Instructions for running Python codes

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Two Python codes are included in this package

1. Capacity-auto-calculate

   Needed input: path of raw data folder, output file name, and name of global information file.

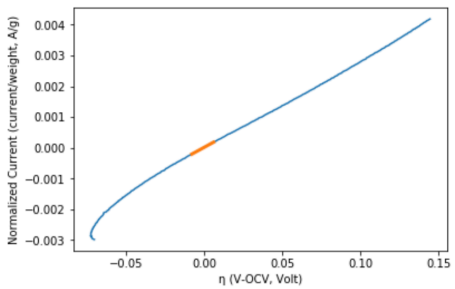
   Output you will get: a csv file that contains the discharge capacity of step 4, full capacity, HRD. It auto-calculates ALL cycles in ALL channels and present with two different calculating method (average and direct)

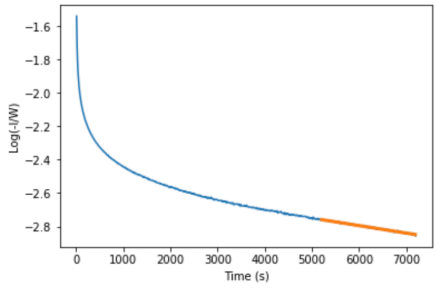
Channel 001							
	weight (g)	Step 4 avg Capacity (mAh/kg	Step 4 direct Capacity (mAh/kg)	Full Capacity (mAh/kg) - Avg method	Full Capacity (mAh/kg) - direct method	HRD - Avg method	HRD - direct method
Cycle 1	0.0451	200.97335475261644	200.972497617	235.82972833	235.8294091208204	0.852193228734	0.8521980167861657
Cycle 2	0.0451	223.3412856632594	223.340873842	249.580643486	249.58119440643014	0.894864564502	0.8948642392485694
Cycle 3	0.0451	229.75768589694016	229.757830666	253.460417872	253.4569501517516	0.906484067985	0.9064958990447014
Cycle 4	0.0451	237.23029045603107	237.232895542	261.091571413	261.0867771103548	0.908619509463	0.9086262164696293
Cycle 5	0.0451	234.16605978946782	234.168385062	257.77201282	257.7685121480266	0.908432154834	0.9084354711835214
Cycle 6	0.0451	237.22346829421284	237.225251863	261.19904574	261.1970225466962	0.908216380311	0.9082165867790571
Cycle 7	0.0451	235.74873131006652	235.748264504	258.978422598	258.98023017563196	0.910300797028	0.910296245972866
Cycle 8	0.0451	233.6489738190909	233.650749492	256.605355246	256.60329206780483	0.91054510249	0.9105455036693432
Cycle 9	0.0451	236.89935759605322	236.905326619	261.771646518	261.76298470485585	0.905007588754	0.9050147325572522
Cycle 10	0.0451	231.28283949705101	231.280334943	257.08478082	257.0870588308204	0.899626707598	0.8996284781850874
Channel 002							
	weight (g)	Step 4 avg Capacity (mAh/kg	Step 4 direct Capacity (mAh/kg)	Full Capacity (mAh/kg) - Avg method	Full Capacity (mAh/kg) - direct method	HRD - Avg method	HRD - direct method
Cycle 1	0.043	185.7402937404186	185.740908038	210.932935532	210.93049520151163	0.880568544545	0.8805758198356872
Cycle 2	0.043	208.54600980260466	208.542784639	228.046242031	228.04542856913955	0.914475865865	0.9144932705343708

2. D-I0-auto-calculate

   Needed input: path of raw data folder, output file name, name of global information file, the range of I_0 (± OCV) and D data (from the end of the curve) for fitting straight line.

   Output you will get: a csv file that contains calculated I_0 and D for ALL channels, plots of normalized current vs. over potential and log(-I/w) vs. time (blue lines), and the fitting straight line for both plot (orange lines), which you can freely change the range of data points.






```
Channel- 016
I0=  0.715427190895 (mA/g)
D=  0.420030974817 (10^(-10)cm^2/s)
```

	D (10^(-10)cm^2/s)	I0 (mA/g)
Channel 016	0.420030974817	0.715427190895
	D (10^(-10)cm^2/s)	I0 (mA/g)
Channel 017	0.431949060296	0.775704090679
	D (10^(-10)cm^2/s)	I0 (mA/g)
Channel 018	0.449110882036	1.19455098625
	D (10^(-10)cm^2/s)	I0 (mA/g)
Channel 019	0.527414480227	0.908004623202
	D (10^(-10)cm^2/s)	I0 (mA/g)
Channel 020	0.415673529947	0.792601434902
	D (10^(-10)cm^2/s)	I0 (mA/g)
Channel 021	0.411214484593	0.877293609976

What you need before running this code

1. Install Python 3 and Jupyter notebook, these two can be done by just downloading and install Anaconda (https://www.anaconda.com/download/#macos), the procedure can be found at here (http://jupyter.org/install)

2. Export the capacity excels file to separated .csv file

If you are using **Mac OS**, you can directly export the raw file (including multi tabs) to separated csv. files by **Numbers**.

If you are using **Windows** and **Excel** it can be done through VBA function of Excel

a. Enable the VBA function in your Excel:

Click File

Click Options

Click Customize Ribbon

Under the list of Main Tabs, select Developer

Click OK

b. Input the exporting code

Click the Developer tab -> Visual Basic

Right-click in the project window -> insert -> Module

In the module window, paste the code below (you can save this in Excel VBA for future use)

```
Public Sub SaveWorksheetsAsCsv()
Dim WS As Excel.Worksheet
Dim SaveToDirectory As String

  SaveToDirectory = "C:\"

  For Each WS In ThisWorkbook.Worksheets
    WS.SaveAs SaveToDirectory & WS.Name, xlCSV
  Next

End Sub
```

Make sure you change the SaveToDirectory to any path that you want to save the separated .csv files

Click the button of Run Sub or press F5 to run this code

You should now see separated .csv files in the targeted folder

3. Now you have the files and Jupyter

a. Click start -> enter "**Anaconda Prompt**" for searching -> open it

b. In the Anaconda Prompt command window, type "**jupyter notebook**"

c. There should be a web page (jupyter) pops up (but it doesn't need internet to start)

d. Locate the folder that you saved this Python code and open it

e. Now you should be able to see the jupyter operation window with cells. If you can't see the cells, back to the web page and click the "new" button on the right-hand side to open a new Python 3 notebook. Then paste the code to the cell of the new window

f. Follow the instruction in the code to change the input parameter (.csv file path, how many channels, output file name, and .csv file name if necessary, usually you don't have to)

g. Press Shift+Enter and the code will be running.

h. You can check results in the output file (.csv), the location of the output file will be the same as this Python code.

Note:

Check the input section before running the codes, the folder path will be different depends on you are using Windows or Mac OS.

For example:

Mac OS path: /Users/HONG-KANG/Documents/BASF/Python-Code/

Windows path: D:\\Users\\HONG-KANG\\Documents\\BASF\\Python-Code

and the file name of global-information has to include ".csv"

In the folder that has separated csv files of raw data, please make sure there are only two kind of files -> Channel file and Global-information file, if there are files other than these two types, the code cannot work.