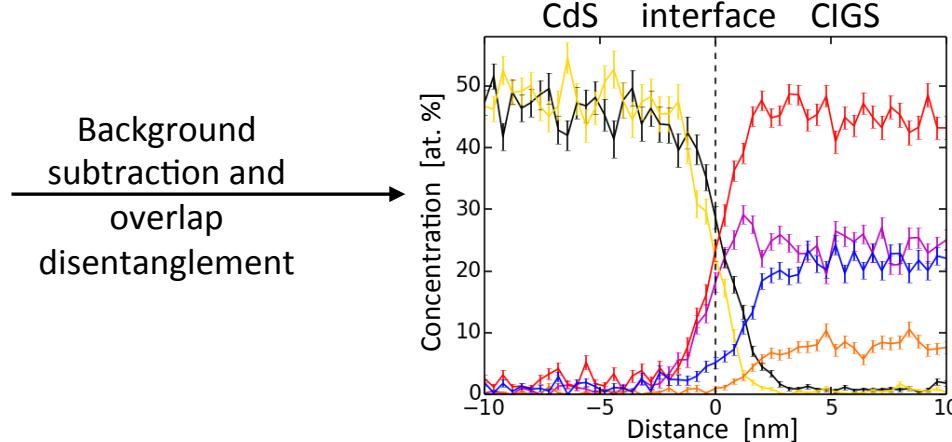
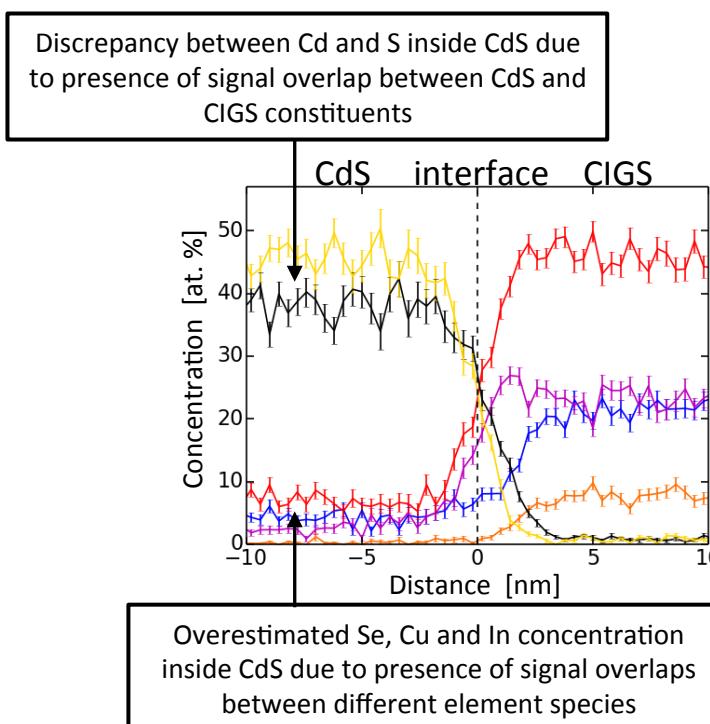
This instruction is shown within Oracle VM VirtualBox (on Ubuntu that contains **Python** program with **Pandas** package).

You can access Oracle VM VirtualBox at : <https://www.virtualbox.org/>

And create a Sharing Forder between Linux and Windows by following this instruction:  
<https://www.youtube.com/watch?v=l5cV0V7vLJw>

# Introduction

Presented here codes are used to create background ranges and for chemical analysis that aims to disentangle overlapping signals at the APT mass spectrum in the CdS/CIGS system. The process of overlap disentangle uses the natural abundance of constituting the overlap elements as well as ability of APT reconstruction program to drown 1D concentration profile in any desired direction along which the analysis is performed. Using the 1D concentration profiles of isotopes that are not affected by any overlap the distribution of isotopes hidden inside the overlapping peak is estimated within each distance interval (distance bin) thereby providing **more reliable and spatially resolved composition**.



# List of Scripts

## For single set of data (small sets of data like interface region)

1. **bgAPT.py** (to create background ranges)
2. **overlap.py** or **bgOverlap-disentangle.py** (analysis – background subtraction and overlap disentangle)
3. **plotProfiles.py** (for automatized plotting)

## Long range diffusion (reconstruction is divided into small sub-pieces that are analyzed individually and further combined together in order to provide whole image of obtained results)

4. **combineCSV.py**
5. **diffusion.py**

# 1. bgAPT.py (what it does)

bg - background

Range\_file.rrng



bgAPT.py

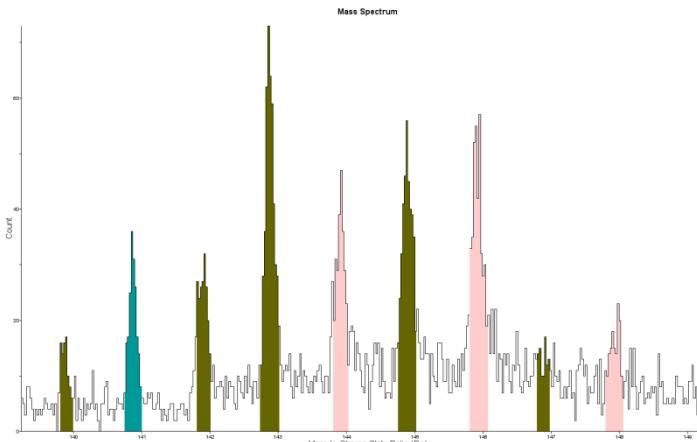
modified\_Range\_file.rrng

With all identified elements, complex ions and overlaps

With all identified elements, complex ions, overlaps and corresponding background ranges

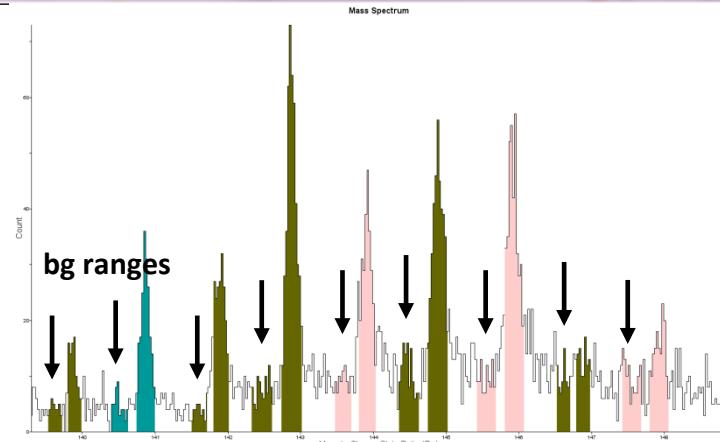
Ref\_M2\_10x10x60.rrng - Notepad

```
File Edit Format View Help
Range11=109.8210 110.0610 vol:0.02159 Cd:1 Color:000000
Range12=110.8250 111.0390 vol:0.02159 Cd:1 Color:000000
Range13=111.8010 112.1000 vol:0.02159 Cd:1 Color:000000
Range14=113.7930 114.0710 vol:0.02159 Cd:1 Color:000000
Range15=105.8200 106.0400 vol:0.02159 Cd:1 Color:000000
Range16=107.7990 108.0260 vol:0.02159 Cd:1 Color:000000
Range17=115.8190 116.0470 vol:0.02159 Cd:1 Color:000000
Range18=161.7130 161.9940 vol:0.05453 Se:2 Color:FF0000
Range19=159.6980 159.9980 vol:0.05453 Se:2 Color:FF0000
Range20=157.7180 158.0010 vol:0.05453 Se:2 Color:FF0000
```



modifiedRef\_M2\_10x10x60.rrng - Notepad

```
File Edit Format View Help
Range21=109.8210 110.0610 vol:0.02159 Cd:1 Color:000000
Range22=109.4610 109.7010 vol:0.02159 Name:Cd1bg Color:000000 ← bg
Range23=110.8250 111.0390 vol:0.02159 Cd:1 Color:000000
Range24=110.5040 110.7180 vol:0.02159 Name:Cd1bg Color:000000 ←
Range25=111.8010 112.1000 vol:0.02159 Cd:1 Color:000000
Range26=111.3525 111.6515 vol:0.02159 Name:Cd1bg Color:000000 ←
Range27=113.7930 114.0710 vol:0.02159 Cd:1 Color:000000
Range28=113.3760 113.6540 vol:0.02159 Name:Cd1bg Color:000000 ←
Range29=105.8200 106.0400 vol:0.02159 Cd:1 Color:000000
Range30=105.4900 105.7100 vol:0.02159 Name:Cd1bg Color:000000 ←
Range31=107.7990 108.0260 vol:0.02159 Cd:1 Color:000000
Range32=107.4585 107.6855 vol:0.02159 Name:Cd1bg Color:000000 ←
Range33=115.8190 116.0470 vol:0.02159 Cd:1 Color:000000
Range34=115.4770 115.7050 vol:0.02159 Name:Cd1bg Color:000000 ←
Range35=161.7130 161.9940 vol:0.05453 Se:2 Color:FF0000
Range36=161.2915 161.5725 vol:0.05453 Name:Se2bg Color:FF0000 ←
Range37=159.6980 159.9980 vol:0.05453 Se:2 Color:FF0000
Range38=159.2480 159.5480 vol:0.05453 Name:Se2bg Color:FF0000 ←
Range39=157.7180 158.0010 vol:0.05453 Se:2 Color:FF0000
Range40=157.2935 157.5765 vol:0.05453 Name:Se2bg Color:FF0000 ←
Range41=156.7350 156.9890 vol:0.05453 Se:2 Color:FF0000 ←
```



# 1. bgAPT.py (how to do)

bg - background

Ubuntu4AK [Running] - Oracle VM VirtualBox

File Machine View Devices Help

[Software Updater] Terminal - ania@ania-Virtu...

Terminal - ania@ania-VirtualBox: /media/WinLinHome/200dgrC\_01-07-14\_M7-chack\_mrp\$ ll

```
total 142
drwxrwxrwx 1 root root 20480 jul 17 13:01 .
drwxrwxrwx 1 root root 28672 jun  9 11:13 ..
-rwxrwxrwx 1 root root 16018 okt 10  2016 15nm_overlap.py*
-rwxrwxrwx 1 root root  8305 sep  9  2016 200dgrC_01-07-14_M7_10x10x60_LR.rrng* ←
-rwxrwxrwx 1 root root  4149 aug 14  2016 bgAPT.py*
drwxrwxrwx 1 root root 12288 jul 17 13:01 data/
drwxrwxrwx 1 root root  4096 dec 21  2016 Diffusion/
-rwxrwxrwx 1 root root     0 okt 10  2016 -i_29.5.txt*
-rwxrwxrwx 1 root root 17051 sep  9  2016 modified200dgrC_01-07-14_M7_10x10x60_LR.rrng* ←
-rwxrwxrwx 1 root root 16046 nov 29  2016 overlap-normalized.py*
-rwxrwxrwx 1 root root 16003 okt 10  2016 overlap.py*
```

ania@ania-VirtualBox: /media/WinLinHome/200dgrC\_01-07-14\_M7-chack\_mrp\$ python bgAPT.py 200dgrC\_01-07-14\_M7\_10x10x60\_LR.rrng

**Range\_file.rrng**

With all identified elements, complex ions and overlaps

Execute:

python bgAPT.py Range\_file.rrng

Wait:

ania@ania-VirtualBox: /media/WinLinHome/200dgrC\_01-07-14\_M7-chack\_mrp\$ ll

```
total 142
drwxrwxrwx 1 root root 20480 jul 17 13:01 .
drwxrwxrwx 1 root root 28672 jun  9 11:13 ..
-rwxrwxrwx 1 root root 16018 okt 10  2016 15nm_overlap.py*
-rwxrwxrwx 1 root root  8305 sep  9  2016 200dgrC_01-07-14_M7_10x10x60_LR.rrng* ←
-rwxrwxrwx 1 root root  4149 aug 14  2016 bgAPT.py*
drwxrwxrwx 1 root root 12288 jul 17 13:01 data/
drwxrwxrwx 1 root root  4096 dec 21  2016 Diffusion/
-rwxrwxrwx 1 root root     0 okt 10  2016 -i_29.5.txt*
-rwxrwxrwx 1 root root 17051 jul 17 13:13 modified200dgrC_01-07-14_M7_10x10x60_LR.rrng* ←
-rwxrwxrwx 1 root root 16046 nov 29  2016 overlap-normalized.py*
-rwxrwxrwx 1 root root 16003 okt 10  2016 overlap.py*
```

ania@ania-VirtualBox: /media/WinLinHome/200dgrC\_01-07-14\_M7-chack\_mrp\$

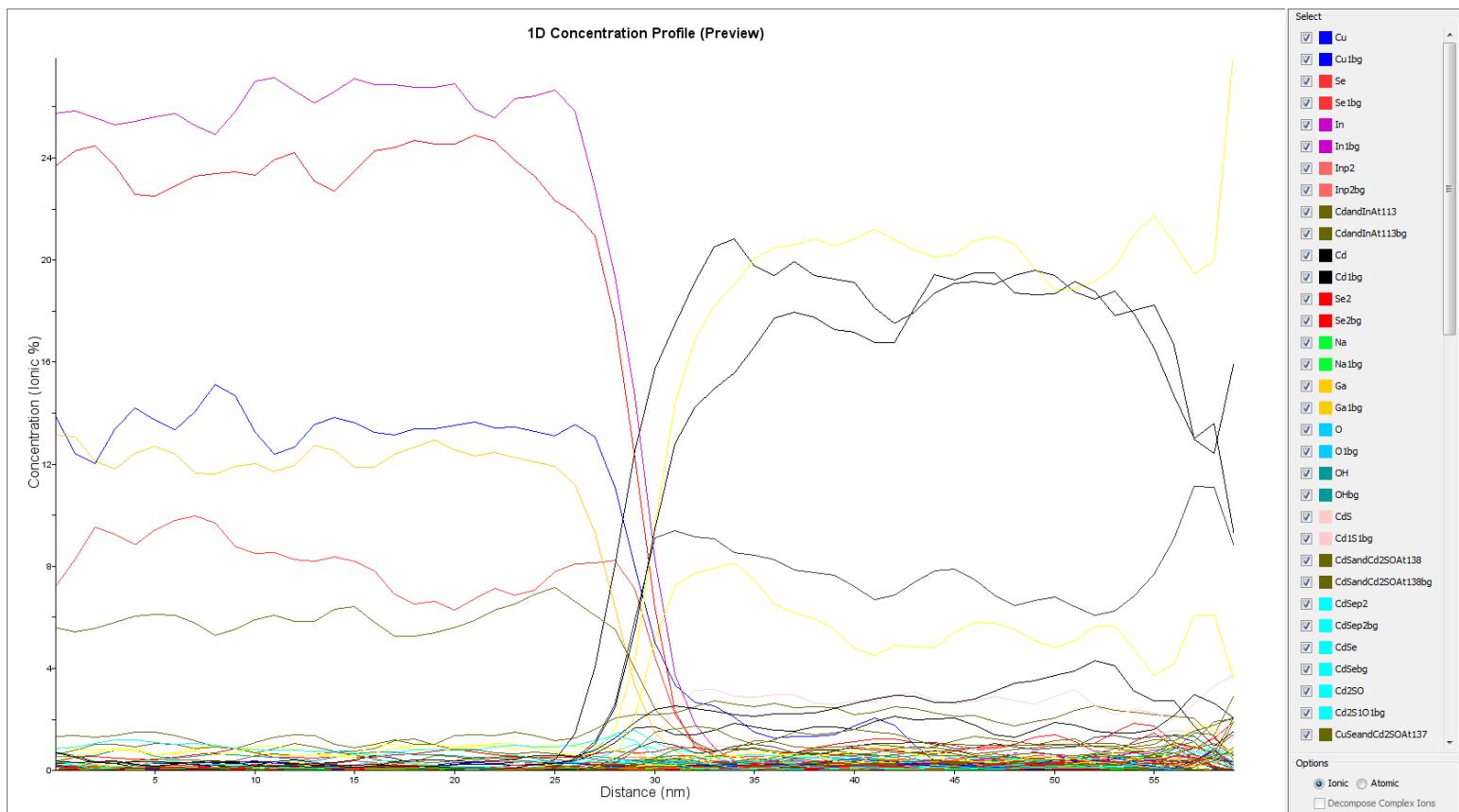
**modified\_Range\_file.rrng**

With all identified elements, complex ions, overlaps and corresponding background ranges

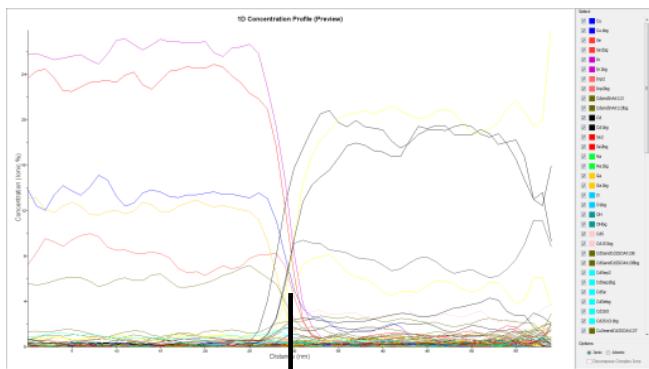
## 2. overlap.py (quick check whether identified overlap for disentangling are correct)

In order to use **bgOverlap-disentangle.py** or **overlap.py** use the modified range file (with bg ranges) and create within reconstruction program 1D concentration profile among chose direction and with a specified distance interval (e.g. 0.4 nm). Important: **DO NOT decompose the complex ions!** Seve the 1D concentration profile as \*csv.file

modified\_Range\_file.rrng → Reconstructing program (here IVAS) → 1D\_concentration\_profile.csv



## 2. overlap.py - get quickly look at the results !



Execute:

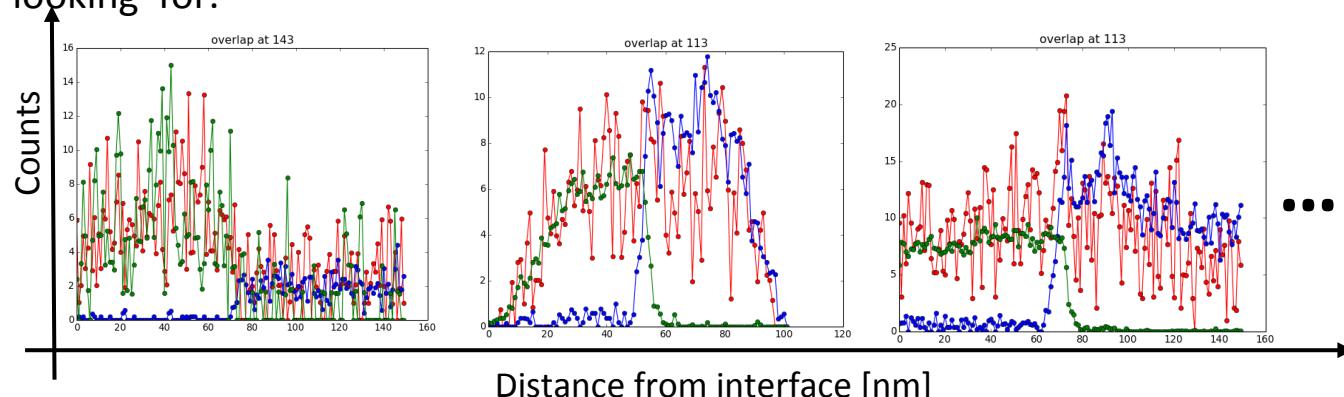
```
python overlap.py -i XX.YY 1D_concentration_profile.csv
```

Wait:

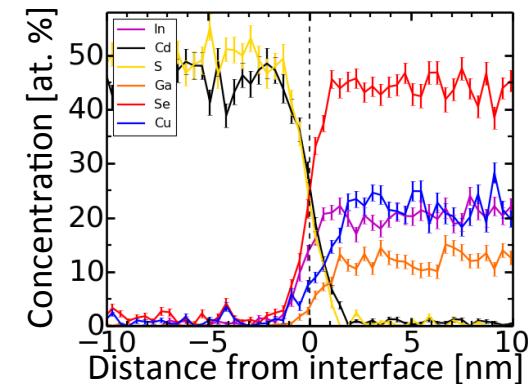
1D\_concentration\_profile.csv  
**(with bg ranges and NOT decomposed!)**

Use **-i XX.YY** (distance) to place the interface in the center (0 nm)

- 1D conc. profiles of identified overlap (red) and the disentangled signals. Green and blue are the distributions of disentangled signals that you are looking for.



- 1D plots for final results after decomposition of complex ions



## 2. overlap.py (background subtraction and overlap disentangle)

File Machine View Devices Help

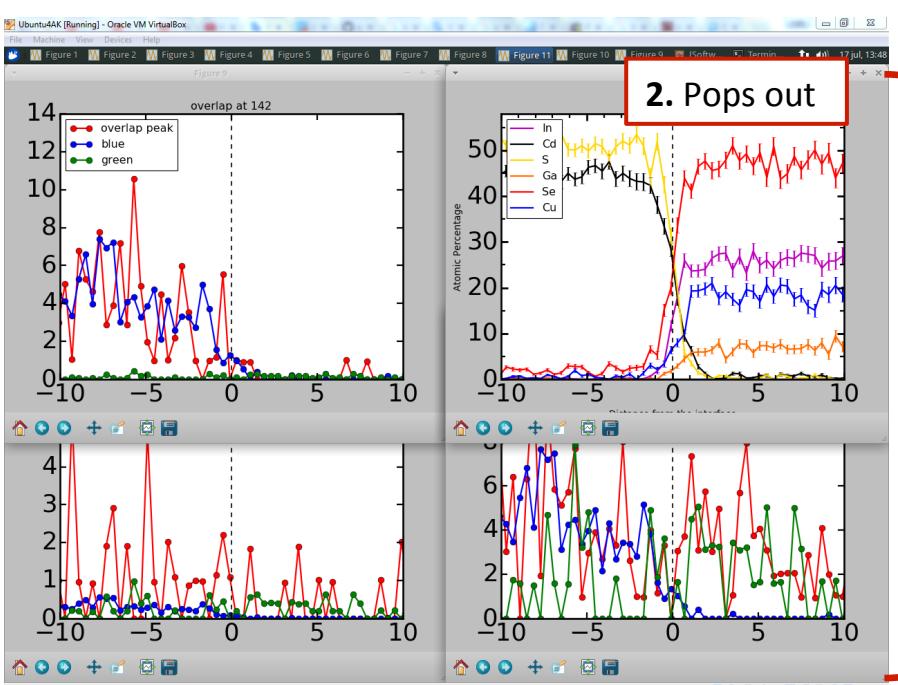
[Software Updater] Terminal - ania@ania-Virtu...

File Edit View Terminal Tabs Help

1. Execute: `python overlap.py -i XX.YY 1D_concentration_profile.csv`

```
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ ll
total 427
drwxrwxrwx 1 root root 20480 jul 17 13:46 /
drwxrwxrwx 1 root root 28672 jun 9 11:13 ..
-rwxrwxrwx 1 root root 16018 okt 10 2016 15nm_overlap.py*
-rwxrwxrwx 1 root root 8305 sep 9 2016 200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rwxrwxrwx 1 root root 4149 aug 14 2016 bgAPT.py*
drwxrwxrwx 1 root root 12288 jul 17 13:01 data/
drwxrwxrwx 1 root root 4096 dec 21 2016 Diffusion/
-rwxrwxrwx 1 root root 0 okt 10 2016 -i_29.5.txt*
-rwxrwxrwx 1 root root 17051 jul 17 13:13 modified200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rwxrwxrwx 1 root root 16046 nov 29 2016 overlap-normalized.py*
-rwxrwxrwx 1 root root 16003 okt 10 2016 overlap.py*
-rwxrwxrwx 1 root root 291340 sep 9 2016 Perp_to_itf_10x10x60_200dgrC_M7_LR.csv
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ python overlap.py -i 29.5 Perp_to_itf_10x10x60_200dgrC_M7_LR.csv
```

Use `-i XX.YY` (distance) to place the interface in the center (0 nm)



3. All images are saved in the directory of execution (unless specified otherwise)

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File Machine View Devices Help

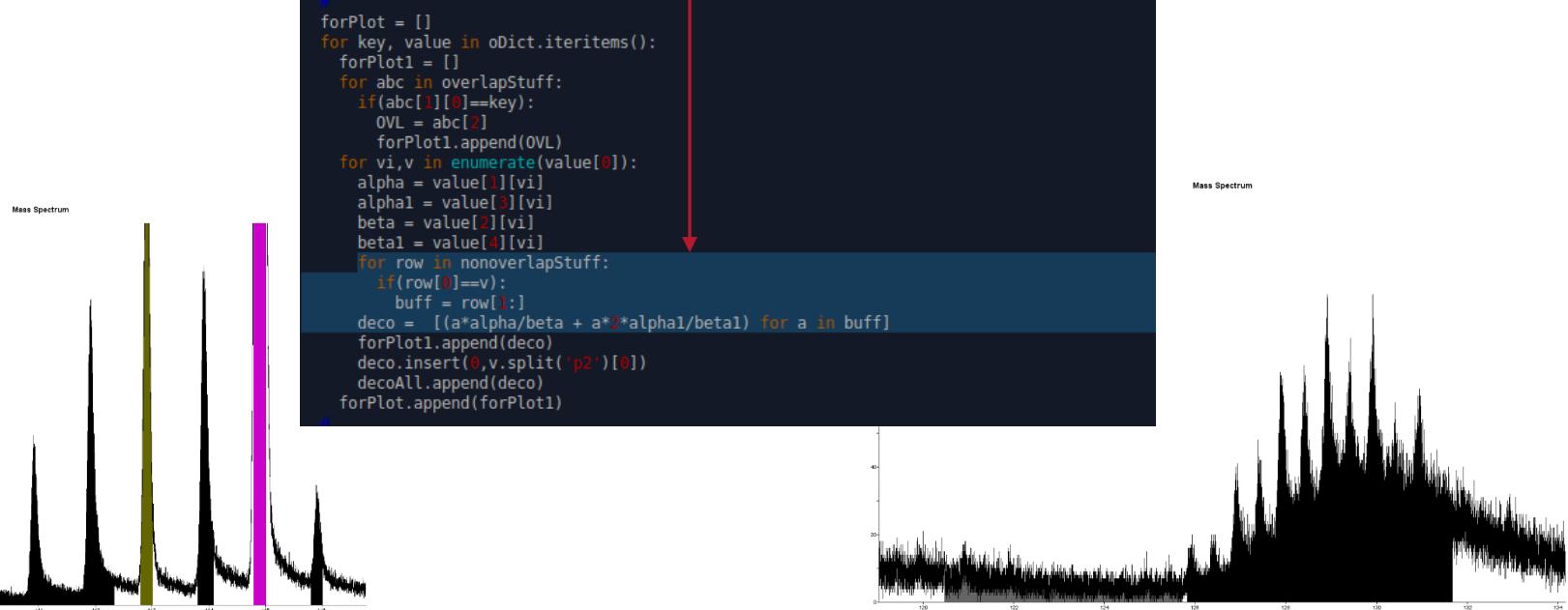
[Software Updater] Terminal - ania@ania-Virtu...

File Edit View Terminal Tabs Help

```
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ ll
total 1998
drwxrwxrwx 1 root root 20480 jul 17 13:46 /
drwxrwxrwx 1 root root 28672 jun 9 11:13 ..
-rwxrwxrwx 1 root root 16018 okt 10 2016 15nm_overlap.py*
-rwxrwxrwx 1 root root 8305 sep 9 2016 200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rwxrwxrwx 1 root root 4149 aug 14 2016 bgAPT.py*
drwxrwxrwx 1 root root 12288 jul 17 13:01 data/
drwxrwxrwx 1 root root 4096 dec 21 2016 Diffusion/
-rwxrwxrwx 1 root root 0 okt 10 2016 -i_29.5.txt*
-rwxrwxrwx 1 root root 17051 jul 17 13:13 modified200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rwxrwxrwx 1 root root 16046 nov 29 2016 overlap-normalized.py*
-rwxrwxrwx 1 root root 16003 okt 10 2016 overlap.py*
-rwxrwxrwx 1 root root 291340 sep 9 2016 Perp_to_itf_10x10x60_200dgrC_M7_LR.csv
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ ls
Perp_to_itf_10x10x60_200dgrC_M7_LR113-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR113-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR137-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR137-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR138-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR138-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR140-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR140-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR142-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR142-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR143-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR143-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR145-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR147-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR56-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR56-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR65-overlapCheck.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR65-overlapCheck.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR_LC-all.png*
Perp_to_itf_10x10x60_200dgrC_M7_LR_C-all.svg*
Perp_to_itf_10x10x60_200dgrC_M7_LR.csv*
```

# Technical remarks

Within provided range file (example of adiff-0.rrng file) as well within the scripts (diffusion.py, overlap.py or bgOverlap-disentangle.py) large ranges are introduced for clusters of Cd<sup>+</sup>, Cd<sup>++</sup> and Cd<sub>2</sub>OH<sup>++</sup>/Cd<sub>2</sub>H<sub>2</sub>O<sup>++</sup> signals (see examples below). Due to presence of large thermal tails – belonging to the same element species – the subtraction of “standard” background range (see slide 4) would cause underestimate of Cd signal that is usually very small inside the CIGS phase. Form technical reason the smallest Cd<sup>+</sup> and Cd<sup>++</sup> signals (i.e. at 53 Da, 54 Da, 106 Da and 108 Da) were not range but covered with the background range. However the (double) loss in the Cd signal is accounted for within the python analysis. The operations on large ranges for Cd as well as accounting for the covered by the bg ranges signal is defined within the scripts as a default. In order to perform analysis without large ranges and accounting for smallest Cd<sup>+</sup> and Cd<sup>++</sup> signal please use option -I 0 (e.g. python bgOverlap-disentangle(overlap.py or diffusion.py).py -I 0 -i XY atomAll.py).



## 2. overlap.py — get quickly the results and check whether selected constituents of an overlap are correct

Remember! If the summer of estimated isotope distributions does not represent distribution of the overlapping peak (before disentangling) it means that identification of constituent elements within the overlap is wrong or some constituents are missing (in the case of underestimation). Hence the mass ranging and overlap identification has to be corrected.

2. `bgOverlap-disentangle.py` - get the results as \*.csv files

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File Machine View Devices Help

[Software Updater] Terminal - ania@ania-Virtu...

Terminal - ania@ania-VirtualBox:/media/WinLinHome/2

```
# and Sigma column
if ('Sigma' not in nameInfoAll):
    # convert the data of the first entry that is a name) into float
    floatData = [float(j) for j in row[1:]]
    # insert the name at the start of the list
    floatData.insert(0, nameInfo)
    dataWbg.append(floatData)

# getting the distance column
# getting the ion count column and smoothing it

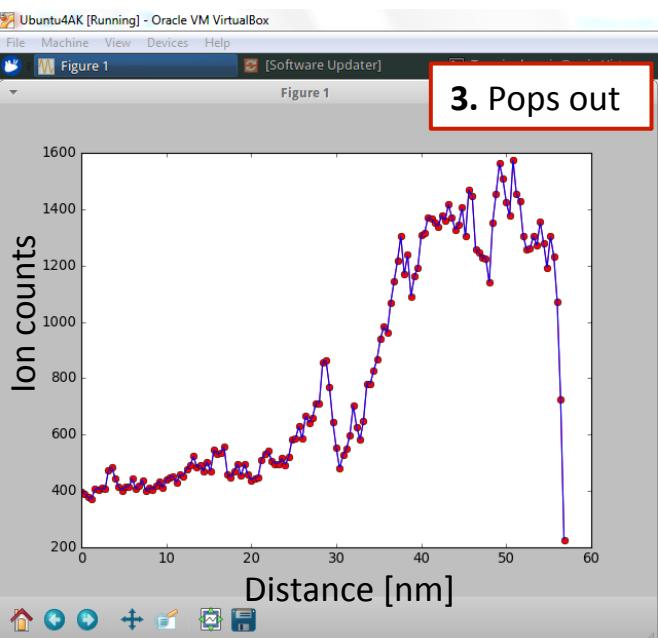
## smoothing the ion counts with moving average and inserting this column
med = list(np.array(dataWbg[0:len(dataWbg)-1]))*0.4
icl = np.array(range(0, len(dataWbg)-1))
wcnl = nonlocal(icl, 0.0, len(icl), len(icl))
icnl = icl

wcnl[1:4] = icnl[1:4]
wcnl[4:41] = icnl[4:41]

icnl.insert(0, ions)
dataWbg.insert(2, icnl)
#
fig, ax1 = plt.subplots()
```

1. Within the bgOverlap-disentangle.py code define the bin size (distance interval) that you choose for 1D projection on file

1. Within the bgOverlap-disentangle.py code define the bin size (distance interval) that you chose for 1 D concentration profile



Ubuntu4AK [Running] - Oracle VM VirtualBox

File Machine View Devices Help

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2. Execute: `python bgOverlap-disentangle.py 1D_concentration_profile.csv`

```
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrps$ ll
total 412
drwxrwxrwx 1 root root 20480 jul 17 14:19 /
drwxrwxrwx 1 root root 28672 jun 9 11:13 .
-rw-rwxrwx 1 root root 8305 sep 9 2016 200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rw-rwxrwx 1 root root 4149 aug 14 2016 bgAPT.py*
-rw-rwxrwx 1 root root 13032 mei 29 15:13 bgOverlap-disentangle.py*
drwxrwxrwx 1 root root 12888 jul 17 14:08 data/
drwxrwxrwx 1 root root 4096 dec 21 2016 Diffusion/
-rw-rwxrwx 1 root root 0 okt 10 2016 -I_29.5.txt*
drwxrwxrwx 1 root root 17051 jul 17 13:13 modified200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rw-rwxrwx 1 root root 16003 okt 10 2016 overlap.py*
-rw-rwxrwx 1 root root 291340 sep 9 2016 Perp_to_itf_10x10x60_200dgrC_M7_LR.csv*
-rw-rwxrwx 1 root root 3878 dec 6 2016 plotProfiles.py*
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrps$ python bgOverlap-disentangle.py Perp_to_itf_10x10x60_200dgrC_M7_LR.csv
```

4. Get saved (in row form! For details open the file):

- **overlap-at-XY(Da).csv** (all disentangled signals),
- **atomAll.csv** (final results: disentangled overlaps and decomposed complex ions into simple ions – **to plot use plotProfiles.py** )

4. Get saved (in row form! For details open the file):

- **overlap-at-XY(Da).csv** (all disentangled signals),
- **atomAll.csv** (final results: disentangled overlaps and decomposed complex ions into simple ions – **to plot use plotProfiles.py** )

```
Ubuntu4AK [~]
File Machine Software
File Edit View
ania@ania-VirtualBox:~/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ ls
total 577
drwxrwxrwx 1 root root 20480 jul 17 14:20 /
drwxrwxrwx 1 root root 28672 jun 9 11:13 /.
-rwxrwxrwx 1 root root 8305 sep 9 2016 200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rwxrwxrwx 1 root root 67925 jul 17 14:20 atomAll.csv* →
-rwxrwxrwx 1 root root 4149 aug 14 2016 bgAPI.py*
-rwxrwxrwx 1 root root 13032 mei 29 15:13 bgOverlap-disentangle.py*
drwxrwxrwx 1 root root 12288 jul 17 14:08 data/
drwxrwxrwx 1 root root 4096 dec 21 2016 Diffusion/
-rwxrwxrwx 1 root root 0 okt 10 2016 -i_29.5.txt*
-rwxrwxrwx 1 root root 17051 jul 17 13:13 modified200dgrC_01-07-14_M7_10x10x60_LR.rrng*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-113.csv*
-rwxrwxrwx 1 root root 7150 jul 17 14:20 overlap-at-137.csv*
-rwxrwxrwx 1 root root 7150 jul 17 14:20 overlap-at-138.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-140.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-142.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-143.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-145.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-147.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-56.csv*
-rwxrwxrwx 1 root root 10725 jul 17 14:20 overlap-at-65.csv*
-rwxrwxrwx 1 root root 16003 okt 10 2016 overlap.py*
-rwxrwxrwx 1 root root 291340 sep 9 2016 Perp_to_itf_10x10x60_200dgrC_M7_LR.csv*
-rwxrwxrwx 1 root root 3878 dec 6 2016 plotProfiles.py*
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ █
```

## 2. bgOverlap-disentangle.py (part II)

```
Ubuntu4AK [Running] - Oracle VM VirtualBox
File Machine View Devices Help
[Software Updater] Terminal - ania@ania-Virtu...
inal - ania@ania-Virtu...
File Edit View Terminal Tabs Help
from __future__ import division
from pylab import plot, ylim, xlim, show, xlabel, ylabel, grid
from numpy import linspace, loadtxt, ones, convolve
import numpy as np
import csv
import matplotlib.pyplot as plt
import re
import os,sys
from optparse import OptionParser
import matplotlib as mpl
mpl.rcParams['axes.linewidth'] = 1.5
mpl.rcParams['lines.linewidth'] = 2.0
import matplotlib.font_manager as font_manager
ticks_font = font_manager.FontProperties(
print('#####')
print('      START')
print('#####')

parser = OptionParser(usage = "usage: %prog [options] filename", \
parser.add_option('-i', '--il', type="float",
    help="interface location",
    dest="IL", default=float(75.00))

(options, filenames) = parser.parse_args()

print('##### Reading data from file #####')

with open(filenames[0], 'rb') as f:
    reader = csv.reader(f)
    allList = list(reader)

print('##### Data read #####')

colors = ['#m', '#k', '#FFD700', '#FF6D00', '#r', '#b']
atomLabels = ['In', 'Cd', 'S', 'Ga', 'Se', 'Cu']
#atomLabels = ['In', 'O', 'Cd', 'S', 'Ga', 'Se', 'Cu', 'Na', 'H']

IL = options.IL

x = np.array([float(d) for d in allList[0]])
x = list((np.array(range(np.shape(allList)[1]))- IL *0.4))
fig,(ax1)=plt.subplots(1,1)
```

1. Within the **plotProfiles.py** code define the bin size (distance interval) that you chose for 1 D concentration profile.

```
Terminal - ania@ania-VirtualBox:/me
dgrC_01-07-14_M7-chack_mrp$ ll
.
.
.
200dgrC_01-07-14_M7_10x10x60_LR.rrng*
atomAll.csv*
bgAPT.py*
bgOverlap-disentangle.py*
data/
Diffusion/
-i_29.5.txt*
modified200dgrC_01-07-14_M7_10x10x60_LR.rrng*
overlap-at-113.csv*
overlap-at-137.csv*
overlap-at-138.csv*
overlap-at-140.csv*
overlap-at-142.csv*
overlap-at-143.csv*
overlap-at-145.csv*
overlap-at-147.csv*
overlap-at-56.csv*
overlap-at-65.csv*
overlap.py*
Perp_to_itf_10x10x60_200dgrC_M7_LR.csv*
plotProfiles.py*
dgrC_01-07-14_M7-chack_mrp$ python plotProfiles.py atomAll.csv
```

2. Execute: **python plotProfiles.py atomall.py**

3. Pops out and get saved under atomAll-Cpall.  
.png,  
.pdf,  
.CSV.

