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Supporting information for article:

**MAP2XANES a Jupiter interactive notebook for elemental mapping
and XANES speciation**

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In this section we present few screenshot from the execution of MAP2XANES.

Configuring your experiment ¶

```
In [19]: e0_conf = 6540 # nominal edge position
ich_conf = [2,39,40,41,42,43,44,5] # [energy, fluo1, fluo2... fluo6, i01]
mode='fluo' # measurement mode for the sample spectra
epra = e0_conf -109 # preedge lower limit range
eprb = e0_conf -19 # preedge middle limit range
eprc = e0_conf -15 # preedge higher limit range
epsa = e0_conf +5 # prostedge lower limit range
epsb = e0_conf +121 # prostedge middle limit range
epsc = e0_conf +600 # prostedge higher limit range
```

Figure S1 Screenshot of parameters configuration in MAP2XANES. E0_conf is the nominal edge position. ich_conf is the list containing the index of energy, fluorescence counters (from 1 to 6), and incident photon flux i01. Mode is the variable that specified how the data have been collected (transmission or fluorescence, i.e. 'transm' and 'fluo' respectively). All the following parameters are for normalization purpose: epra, eprb, eprc (the lower, the intermediate, and the higher pre-edge energy values), epsa, epsb, epsc (the lower, the intermediate, and the higher post-edge energy values).

Deglitching the spectra (optional)

```
In [21]: spectra['glitches'] = [] # [[6540, 6542],...]
```

Correct for self absorption (optional)

```
In [22]: display(button_open_SAc)
display(button_correct_SA)
```

Open fluo.inp

SA correction

```
writing absorption file 0
writing absorption file 1
writing absorption file 2
```

Figure S2 Optional procedure for data deglitching and self-absorption correction

Normalization Parameters (on sample spectra)

```
In [23]: interactive_plot = interactive(f, pr_es=(epra,eprb),
                                     pr_ee=(eprb,eprc),
                                     po_es=(epsa,epsb),
                                     po_ee=(epsb,epsd),
                                     number=(0,len(spectra['raw'])-1),
                                     plot=[('raw', 10), ('normalize', 20)]
                                     )

output = interactive_plot.children[-1]
output.layout.width = '24500px'
interactive_plot
```

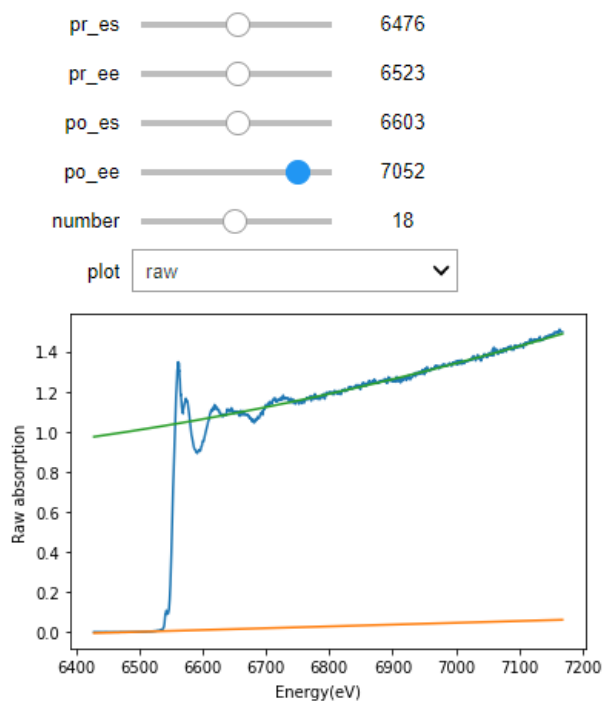


Figure S3 Normalization procedure in MAP2XANES on sample spectra. These are the normalization parameters (“sliders”): pre_es, pr_ee (lower and higher values for pre-edge energy), po_es, and po_ee (lower and higher values for post-edge energy). “number” is the index corresponding to the sample spectrum plot. The combobox “plot” allow the users to pass from raw data to normalized data.

Normalizing of references

```
In [25]: #references
interactive_plot2 = interactive(frefs, number=(0,len(spectra['refs']['raw'])-1),
                              plot=[('raw', 10), ('normalize', 20)])
output = interactive_plot2.children[-1]
output.layout.width = '1250px'
interactive_plot2
```

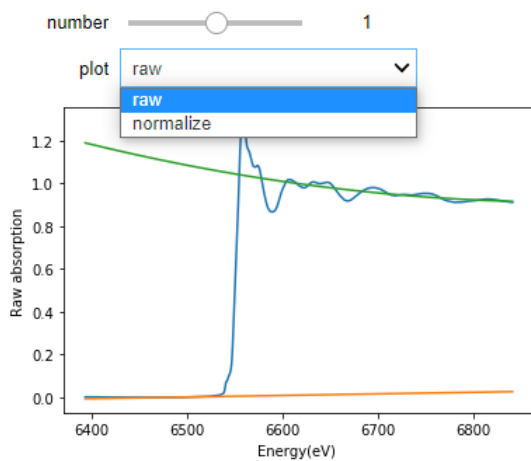


Figure S4 Normalization procedure in MAP2XANES applied to references' spectra. “number” is the index corresponding to the reference plotted. The combobox “plot” allows the users to pass from raw data to normalized data

Guessing LCF parameters

```
In [27]: interactive_plot3 = interactive(guess_lca,  
                                       lim1=(epra,eprb),  
                                       lim2=(epsb,epsc),  
                                       a=(0,1, 0.1),  
                                       b=(0,1, 0.1),  
                                       c=(0,1, 0.1),  
                                       d=(0,1, 0.1),  
                                       number=(0,len(spectra['raw'])-1)  
                                       )
```

```
In [28]: output = interactive_plot3.children[-1]  
output.layout.width = '2450px'  
interactive_plot3
```

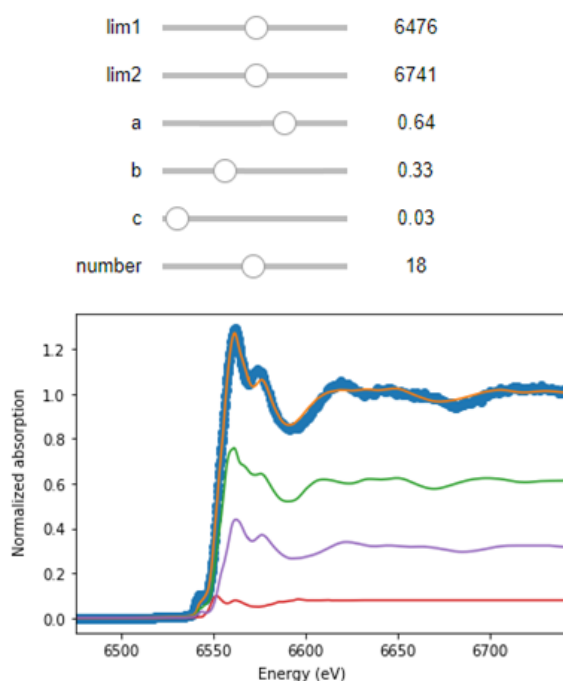


Figure S5 Guessing procedure for the linear combination fits. A, b, c are the weight of the three references loaded. “number” is the index corresponding to the sample spectrum plotted.

Making LCF

```
In [29]: display(button_lcf)
```

LCF all spectra

lcf of all spectra have been calculated

```
In [30]: interactive_plot4 = interactive(show_lca,  
                                         number=(0, len(spectra['raw'])-1)  
                                         )  
interactive_plot4
```

number 12

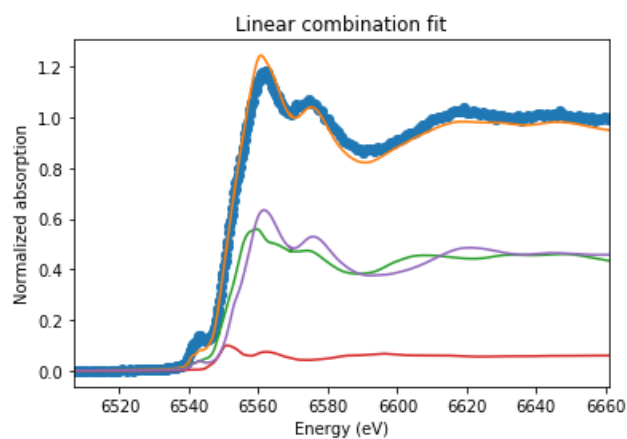


Figure S6 Linear combination fit for all the sample spectra. Interactive plot displaying the results for each sample spectrum. “number” is the index corresponding to the sample spectrum plot.

Displayed loaded maps

```
In [33]: interactive_plot6 = interactive(make_map, number=(0,len(spectra['Map'])-1))
output = interactive_plot6.children[-1]
output.layout.width = '12500px'
display(button_save_map)
interactive_plot6
```

Save map

number 1

you enter a single counter
(1200, 1200)

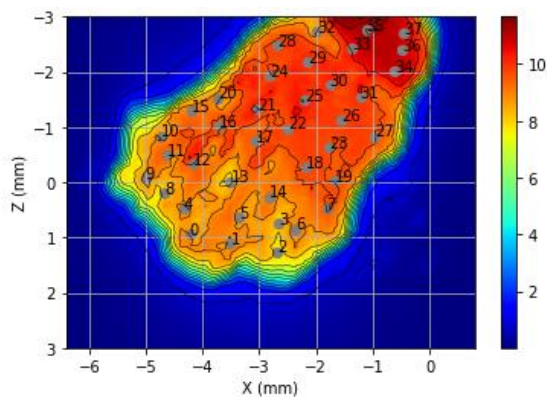


Figure S7 Function for map plotting in MAP2XANES. Each displayed map can be saved as image.

“number” is the index corresponding to the sample map plotted.

Overlap LCF on elemental map

```
In [35]: interactive_plot7 = interactive(map_lca, n_map =(0,len(spectra['Map'])-1), n_comp=(0,len(spectra['Map'])-1))
output = interactive_plot7.children[-1]
display(button_save_mapLCF)
interactive_plot7
```

Save LCF map

n_map 1

n_comp 0

C:/Users/hp/Desktop/data/XAS_husmanite/map/position_Mn.txt
3876 (3876, 2) 3876 3876
38 (38, 2) 38 38

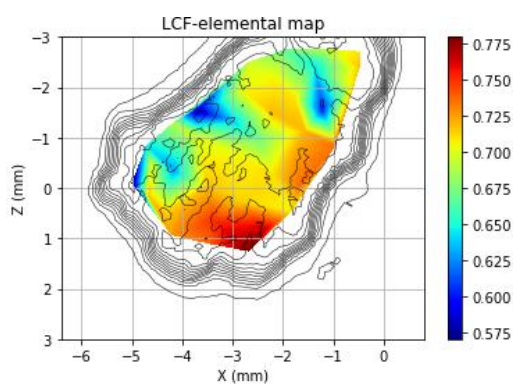


Figure S8 Function to overlap linear component fit results on elemental map. “n_map” and “n_comp” are the index of elemental map and linear combination component respectively