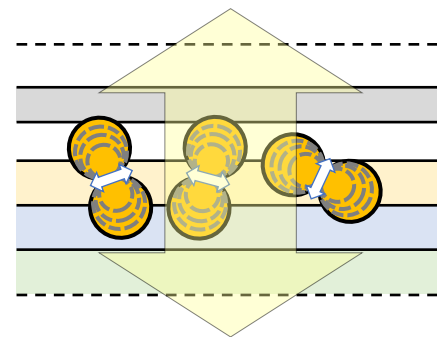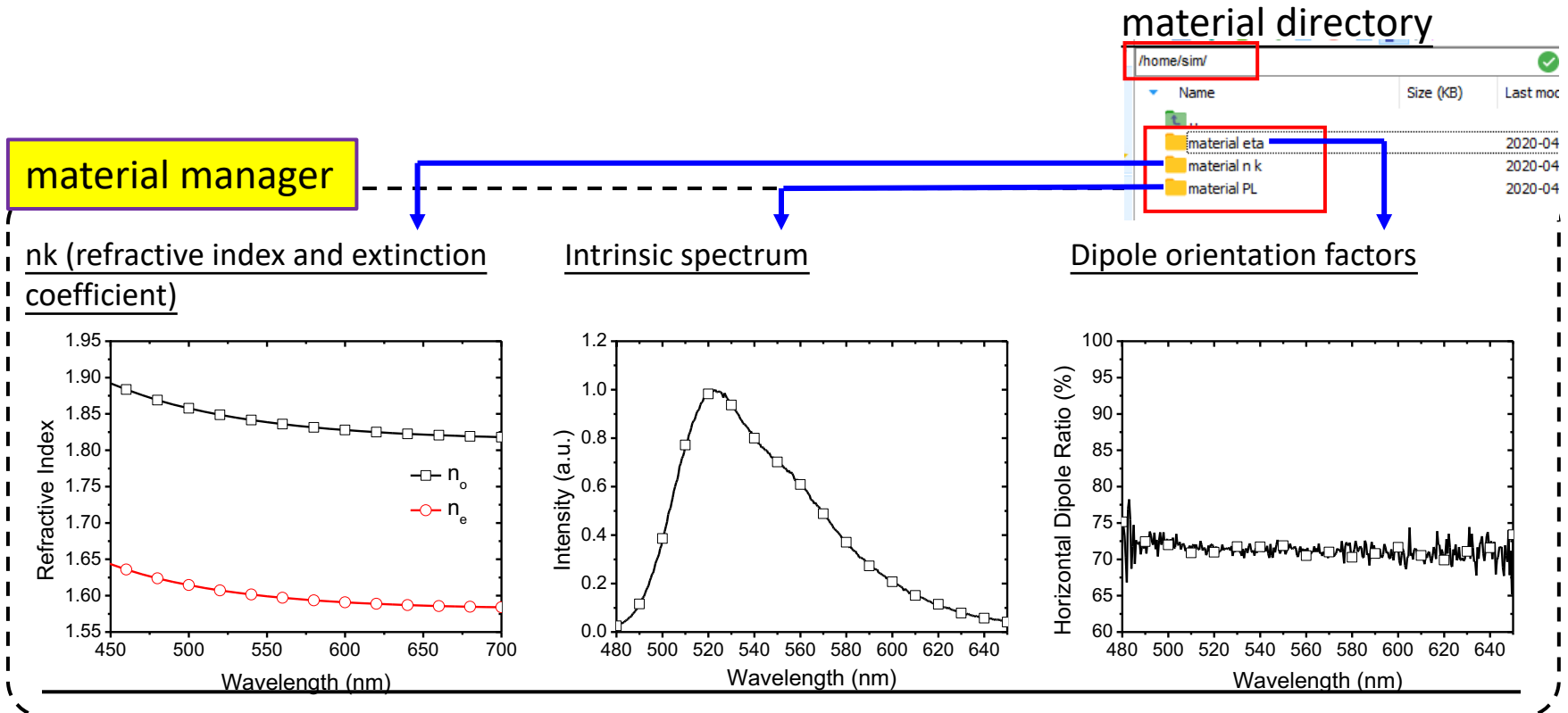# Material Manager System

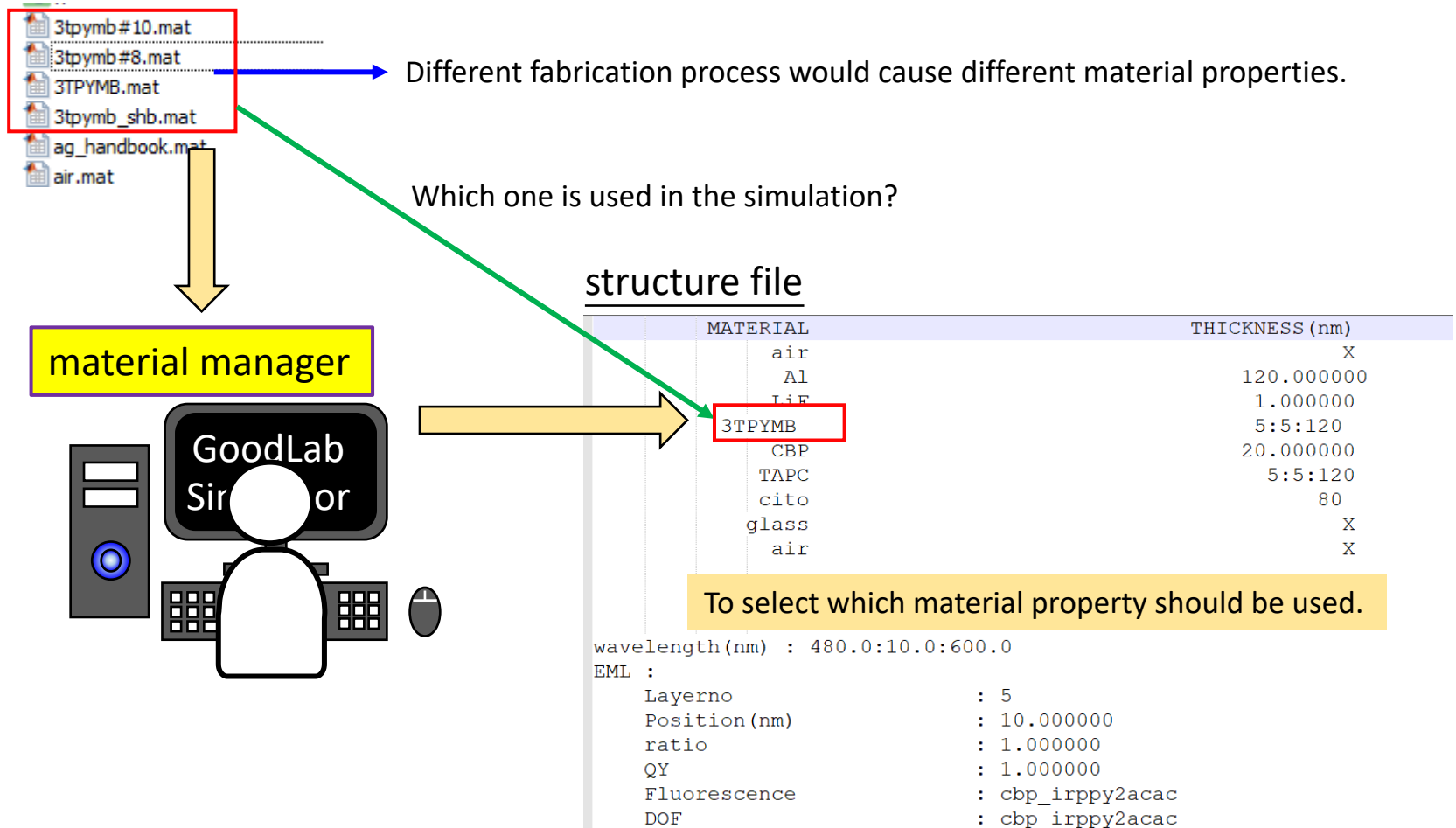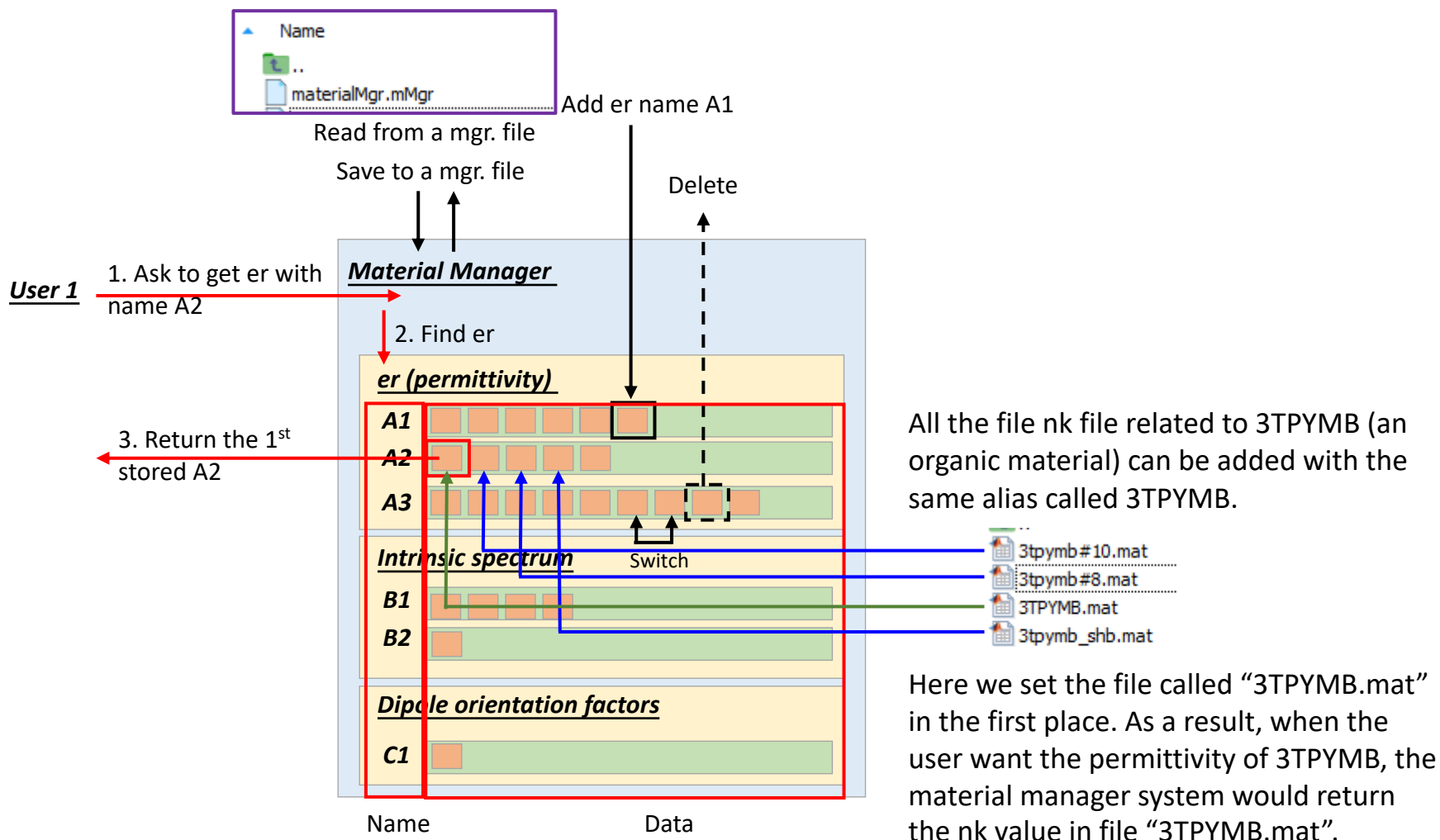**-materialMgrCmd.pyc**

Author: Wei-Kai Lee

Objective

- Material manager system is to help control the material properties, such refractive index, intrinsic spectrum, and dipole orientation factors.

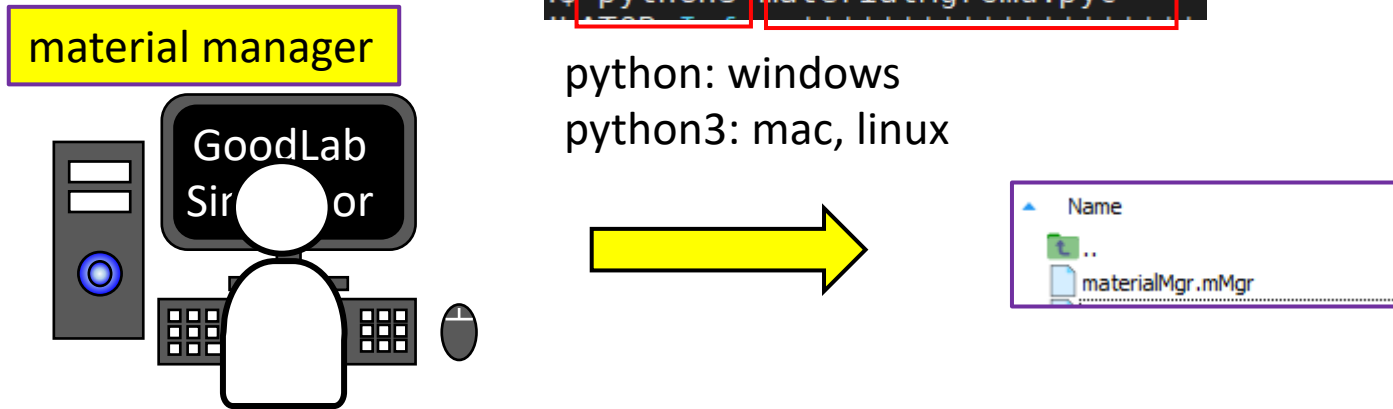material directory

material manager

nk (refractive index and extinction coefficient)

Intrinsic spectrum

Dipole orientation factors

Objective

3tpymb#10.mat
3tpymb#8.mat
3TPYMB.mat
3tpymb_shb.mat
ag_handbook.mat
air.mat

Different fabrication process would cause different material properties.

Which one is used in the simulation?

material manager

GoodLab Simulator

structure file

MATERIAL	THICKNESS(nm)
air	X
Al	120.000000
LiF	1.000000
3TPYMB	5:5:120
CBP	20.000000
TAPC	5:5:120
cito	80
glass	X
air	X

To select which material property should be used.

```
wavelength(nm) : 480.0:10.0:600.0
EML :
    Layerno                 : 5
    Position(nm)            : 10.000000
    ratio                   : 1.000000
    QY                      : 1.000000
    Fluorescence            : cbp_irppy2acac
    DOF                     : cbp_irppy2acac
```

Material Manager Workflow

All the file nk file related to 3TPYMB (an organic material) can be added with the same alias called 3TPYMB.

Here we set the file called "3TPYMB.mat" in the first place. As a result, when the user want the permittivity of 3TPYMB, the material manager system would return the nk value in file "3TPYMB.mat".
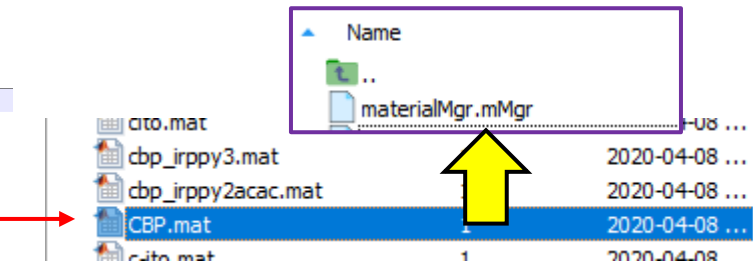
How to use the system

1. The user can directly control the material manager system by execution file "materialMgrCmd.pyc".

material manager

GoodLab Simulator

python: windows
python3: mac, linux

Name
..
materialMgr.mMgr

2. Or do not use the material manager system, the simulator would directly load the file with the same name as the material in the structure file in the default directory and save into the material manager setting file.

structure file

MATERIAL	THICKNESS(nm)
air	X
Al	120.000000
LiF	1.000000
3TPYMB	5:5:120
CBP	20.000000
TAPC	5:5:120
cito	80
glass	X
air	X

Name
..
materialMgr.mMgr

cito.mat
cbp_irppy3.mat   2020-04-08 ...
cbp_irppy2acac.mat   2020-04-08 ...
CBP.mat   2020-04-08 ...
c-ito.mat   1   2020-04-08

nk file format

Isotropic refractive index

Wavelength (nm)	n	k
350	1.808045	0
360	1.791156	0
370	1.776248	0
380	1.763036	0
390	1.751282	0
400	1.74079	0
410	1.731392	0
420	1.722947	0
430	1.715336	0
440	1.708455	0
450	1.702218	0
460	1.69655	0
470	1.691386	0
480	1.686669	0
490	1.682351	0
500	1.67839	0

Wavelength (nm)   n   k

wavelength	n	k
350	1.808045	0
360	1.791156	0
370	1.776248	0
380	1.763036	0
390	1.751282	0
400	1.74079	0
410	1.731392	0
420	1.722947	0
430	1.715336	0
440	1.708455	0
450	1.702218	0

Wavelength (nm)   n   k

This line is optional. If this line is given, the column can be randomly switched.

nk file format

Uniaxial refractive index (optical axis is parallel to the z axis)

This line is optional. If this line is given, the column can be randomly switched.

```
B3PYMPM_uniaxial.mat
 1    400 1.9576   0 1.66512266   0
 2    410 1.9479   0 1.65684127   0
 3    420 1.9388   0 1.64967952   0
 4    430 1.9302   0 1.6434751 0
 5    440 1.9221   0 1.63809165   0
 6    450 1.9145   0 1.63341424   0
 7    460 1.9072   0 1.62934559   0
 8    470 1.9004   0 1.62580317   0
 9    480 1.894    0 1.62271668   0
10    490 1.8879   0 1.6200261 0
11    500 1.8821   0 1.61768    0
12    510 1.8767   0 1.61563423   0
13    520 1.8715   0 1.61385077   0
14    530 1.8666   0 1.61229681   0
15    540 1.8619   0 1.61094394   0
16    550 1.8574   0 1.60976756   0
17    560 1.8532   0 1.60874626   0
18    570 1.8492   0 1.60786141   0
19    580 1.8454   0 1.60709676   0
20    590 1.8417   0 1.6064381 0
```

Wavelength (nm) n_o k_o n_e k_e

```
B3PYMPM_uniaxial.mat
 1    wavelength no ne ko ke
 2    400 1.9576   0 1.66512266   0
 3    410 1.9479   0 1.65684127   0
 4    420 1.9388   0 1.64967952   0
 5    430 1.9302   0 1.6434751 0
 6    440 1.9221   0 1.63809165   0
 7    450 1.9145   0 1.63341424   0
 8    460 1.9072   0 1.62934559   0
 9    470 1.9004   0 1.62580317   0
10    480 1.894    0 1.62271668   0
11    490 1.8879   0 1.6200261 0
12    500 1.8821   0 1.61768    0
13    510 1.8767   0 1.61563423   0
14    520 1.8715   0 1.61385077   0
15    530 1.8666   0 1.61229681   0
```

Wavelength (nm) n_o k_o n_e k_e

$$\epsilon_r = \begin{bmatrix} (n_o + jk_o)^2 & 0 & 0 \\ 0 & (n_o + jk_o)^2 & 0 \\ 0 & 0 & (n_e + jk_e)^2 \end{bmatrix}$$

nk file format

Uniaxial refractive index

B3PYMPM_uniaxial.mat							
1	400	1.9576	0	1.66512266	0	30	30
2	410	1.9479	0	1.65684127	0	30	30
3	420	1.9388	0	1.64967952	0	30	30
4	430	1.9302	0	1.6434751	0	30	30
5	440	1.9221	0	1.63809165	0	30	30
6	450	1.9145	0	1.63341424	0	30	30
7	460	1.9072	0	1.62934559	0	30	30
8	470	1.9004	0	1.62580317	0	30	30
9	480	1.894	0	1.62271668	0	30	30
10	490	1.8879	0	1.6200261	0	30	30

Wavelength (nm) n_o k_o n_e k_e β/beta γ/gamma

Euler Angle

β/beta $\rightarrow \boldsymbol{R}_x(\beta)$
γ/gamma $\rightarrow \boldsymbol{R}_z(\gamma)$

$$\boldsymbol{R} = \boldsymbol{R}_z(\gamma)\boldsymbol{R}_x(\beta)$$

$$\epsilon_r = \boldsymbol{R} \begin{bmatrix} (n_o + jk_o)^2 & 0 & 0 \\ 0 & (n_o + jk_o)^2 & 0 \\ 0 & 0 & (n_e + jk_e)^2 \end{bmatrix} \boldsymbol{R}^{-1}$$

Intrinsic Spectrum

```
cbp_irppy2acac.spc
 1   380 0.00358
 2   410 0.00201
 3   411 0
 4   412 0.00244
 5   413 0.00125
 6   414 0.00339
 7   415 0.00422
 8   416 0.00713
 9   417 0.00327
10   418 0.00277
11   419 8.00308E-4
12   420 0.00427
13   421 0.00166
14   422 0.00536
15   423 0.005
16   424 0.00572
17   425 0.00512
18   426 0.00249
19   427 0.00377
20   428 0.00401
21   429 0.00247
```

Wavelength (nm)   spectrum

```
cbp_irppy2acac.spc
 1   wavelength Intensity
 2   380 0.00358
 3   410 0.00201
 4   411 0
 5   412 0.00244
 6   413 0.00125
 7   414 0.00339
 8   415 0.00422
 9   416 0.00713
10   417 0.00327
11   418 0.00277
12   419 8.00308E-4
13   420 0.00427
14   421 0.00166
15   422 0.00536
```

This line is optional. If this line is given, the column can be randomly switched.

Wavelength (nm)   spectrum

Dipole Orientation Factors

This line is optional. If this line is given, the column can be randomly switched.

	cbp_irppy2acac.eta					
1	420	0.5218	0	0	0	0
2	421	0.5198	0	0	0	0
3	422	0.5252	0	0	0	0
4	423	0.526	0	0	0	0
5	424	0.5259	0	0	0	0
6	425	0.5252	0	0	0	0
7	426	0.5184	0	0	0	0
8	427	0.5251	0	0	0	0
9	428	0.5199	0	0	0	0
10	429	0.518	0	0	0	0
11	430	0.5195	0	0	0	0
12	431	0.5139	0	0	0	0
13	432	0.5164	0	0	0	0
14	433	0.5209	0	0	0	0

Wavelength (nm) DOF1   DOF3   DOF5
                  DOF2   DOF4

DOF2~DOF5 is optional and the default values are zeros.

	cbp_irppy2acac.eta						
1	wavelength		DOF1	DOF2	DOF3	DOF4	DOF5
2	420	0.5218	0	0	0	0
3	421	0.5198	0	0	0	0
4	422	0.5252	0	0	0	0
5	423	0.526	0	0	0	0
6	424	0.5259	0	0	0	0
7	425	0.5252	0	0	0	0
8	426	0.5184	0	0	0	0
9	427	0.5251	0	0	0	0
10	428	0.5199	0	0	0	0
11	429	0.518	0	0	0	0
12	430	0.5195	0	0	0	0
13	431	0.5139	0	0	0	0
14	432	0.5164	0	0	0	0

$DOF1 = < \frac{1}{2}\sin^2\theta >$ (half of horizontal dipole orientation ratio)

$DOF2 = < \frac{1}{2}\sin^2\theta\,(\cos^2\phi - \sin^2\phi) >$

$DOF3 = < \sin^2\theta\cos\phi\sin\phi >$

$DOF4 = < \cos\theta\sin\theta\cos\phi >$

$DOF5 = < \cos\theta\sin\theta\sin\phi >$

$<\cdot>$ the average over θ and ϕ

Material Manager File

The material manager file can share to others and the other can use the same material manager setting.

Name
..
materialMgr.mMgr

```
 1  er|air|0|[PATH]../Material/Example|[FILENAME]air
 2  er|Al|0|[PATH]../Material/Example|[FILENAME]Al
 3  er|LiF|0|[PATH]../Material/Example|[FILENAME]LiF
 4  er|B3PYMPM_uniaxial|0|[PATH]../Material/Example|[FILENAME]B3PYMPM_uniaxial
 5  er|B3PYMPM_isotropic|0|[PATH]../Material/Example|[FILENAME]B3PYMPM_isotropic
 6  er|B3PYMPM_ne|0|[PATH]../Material/Example|[FILENAME]B3PYMPM_ne
 7  er|B3PYMPM_no|0|[PATH]../Material/Example|[FILENAME]B3PYMPM_no
 8  er|B3PYMPM|0|[PATH]../Material/Example|[FILENAME]B3PYMPM_uniaxial
 9  er|3TPYMB|0|[PATH]../Material/Example|[FILENAME]3tpymb
10  er|TPBi|0|[PATH]../Material/Example|[FILENAME]TPBi_irppy
11  er|bmpypb_ne|0|[PATH]../Material/Example|[FILENAME]bmpypb_ne
12  er|bmpypb_no|0|[PATH]../Material/Example|[FILENAME]bmpypb_no
13  er|bmpypb_uniaxial|0|[PATH]../Material/Example|[FILENAME]bmpypb_uniaxial
14  er|BMPYPB|0|[PATH]../Material/Example|[FILENAME]bmpypb_uniaxial
15  er|mCPCN|0|[PATH]../Material/Example|[FILENAME]mCPCN
16  er|CBP|0|[PATH]../Material/Example|[FILENAME]cbp_irppy2acac
17  er|mCP|0|[PATH]../Material/Example|[FILENAME]mCP
18  er|TAPC|0|[PATH]../Material/Example|[FILENAME]tapc_shb
19  er|MoO3|0|[PATH]../Material/Example|[FILENAME]moo3
20  er|cITO|0|[PATH]../Material/Example|[FILENAME]c-ito
21  er|sITO|0|[PATH]../Material/Example|[FILENAME]sito
22  er|glass|0|[PATH]../Material/Example|[FILENAME]glass
```

property   alias   order   filepath   filename

Execute the material manager system control software


```
william7699@instance-1:~$ cd LegendDesign/src/Execution/
william7699@instance-1:~/LegendDesign/src/Execution$ ls
DOFExtractor.pyc              DeviceFieldCmd.pyc    FarFieldCmd.pyc      PowerDensityCmd.pyc    TextExecute.pyc    rtauCmd.pyc
DOFExtractorExample.pyc       DeviceOpticsCmd.pyc   LazyCmd.py           PurcellFactorCmd.pyc   materialMgrCmd.pyc
DataMatrixAnalyzerScript.pyc  Example               ModeDistributionAnalyzerCmd.pyc  TRACmd.pyc             materialOpticsCmd.pyc
william7699@instance-1:~/LegendDesign/src/Execution$ python3 materialMgrCmd.pyc
********************************    GOODLAB SIMULATOR Info    ********************************
Optical Planar OLED Simulation Tool/Console interface - Mate
Anisotropic Version 1.0
Author : Wei-Kai Lee
Publication Date : 2019/01/04

Copyright(c) 2019 Wei-Kai Lee. All right reserved.

This program is a material manager system supporting add, delete, switch and print,
which including all the things about material properties management.
********************************    GOODLAB SIMULATOR Info    ********************************


>>> Please insert username : user-1
--------------------------------------------------------------------------------
Start running GOODLAB anisotropic simulator ver1.0 Thu Apr 09 07:34:24 2020
--------------------------------------------------------------------------------


Successfully reading materialMgr.mMgr
Now printing the information stored in the material manager...
[A]: er                  /*Empty*/
--------------------------------------------------------------------------------
[A]: Fluorescence        /*Empty*/
--------------------------------------------------------------------------------
[A]: Phosphorescence     /*Empty*/
--------------------------------------------------------------------------------
[A]: DOF                 /*Empty*/
--------------------------------------------------------------------------------
[A]: wavelengthunitstr   [N]nm(#1)
                         [N]um(#1)
                         [N]m(#1)
--------------------------------------------------------------------------------
[A]: Attribute/ [N]: Name(# of data)


<materialMgrCmd>
```

1. Go into the execution file directory

2. Execute the material manager system

3. Type user name

4. Waiting for the command from user

Help function

Use "?" or "help" to list all the command in the material manager system.

```
<materialMgrCmd> ?

Documented commands (type help <topic>):
========================================
addDOFMaterial     deleteDOFMaterial    printDOFInfo     saveMgr
addFluoMaterial    deleteFluoMaterial   printFluoInfo    setdefaultPath
addNKMaterial      deleteNKMaterial     printMgr         switchDOFOrder
changeDOFPath      deletePhosMaterial   printNKInfo      switchNKOrder
changeNKPath       exit                 printPath        switchPhosOrder
changePLPath       help                 printPhosInfo    switcheFluoOrder
changeUser         printAttributes      resetMgr

<materialMgrCmd> Help
*** Unknown syntax: Help
<materialMgrCmd> help

Documented commands (type help <topic>):
========================================
addDOFMaterial     deleteDOFMaterial    printDOFInfo     saveMgr
addFluoMaterial    deleteFluoMaterial   printFluoInfo    setdefaultPath
addNKMaterial      deleteNKMaterial     printMgr         switchDOFOrder
changeDOFPath      deletePhosMaterial   printNKInfo      switchNKOrder
changeNKPath       exit                 printPath        switchPhosOrder
changePLPath       help                 printPhosInfo    switcheFluoOrder
changeUser         printAttributes      resetMgr
```

commands

Material File Path

```
<materialMgrCmd> printPath
NKPath : /home/sim/material n k/
PLPath : /home/sim/material PL/
DOFPath : /home/sim/material eta/
```

Linux user

Execution Files Directory

home — test1 — LegendDesign — src — Execution

sim — material n k

Default material file path

material PL (intrinsic spectrum)

material eta (dipole orientation factors)

Directory Tree
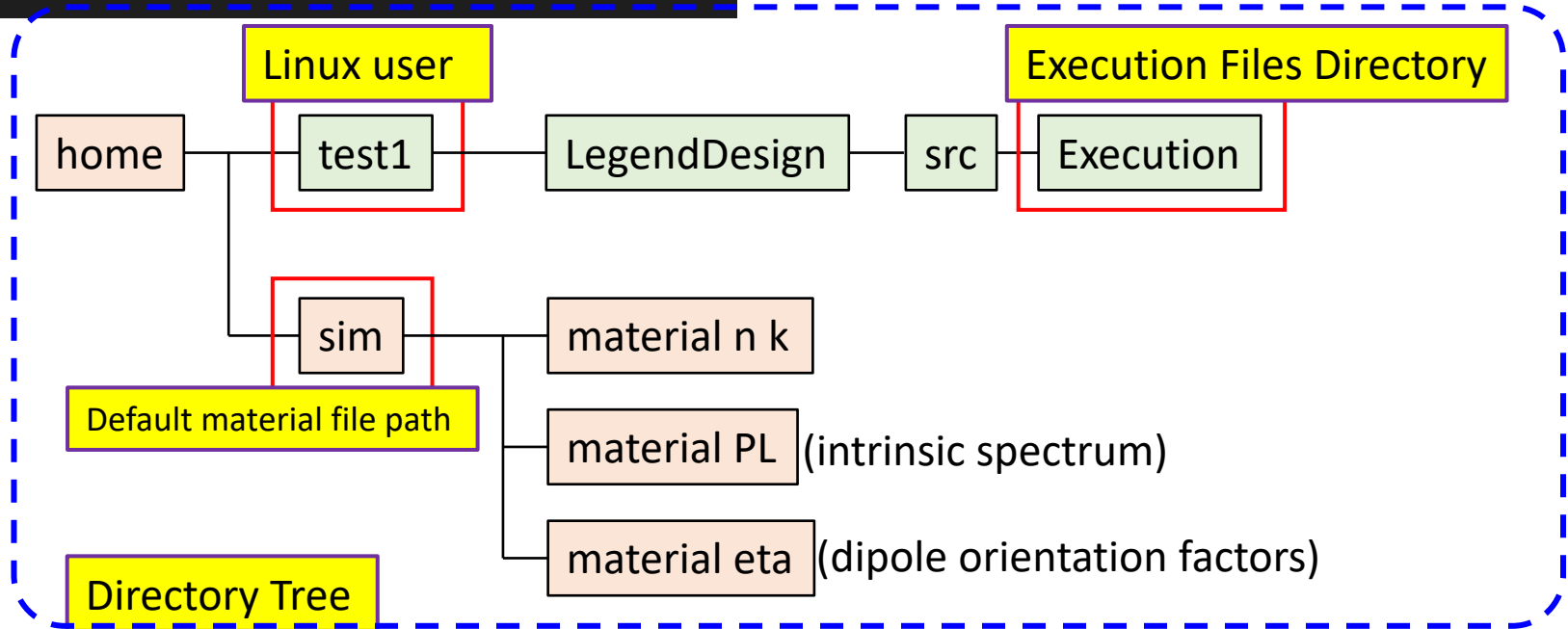
```
<materialMgrCmd> help changeNKPath
Change the NKPath.
[Usage] changeNKPath [path]
```

The reading path can be changed by "changeNKPath", "changePLPath", and "changeDOFPath".

Add new material
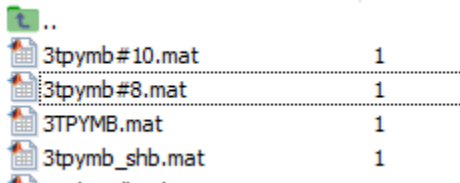
"help + [command name]" to print the function of the specified command.

```
<materialMgrCmd> help printPath
Show the path of material.

<materialMgrCmd> help add NKMaterial
*** No help on add NKMaterial
<materialMgrCmd> help addNKMaterial
Add new nk material into material manager.
[Usage 1] addNKMaterial [Name]
[Usage 2] addNKMaterial [Name] [FileName]

<materialMgrCmd>
```

Add new material


```
<materialMgrCmd> addNKMaterial 3TPYMB 3TPYMB
Now reading nk file (/home/sim/material_n_k/3TPYMB.mat)
<materialMgrCmd> addNKMaterial 3TPYMB 3tpymb#10
Now reading nk file (/home/sim/material_n_k/3tpymb#10.mat)
<materialMgrCmd> addNKMaterial 3TPYMB 3tpymb#8
Now reading nk file (/home/sim/material_n_k/3tpymb#8.mat)
<materialMgrCmd> addNKMaterial 3TPYMB 3tpymb_shb
Now reading nk file (/home/sim/material_n_k/3tpymb_shb.mat)
<materialMgrCmd>
```

Alias   Filename

This 4 nk files are given the same alias. The 1st one in material manager system is "3TPYMB.mat"

Print Mgr

Before add new material into the system.   After

```
Now printing the information stored in the material manager...
[A]: er                  /*Empty*/
-------------------------------------------
[A]: Fluorescence        /*Empty*/
-------------------------------------------
[A]: Phosphorescence     /*Empty*/
-------------------------------------------
[A]: DOF                 /*Empty*/
-------------------------------------------
[A]: wavelengthunitstr   [N]nm(#1)
                         [N]um(#1)
                         [N]m(#1)
-------------------------------------------
[A]: Attribute/ [N]: Name(# of data)
```

```
<materialMgrCmd> printMgr
[A]: er                  [N]3TPYMB(#4)
-------------------------------------------
[A]: Fluorescence
-------------------------------------------
[A]: Phosphorescence
-------------------------------------------
[A]: DOF                 /*Empty*/
-------------------------------------------
[A]: wavelengthunitstr   [N]nm(#1)
                         [N]um(#1)
                         [N]m(#1)
-------------------------------------------
[A]: Attribute/ [N]: Name(# of data)
<materialMgrCmd>
```

There 4 data in 3TPYMB.

Print Info

```
>>> help printNKInfo

Print the information of material nk.
[Usage 1] printNKInfo [Name]
[Usage 2] printNKInfo [Name] [Index]

>>> printNKInfo 3TPYMB
TYPE: ISOTROPIC
In Note :
   PATH:/home/sim/material n k/
   FILENAME:3TPYMB
-----------------------------------------
   Wavelength(nm)        Re(e)        Im(e)
         350.00000     3.26903      0.00000
         360.00000     3.20824      0.00000
         370.00000     3.15506      0.00000
         380.00000     3.10830      0.00000
         390.00000     3.06699      0.00000
         400.00000     3.03035      0.00000
         410.00000     2.99772      0.00000
         420.00000     2.96855      0.00000
         430.00000     2.94238      0.00000
         440.00000     2.91882      0.00000
         450.00000     2.89755      0.00000
         460.00000     2.87828      0.00000
         470.00000     2.86079      0.00000
         480.00000     2.84485      0.00000
         490.00000     2.83030      0.00000
         500.00000     2.81699      0.00000
         510.00000     2.80478      0.00000
         520.00000     2.79355      0.00000
```

Print the 1st data in 3TPYMB

```
>>> printNKInfo 3TPYMB 1

TYPE: ISOTROPIC
In Note :
   PATH:/home/sim/material n k/
   FILENAME:3TPYMB
-----------------------------------------
   Wavelength(nm)        Re(e)        Im(e)
         350.00000     3.26903      0.00000
         360.00000     3.20824      0.00000
         370.00000     3.15506      0.00000
         380.00000     3.10830      0.00000
         390.00000     3.06699      0.00000
         400.00000     3.03035      0.00000
         410.00000     2.99772      0.00000
         420.00000     2.96855      0.00000
         430.00000     2.94238      0.00000
         440.00000     2.91882      0.00000
         450.00000     2.89755      0.00000
         460.00000     2.87828      0.00000
         470.00000     2.86079      0.00000
         480.00000     2.84485      0.00000
         490.00000     2.83030      0.00000
         500.00000     2.81699      0.00000
         510.00000     2.80478      0.00000
         520.00000     2.79355      0.00000
         530.00000     2.78321      0.00000
         540.00000     2.77366      0.00000
         550.00000     2.76483      0.00000
         560.00000     2.75665      0.00000
```

Print Info


```
>>> printNKInfo 3TPYMB 2

TYPE: ISOTROPIC
In Note :
   PATH:/home/sim/material n k/
   FILENAME:3tpymb#10
-------------------------------------------
   Wavelength(nm)        Re(e)      Im(e)
        350.00000      3.36463    0.00000
        360.00000      3.29294    0.00000
        370.00000      3.23019    0.00000
        380.00000      3.17498    0.00000
        390.00000      3.12619    0.00000
        400.00000      3.08288    0.00000
        410.00000      3.04427    0.00000
        420.00000      3.00973    0.00000
        430.00000      2.97871    0.00000
        440.00000      2.95076    0.00000
        450.00000      2.92550    0.00000
        460.00000      2.90260    0.00000
        470.00000      2.88178    0.00000
        480.00000      2.86280    0.00000
        490.00000      2.84545    0.00000
        500.00000      2.82955    0.00000
        510.00000      2.81496    0.00000
        520.00000      2.80152    0.00000
        530.00000      2.78913    0.00000
        540.00000      2.77768    0.00000
        550.00000      2.76708    0.00000
```
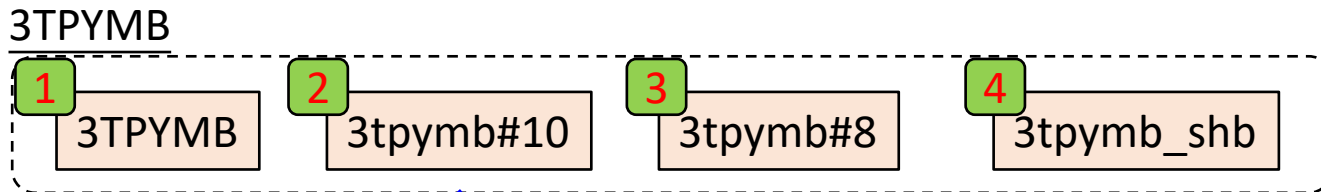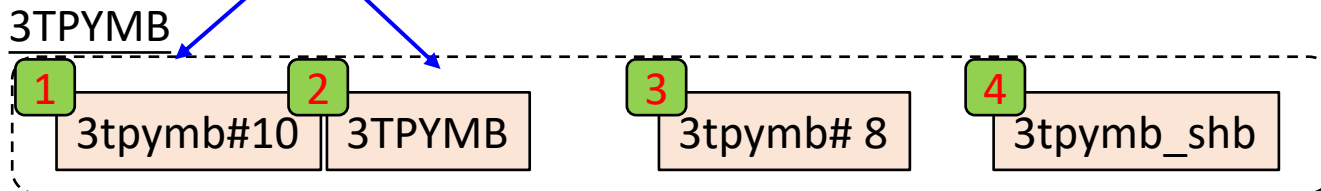
Print the 2nd data in 3TPYMB

Switch Order

```
>>> help switchNKOrder

Switch the order of nk material data.
[Usage 1] switchNKOrder [Name] [n2] (switch with n1=1)
[Usage 2] switchNKOrder [Name] [n1] [n2]

>>> switchNKOrder 3TPYMB 1 2
```

Before

3TPYMB

| 1 3TPYMB | 2 3tpymb#10 | 3 3tpymb#8 | 4 3tpymb_shb |

After

3TPYMB

| 1 3tpymb#10 | 2 3TPYMB | 3 3tpymb# 8 | 4 3tpymb_shb |

Switch Order

Before

After

21

Path/Add/Switch


```
 cumented commands (type help <topi
 ====================================
addDOFMaterial      deleteDOFMaterial     printDOFInfo    saveMgr
addFluoMaterial     deleteFluoMaterial    printFluoInfo   setdefaultPath
addNKMaterial       deleteNKMaterial      printMgr        switchDOFOrder
changeDOFPath       deletePhosMaterial    printNKInfo     switchNKOrder
changeNKPath        exit                  printPath       switchPhosOrder
changePLPath        help                  printPhosInfo   switcheFluoOrder
changeUser          printAttributes       resetMgr
```

add

print

change path

switch order

Reset Material Manager System

Save Material Manager System

```
>>> help saveMgr

Save the information.
>>> saveMgr
```

Save the material manager system in the user's setting directory.

Exit the material manager system

Exit the material manager system.
*** The material manager system would be automatically saved into the user's setting directory.

```
>>> exit
-------------------------------------------------------------------------------
End running GOODLAB anisotropic simulator ver1.0 Thu Apr 09 13:38:57 2020
Elapsed time : 0 day(s)/ 0 hr(s)/ 0 min(s)/ 0.01470637321472168 sec(s)
-------------------------------------------------------------------------------


william7699@instance-1:~/LegendDesign/src/Execution$
```

Command Structure File

One can type the command lists in a file. The file can be executed by the execution file.

```
materialMgrCmd-Example-1.txt ☒
 1  ?
 2  resetMgr
 3  help
 4  printPath
 5  help printNKPath
 6  help printPath
 7  help addNKMaterial
 8  addNKMaterial 3TPYMB 3TPYMB
 9  addNKMaterial 3TPYMB 3tpymb#10
10  addNKMaterial 3TPYMB 3tpymb#8
11  addNKMaterial 3TPYMB 3tpymb_shb
12  printMgr
13  help printNKInfo
14  printNKInfo 3TPYMB
15  printNKInfo 3TPYMB 1
16  printNKInfo 3TPYMB 2
17  printNKInfo 3TPYMB 3
18
19
20  help switchNKOrder
21  switchNKOrder 3TPYMB 1 2
22  printNKInfo 3TPYMB 1
23  printNKInfo 3TPYMB 2
24  help resetMgr
25  resetMgr
26  help printMgr
27  printMgr
28  help saveMgr
29  saveMgr
30  exit
```

Execution file

Command file

```
william7699@instance-1:~/LegendDesign/src/Execution$ python3 materialMgrCmd.pyc ./Example/materialMgrCmd-Example-1.txt
```