

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:

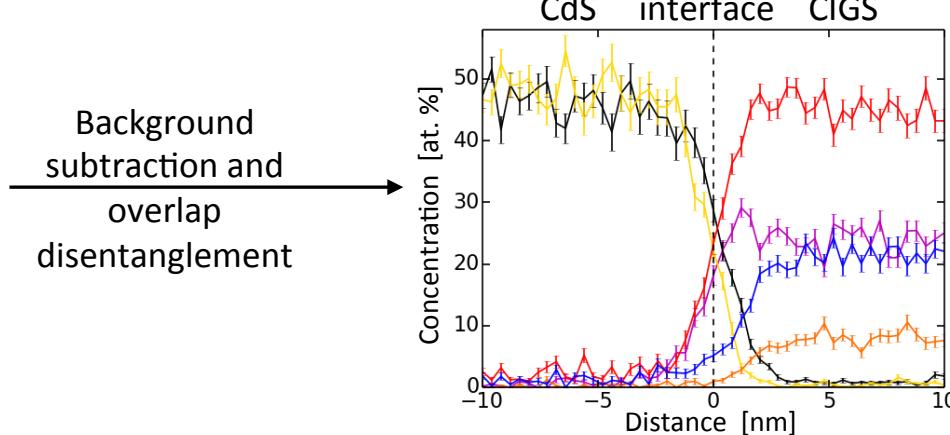
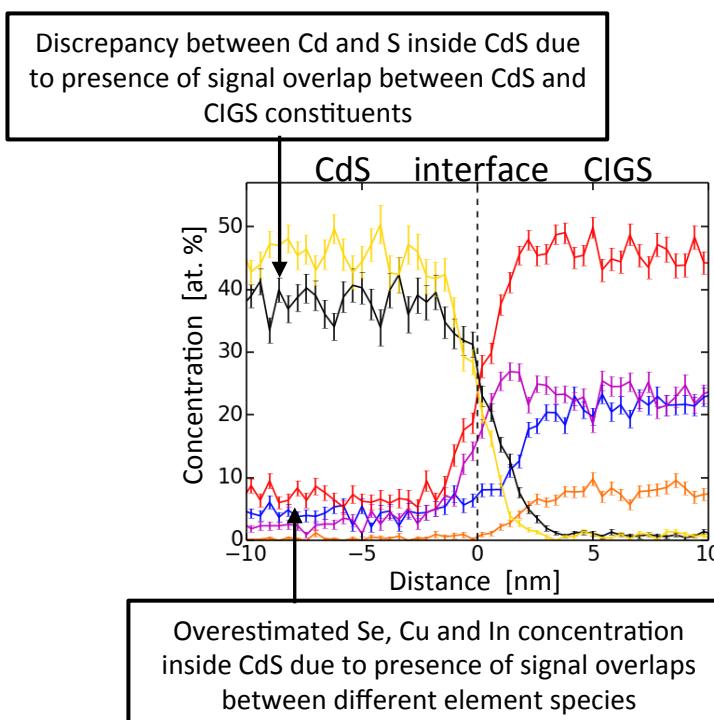
This instruction is shown within Oracle VM VirtualBox (on Ubuntu that contains **Python** program with **Pandas** package).

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.**



- Cu
- In
- Ga
- Se
- Cd
- S

Long range diffusion (small pieces of data combined to one after analysis)

1. **bgAPT.py** (to create background ranges)
2. **combineCSV.py** (to combine pre-prepared
sub-1D_concentration_profile.csv coming from each 3D subset (after mass spectrum
ranging and bg ranging) into one *.csv files on which further analysis is performed)
3. **diffusion.py** (analysis – background subtraction and overlap disentangle –
with taking into account specific distance interval taken for the 1D concentration
profiles)
4. **plotProfiles.py** (to plot final results – final composition)

1. bgAPT.py (what it does)

bg - background

Range_file.rrng

With all identified elements, complex ions and overlaps

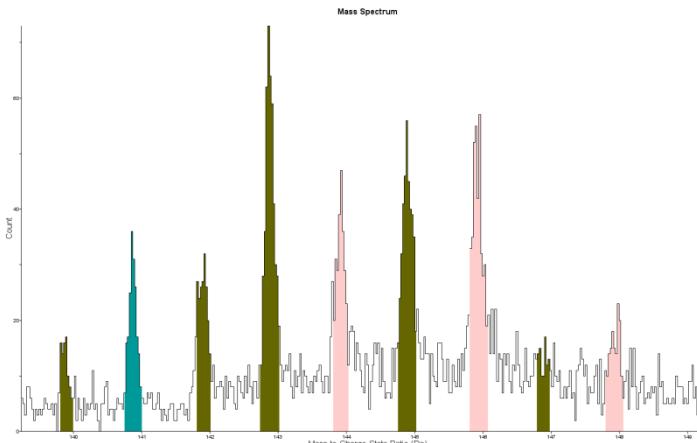
bgAPT.py

modified_Range_file.rrng

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

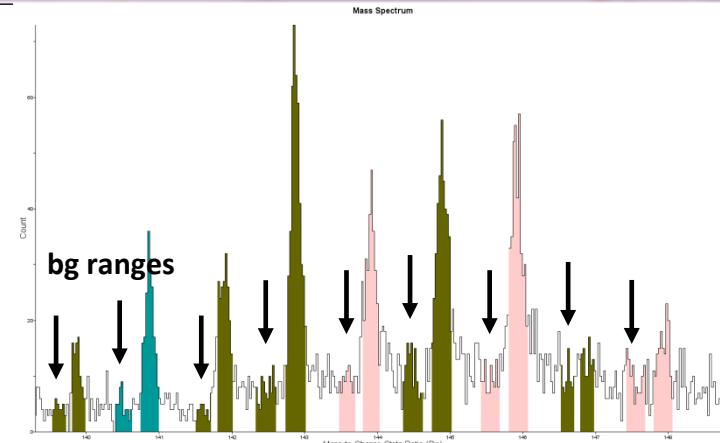
Ref_M2_10x10x60.rrng - Notepad

```
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

```
Terminal - ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp$ ll  
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$
```

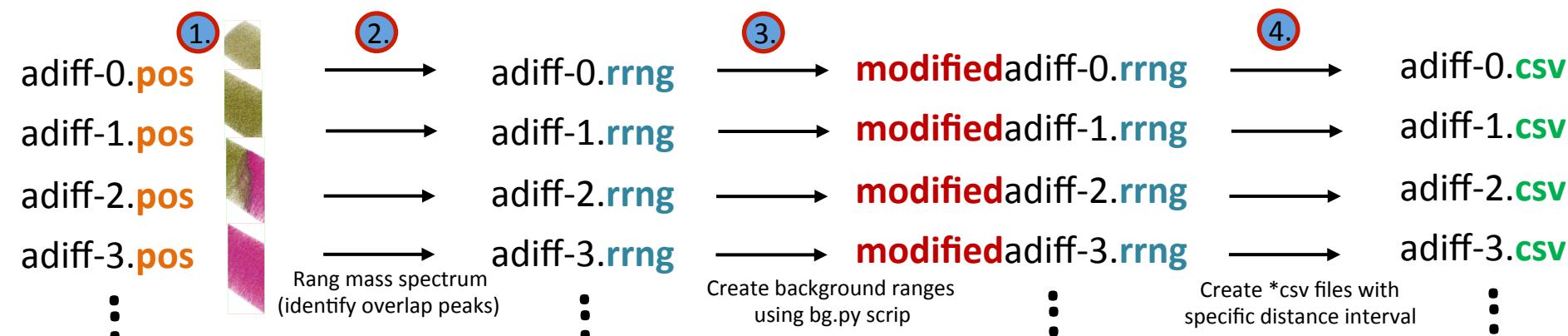
modified_Range_file.rrng

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

Long range diffusion analysis – scope part I

In order to perform background subtraction and overlap disentangle on a long set of data:

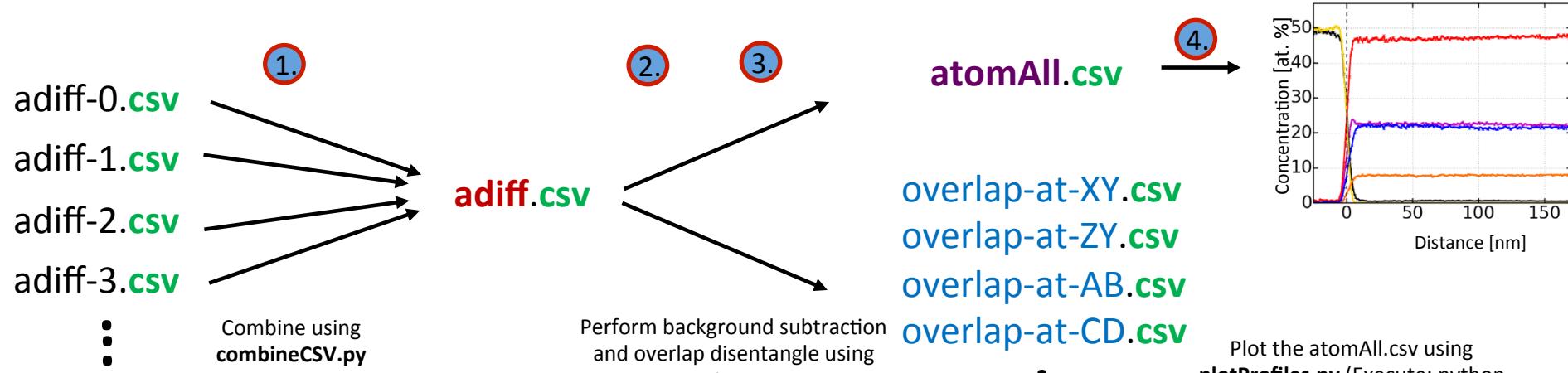
1. Chop the 3D reconstruction into ≈ 20 nm wide slices (or different if preferred) across desired direction. Export each of the slice into separate *.pos file. In order to facilitate data analysis name each of the slice as adiff-Number.pos. Start numbering from 0 (python requirement). The procedure of sectioning the data into separate *.pos files is needed to track the changes in the composition as well as peaks shape with the increasing distance.
2. Within each *.pos file range the mass spectrum and mark the overlaps*. A default/example range file can be found in the list of python scripts.
3. Export all ranges to the analysis directory (as adiff-Number.rrng). Using python script **bg.py** create modified range files (modifiedadiff-Number.rrng) that contain background ranges.
4. Import the modifiedadiff-Number.rrng into particular slice (separated part of the reconstruction) and create 1D-concentration profile along desired direction and with a specified distance bin (distance interval).



*Each peak and overlap should be ranged according to its charge state. A default range file is attached to the list of python scripts.

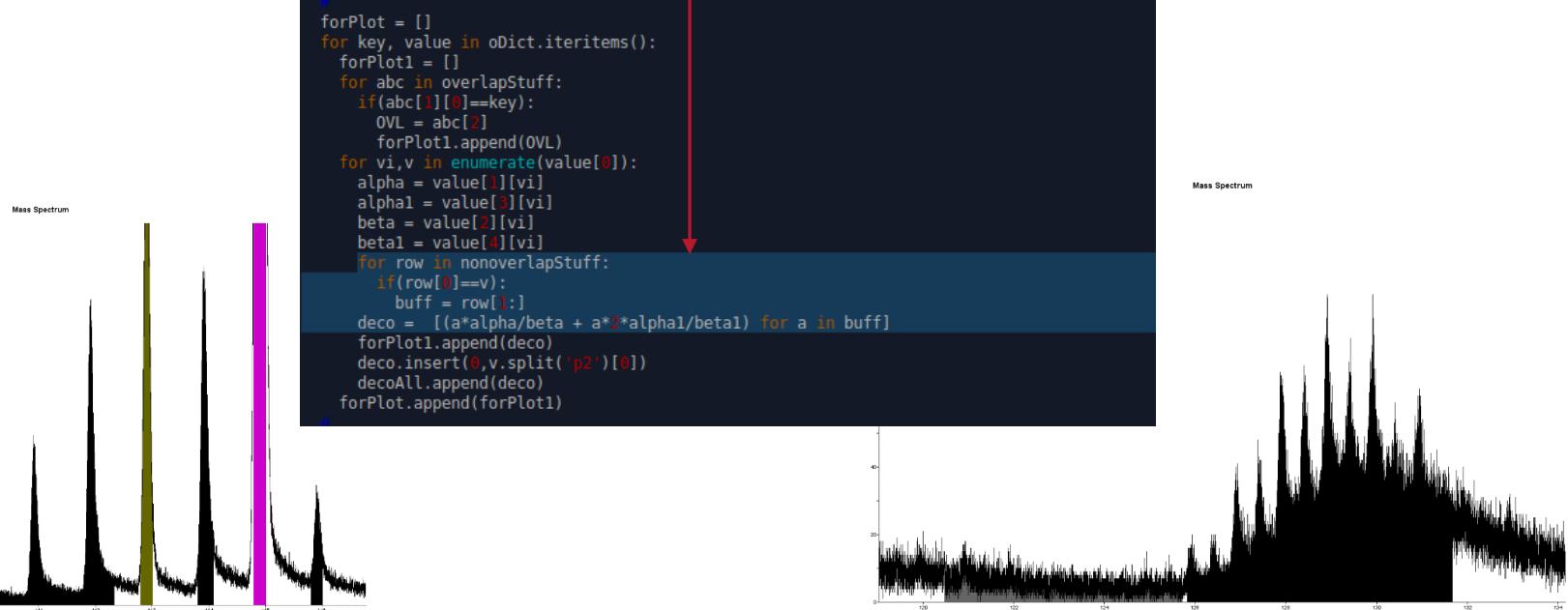
Long range diffusion analysis – scope part II

1. Open the **combineCSV.py** script in the directory where all adiff_Number.csv files are saved. Within the script set the number of **adiff-Number.csv** files that should be combined and used for analysis (see slide 9). Pay attention that the input number will always be larger by unity as compared to the number appearing in the name of the last adiff-Number.csv file. Since every operation in python starts from 0, first *.csv file is named as adiff-0.csv and therefore you have to input Number+1 (see slide 9).
2. Open the diffusion.py code and define within the code the distance interval that is used for all *.csv files (see next slide 10).
3. Perform the analysis (background subtraction and overlap disentangle) by executing the diffusion.py script on adiff.csv file (see slide 11) . As an outcome you will obtain:
 - final results (composition) in the form of **atomAll.csv** files and,
 - set of **overlap-at-XY.csv** files that contain the disentangled signals.The data presented in the line form suitable for python. If using Excel, Origin or others you need to transpose the rows into columns. First raw is always distance (in nm).
4. Use **plotProfiles.py** to plot the data from atomAll.csv (Execute: python plotProfiles.py –i XY atomAll.csv where –i XY defines the position of the interface).



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⁺, Cd⁺⁺ and Cd₂OH⁺⁺/Cd₂H₂O⁺⁺ 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⁺ and Cd⁺⁺ 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⁺ and Cd⁺⁺ signal please use option -I 0 (e.g. python bgOverlap-disentangle(overlap.py or diffusion.py).py -I 0 -i XY atomAll.py).



combineCSV.py - Combine files

```
File Edit View Terminal Tabs Help
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$ ls
total 333
-rwxrwxrwx 1 root root 28672 jul 26 22:15 /
-rwxrwxrwx 1 root root 4096 dec 21 2016 ./combineCSV.py*
-rwxrwxrwx 1 root root 14757 nov 29 2016 adiff-0.csv*
-rwxrwxrwx 1 root root 14845 nov 29 2016 adiff-10.csv*
-rwxrwxrwx 1 root root 14919 nov 29 2016 adiff-11.csv*
-rwxrwxrwx 1 root root 15075 nov 29 2016 adiff-12.csv*
-rwxrwxrwx 1 root root 14934 nov 29 2016 adiff-13.csv*
-rwxrwxrwx 1 root root 11798 nov 29 2016 adiff-14.csv*
-rwxrwxrwx 1 root root 14396 nov 29 2016 adiff-1.csv*
-rwxrwxrwx 1 root root 14621 nov 29 2016 adiff-2.csv*
-rwxrwxrwx 1 root root 14530 nov 29 2016 adiff-3.csv*
-rwxrwxrwx 1 root root 14592 nov 29 2016 adiff-4.csv*
-rwxrwxrwx 1 root root 14829 nov 29 2016 adiff-5.csv*
-rwxrwxrwx 1 root root 14863 nov 29 2016 adiff-6.csv*
-rwxrwxrwx 1 root root 14880 nov 29 2016 adiff-7.csv*
-rwxrwxrwx 1 root root 14824 nov 29 2016 adiff-8.csv*
-rwxrwxrwx 1 root root 14892 nov 29 2016 adiff-9.csv*
-rwxrwxrwx 1 root root 4096 dec 21 2016 bd/
-rwxrwxrwx 1 root root 603 dec 8 2016 combineCSV.py* ←
-rwxrwxrwx 1 root root 12288 jul 26 19:29 Conc prof with bg/
-rwxrwxrwx 1 root root 24576 jul 26 19:30 data/
-rwxrwxrwx 1 root root 13035 dec 6 2016 diffusion.py*
-rwxrwxrwx 1 root root 0 dec 12 2016 -i atomAll_3.62.txt*
-rwxrwxrwx 1 root root 4096 dec 21 2016 overlapChecks/
-rwxrwxrwx 1 root root 15113 dec 8 2016 overlap.py*
-rwxrwxrwx 1 root root 5865 sep 18 2016 plot4mCSV.py*
-rwxrwxrwx 1 root root 3938 dec 12 2016 plotConcProf.py*
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$
```

1. Open combineCSV.py using: vi

```
File Edit View Terminal Tabs Help
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$ ls
total 518
-rwxrwxrwx 1 root root 28672 jul 26 22:18 /
-rwxrwxrwx 1 root root 4096 dec 21 2016 ./adiff.csv*
-rwxrwxrwx 1 root root 14757 nov 29 2016 ad
-rwxrwxrwx 1 root root 14845 nov 29 2016 ad
-rwxrwxrwx 1 root root 14919 nov 29 2016 ad
-rwxrwxrwx 1 root root 15075 nov 29 2016 ad
-rwxrwxrwx 1 root root 14934 nov 29 2016 ad
-rwxrwxrwx 1 root root 11798 nov 29 2016 ad
-rwxrwxrwx 1 root root 14396 nov 29 2016 ad
-rwxrwxrwx 1 root root 14621 nov 29 2016 ad
-rwxrwxrwx 1 root root 14530 nov 29 2016 ad
-rwxrwxrwx 1 root root 14592 nov 29 2016 ad
-rwxrwxrwx 1 root root 14829 nov 29 2016 ad
-rwxrwxrwx 1 root root 14863 nov 29 2016 ad
-rwxrwxrwx 1 root root 14880 nov 29 2016 ad
-rwxrwxrwx 1 root root 14824 nov 29 2016 ad
-rwxrwxrwx 1 root root 14892 nov 29 2016 ad
-rwxrwxrwx 1 root root 189285 jul 26 22:18 adif
-rwxrwxrwx 1 root root 4096 dec 21 2016 ad
-rwxrwxrwx 1 root root 603 dec 8 2016 combineCSV.py* ←
-rwxrwxrwx 1 root root 12288 jul 26 19:29 Conc prof with bg/
-rwxrwxrwx 1 root root 24576 jul 26 19:30 data/
-rwxrwxrwx 1 root root 13035 dec 6 2016 diffusion.py*
-rwxrwxrwx 1 root root 0 dec 12 2016 -i atomAll_3.62.txt*
-rwxrwxrwx 1 root root 4096 dec 21 2016 overlapChecks/
-rwxrwxrwx 1 root root 15113 dec 8 2016 overlap.py*
-rwxrwxrwx 1 root root 5865 sep 18 2016 plot4mCSV.py*
-rwxrwxrwx 1 root root 3938 dec 12 2016 plotConcProf.py*
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$
```

3. Execute the combineCSV.py in the directory where all adiff-Number.csv files are. Use: **python combineCSV.py**. As a result you will obtain adiff.csv file that consists of all adiff-Number.csv files written one after another starting from adiff-0.csv.

2. Define number of *.csv files that you want to use for analysis. Bear in mind that python starts counting from 0. If your last file is adiff-14.csv put inside the combineCSV.py 15 (as in the example).

```
import re
import os,sys
from optparse import OptionParser
# import statsmodels.api as sm

fout=open("adiff.csv","a")
# first file:
for line in open("adiff-0.csv"):
    fout.write(line)
# now the rest:
for num in range(1,15): ←
    f = open("adiff-"+str(num)+".csv")
    f.next() # skip the header
    for line in f:
        fout.write(line)
    f.close() # not really needed
fout.close()
~
```

Define distance interval

In order to perform background subtraction and overlaps disentangle please open the **diffusion.py** script (vi diffusion.py) and within the code define the distance interval that you choose for 1D concentration profile in each of the adiff-Number.csv files (as in the example for 5 nm sampling interval).

```
Terminal - ania@ania-VirtualBox: /media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm
File Edit View Terminal Tabs Help
(options, filenames) = parser.parse_args()
#
# syntax 'rule' for loading a file in a particular format
with open(filenames[0], 'rb') as f:
    reader = csv.reader(f)
    allList = list(reader)

allData = []
# transpose all list
T_allList = map(list,zip(*allList))
totColumns = len(T_allList)

ionNames = []
dataWbg = []

for i, row in enumerate(T_allList):
    nameInfoAll = row[0].split()
    nameInfo = row[0].split()[0]
    # ignore the first few columns distance, ion cont , atom count
    if('Sigma' not in nameInfoAll):
        # convert the data (not 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)

# smoothing the ion counts with moving average and inserting this column
#d = list(np.array(len(dataWbg[0][1:]))*0.4)
d = np.array(range(0, len(dataWbg[0][1:]))*5
ic1 = dataWbg[1][1:]
if (options.NMA==1):
    icnl = ic1
else:
    icnl = maAK(ic1,options.binSize)
    icnl = list(icnl)
icnl.insert(0, 'IonS')
dataWbg.insert(2,icnl)

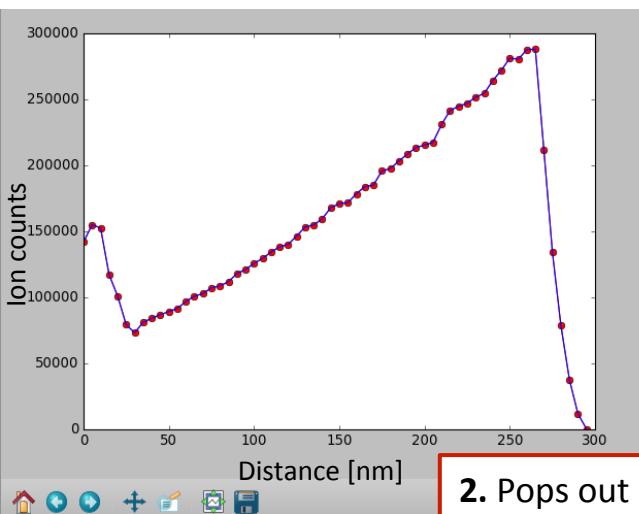
#
dataWObg = dataWbg[0:3]
for i, row in enumerate(dataWbg):
    nameInfoAll = row[0].split()
    nameInfo = row[0].split()[0]
    # # ignore the first few columns distance, ion cont , atom count
    if((nameInfo not in ['Distance', 'Ion', 'Atom']) and \
       bg not in nameInfo):
        orig = row[1:]
        BG = dataWbg[i+1][1:]
        # #Bgsub = orig-BG
        BGsub = [max(0.01*c*(a-b),float(0)) for a,b,c in zip(orig,BG,icnl[1:])]
        BGsub.insert(0,nameInfo)
        dataWObg.append(BGsub)
```

5 nm distance interval

diffusion.py - perform the analysis

1. Execute: python diffusion.py adiff.csv

```
File Edit View Terminal Tabs Help
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$ ll
total 518
drwxrwxrwx 1 root root 28672 jul 26 22:18 /
drwxrwxrwx 1 root root 4096 dec 21 2016 /_
-rw-rwxrwx 1 root root 14757 nov 29 2016 adiff-0.csv*
-rw-rwxrwx 1 root root 14845 nov 29 2016 adiff-10.csv*
-rw-rwxrwx 1 root root 14919 nov 29 2016 adiff-11.csv*
-rw-rwxrwx 1 root root 15075 nov 29 2016 adiff-12.csv*
-rw-rwxrwx 1 root root 14934 nov 29 2016 adiff-13.csv*
-rw-rwxrwx 1 root root 11798 nov 29 2016 adiff-14.csv*
-rw-rwxrwx 1 root root 14396 nov 29 2016 adiff-1.csv*
-rw-rwxrwx 1 root root 14621 nov 29 2016 adiff-2.csv*
-rw-rwxrwx 1 root root 14530 nov 29 2016 adiff-3.csv*
-rw-rwxrwx 1 root root 14592 nov 29 2016 adiff-4.csv*
-rw-rwxrwx 1 root root 14829 nov 29 2016 adiff-5.csv*
-rw-rwxrwx 1 root root 14863 nov 29 2016 adiff-6.csv*
-rw-rwxrwx 1 root root 14880 nov 29 2016 adiff-7.csv*
-rw-rwxrwx 1 root root 14824 nov 29 2016 adiff-8.csv*
-rw-rwxrwx 1 root root 14892 nov 29 2016 adiff-9.csv*
-rw-rwxrwx 1 root root 189285 jul 26 22:18 adiff.csv*
drwxrwxrwx 1 root root 4096 dec 21 2016 bg/
-rw-rwxrwx 1 root root 603 dec 8 2016 combineCSV.py*
drwxrwxrwx 1 root root 12288 jul 26 19:29 Conc_prof_with_bg/
drwxrwxrwx 1 root root 24576 jul 26 19:30 data/
-rw-rwxrwx 1 root root 13035 dec 6 2016 diffusion.py*
-rw-rwxrwx 1 root root 0 dec 12 2016 -i atomAll_3.62.txt*
drwxrwxrwx 1 root root 4096 dec 21 2016 overlapChecks/
-rw-rwxrwx 1 root root 15113 dec 8 2016 overlap.py*
-rw-rwxrwx 1 root root 5865 sep 18 2016 plot4mCSV.py*
-rw-rwxrwx 1 root root 3938 dec 12 2016 plotConcProf.py*
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$ python diffusion.py adiff.csv
```



3. Main result (final composition) will be generated as atomAll.csv together with set of overlap-at-XY.csv files that contain distribution of disentangled signals. First row always corresponds to distance (in

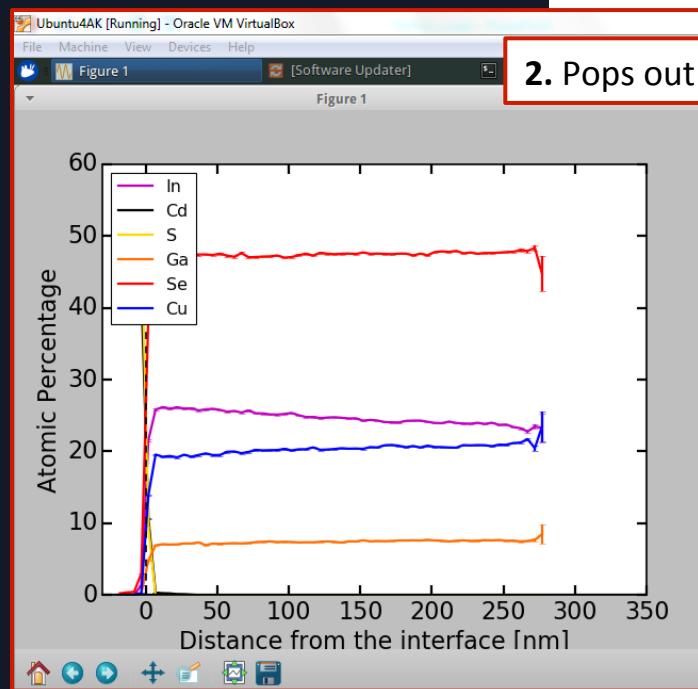
```
File Edit View Terminal Tabs Help
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$ ll
total 588
drwxrwxrwx 1 root root 11539 nov 29 2016 adiff-3.csv*
drwxrwxrwx 1 root root 14592 nov 29 2016 adiff-4.csv*
drwxrwxrwx 1 root root 14829 nov 29 2016 adiff-5.csv*
drwxrwxrwx 1 root root 14863 nov 29 2016 adiff-6.csv*
drwxrwxrwx 1 root root 14880 nov 29 2016 adiff-7.csv*
drwxrwxrwx 1 root root 14824 nov 29 2016 adiff-8.csv*
drwxrwxrwx 1 root root 14892 nov 29 2016 adiff-9.csv*
drwxrwxrwx 1 root root 189285 jul 26 22:18 adiff.csv*
drwxrwxrwx 1 root root 28500 jul 26 22:21 atomAll.csv*
drwxrwxrwx 1 root root 4096 dec 21 2016 bg/
drwxrwxrwx 1 root root 603 dec 8 2016 combineCSV.py*
drwxrwxrwx 1 root root 12288 jul 26 19:29 Conc_prof_with_bg/
drwxrwxrwx 1 root root 24576 jul 26 19:30 data/
drwxrwxrwx 1 root root 13035 dec 6 2016 diffusion.py*
drwxrwxrwx 1 root root 0 dec 12 2016 -i atomAll_3.62.txt*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-113.csv*
drwxrwxrwx 1 root root 3000 jul 26 22:21 overlap-at-137.csv*
drwxrwxrwx 1 root root 3000 jul 26 22:21 overlap-at-138.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-140.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-142.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-143.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-145.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-147.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-56.csv*
drwxrwxrwx 1 root root 4500 jul 26 22:21 overlap-at-65.csv*
drwxrwxrwx 1 root root 4096 dec 21 2016 overlapChecks/
drwxrwxrwx 1 root root 15113 dec 8 2016 overlap.py*
drwxrwxrwx 1 root root 5865 sep 18 2016 plot4mCSV.py*
drwxrwxrwx 1 root root 3938 dec 12 2016 plotConcProf.py*
ania@ania-VirtualBox:/media/WinLinHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$
```

plotProfiles.py - plot the final results

To plot and save final results in the form of an image execute: `python plotProfiles.py -i XY atomAll.csv` (as shown in the example).

1. Execute: `python plotProfiles.py -i XY atomAll.csv`

```
27 18:30 ./
21 2016 ../
29 2016 adiff-0.csv*
29 2016 adiff-10.csv*
29 2016 adiff-11.csv*
29 2016 adiff-12.csv*
29 2016 adiff-13.csv*
29 2016 adiff-14.csv*
29 2016 adiff-1.csv*
29 2016 adiff-2.csv*
29 2016 adiff-3.csv*
29 2016 adiff-4.csv*
29 2016 adiff-5.csv*
29 2016 adiff-6.csv*
29 2016 adiff-7.csv*
29 2016 adiff-8.csv*
29 2016 adiff-9.csv*
26 22:18 adiff.csv*
27 18:32 atomAll-CPall.pdf*
27 18:32 atomAll-CPall.png*
27 18:32 atomAll-CPall.svg*
26 22:21 atomAll.csv*
21 2016 bq/
8 2016 combineCSV.py*
26 19:29 Conc prof with bd/
26 19:30 data/
27 16:14 diffusion.py*
12 2016 -i_atomAll_3.62.txt*
26 22:21 overlap-at-113.csv*
26 22:21 overlap-at-137.csv*
26 22:21 overlap-at-138.csv*
26 22:21 overlap-at-140.csv*
26 22:21 overlap-at-142.csv*
26 22:21 overlap-at-143.csv*
26 22:21 overlap-at-145.csv*
26 22:21 overlap-at-147.csv*
26 22:21 overlap-at-56.csv*
26 22:21 overlap-at-65.csv*
21 2016 overlapChecks/
8 2016 overlap.py*
18 2016 plot4mCSV.py*
27 16:15 plotProfiles.py*
nHome/200dgrC_01-07-14_M7-chack_mrp/Diffusion/5nm$ python plotProfiles.py -i 3.62 atomAll.csv
```



3. Images get saved

Time	User	File	Date	File
2016	adiff-4.csv*			
2016	adiff-5.csv*			
2016	adiff-6.csv*			
2016	adiff-7.csv*			
2016	adiff-8.csv*			
2016	adiff-9.csv*			
2016	adiff.csv*			
2016	atomAll-CPall.pdf*			
2016	atomAll-CPall.png*			
2016	atomAll-CPall.svg*			
2016	atomAll.csv*			