Internal Light Source-Field Distribution

-DeviceFieldCmd.pyc

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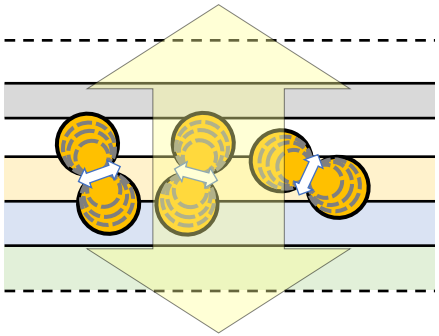
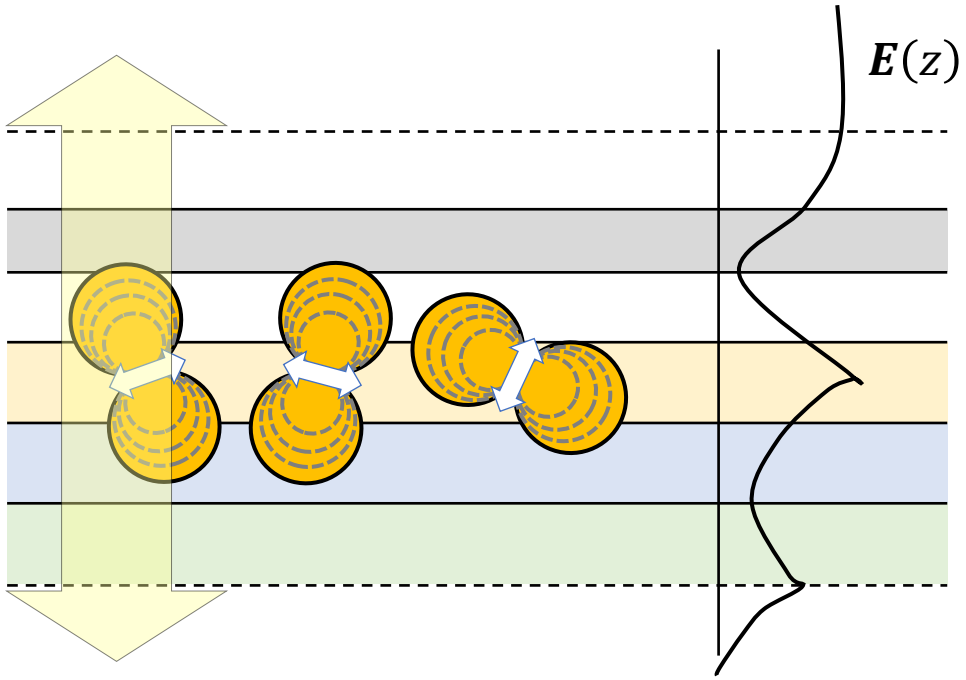
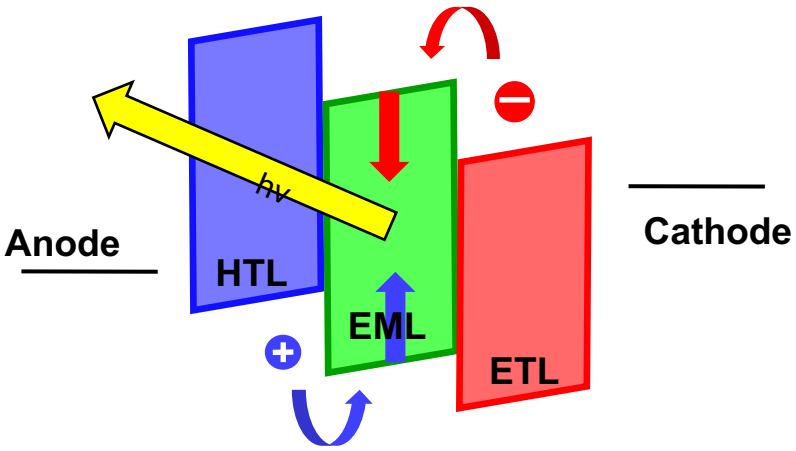


Objective

- This function is to calculate the ensemble average of the field distribution along z-axis.

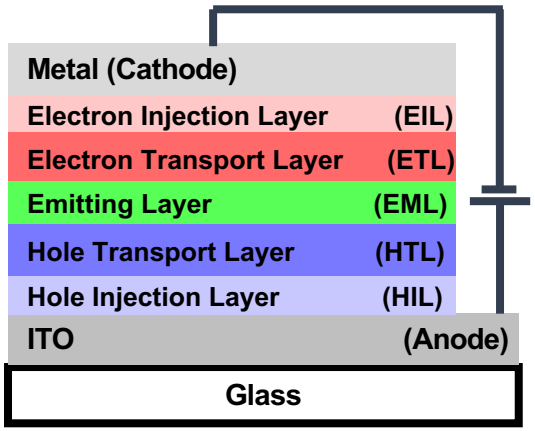


Organic Light Emitting Diodes (OLEDs)



Under forward bias

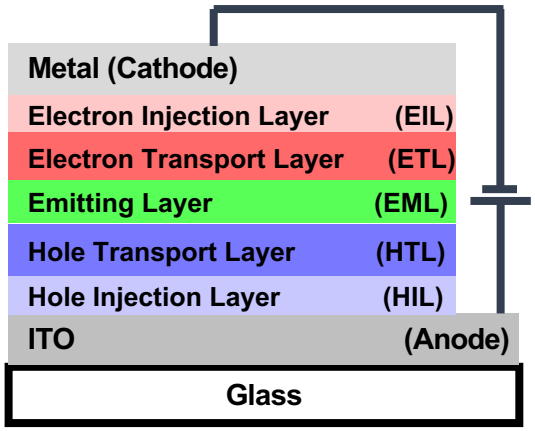
- Charge injection
- Charge transport
- Exciton formation
- Light emission



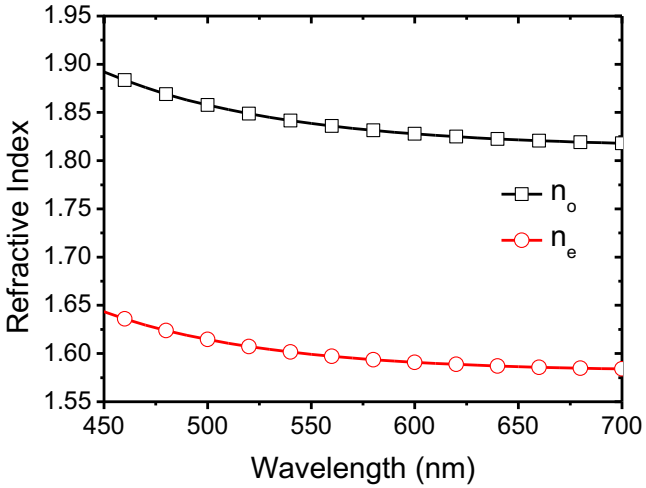
The advantage of OLEDs

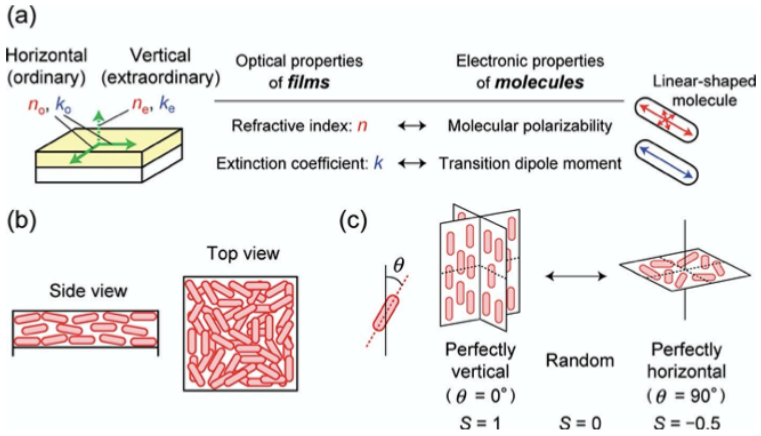
- R,G,B available
- High brightness, low voltage, high efficiency
- Fast response, wide viewing angle
- High Contrast
- Lightweight
- Display, lighting, other applications

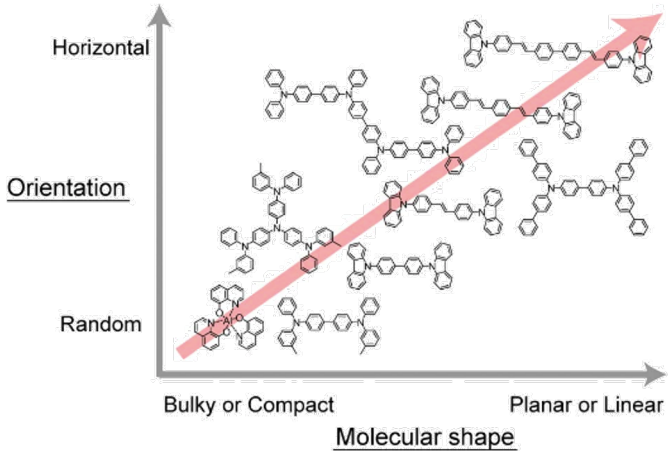
Uniaxial Refraction Index



Uniaxial refractive index

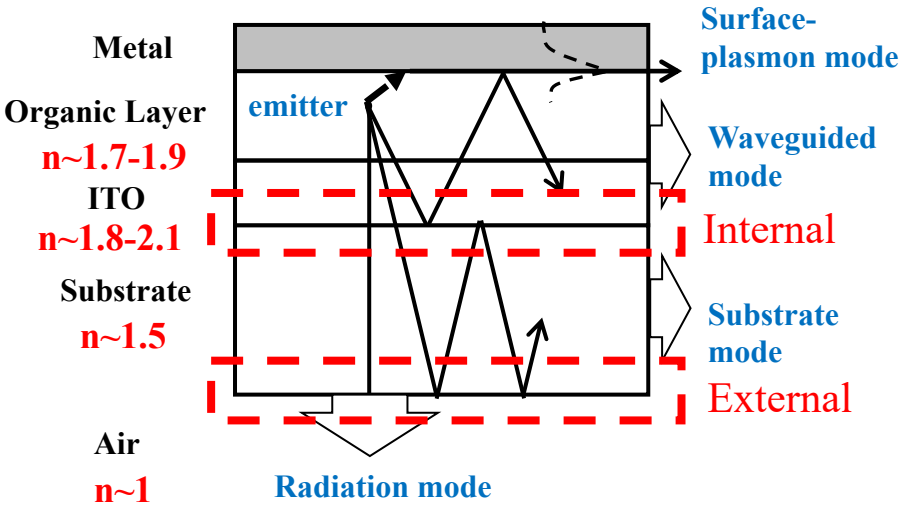


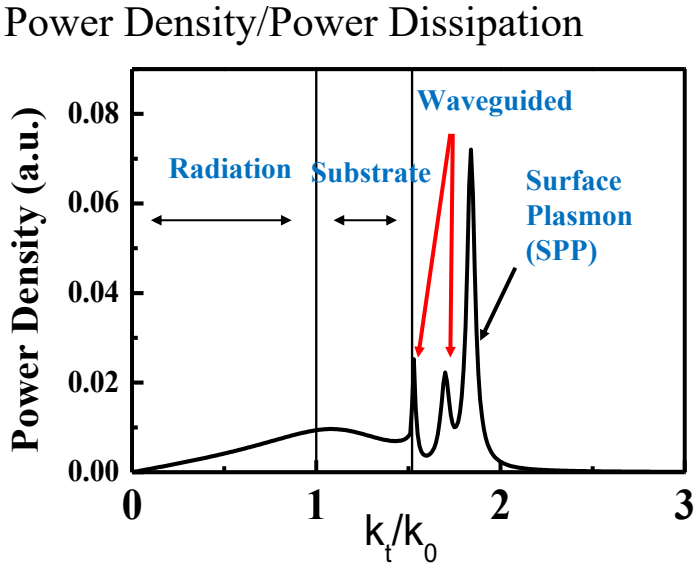




Ref. D. Yokoyama, *J. Mater. Chem.*, 2011, **21**, 19187

Outcoupling Issue





Rigorous EM wave model

$$\eta_{EQE} = \gamma \times \eta_{exc.} \times \eta_{out}(\Theta, \Gamma) = \eta_{int.} \times \eta_{out}(\Theta, \Gamma)$$

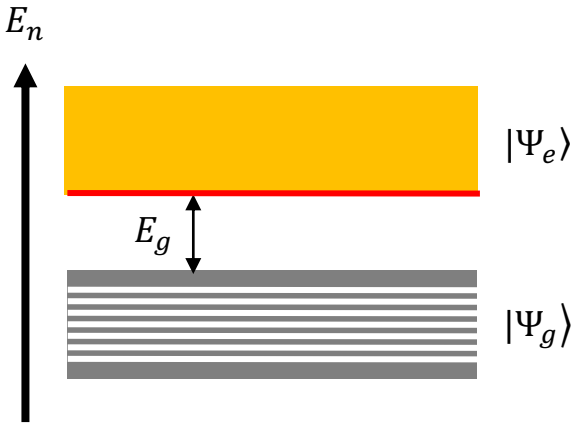
- Due to index mismatches of OLED layers, out-coupling efficiency is **20%~30%** for a typical bottom-emitting OLED.
- Nearly **100%** internal quantum efficiency nowadays.
- Making use of **not out-coupled internal radiation** is a current issue.

Optics in OLED

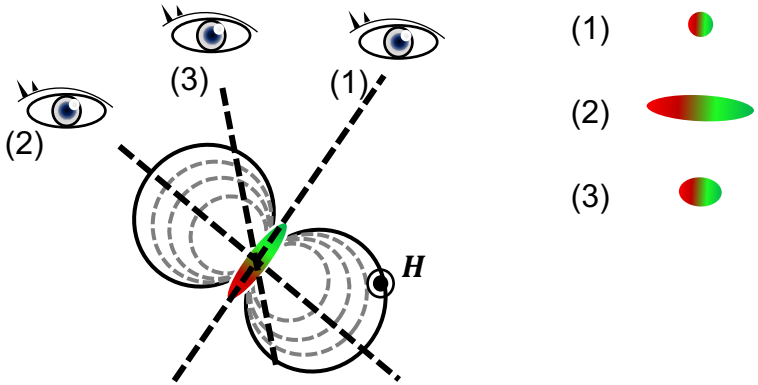
- **Transition Dipole Moment (TDM)**
  ↔Classical Electromagnetic Oscillating Dipole

$$\boldsymbol{d}(\omega) = \langle \Psi_e | q\boldsymbol{r} | \Psi_g \rangle \langle \Phi_e | \Phi_g \rangle$$

$$R_t = \frac{\pi}{\hbar^2} \rho(\omega) |\boldsymbol{d}(\omega) \cdot \boldsymbol{E}(\boldsymbol{k})|^2$$



- **Classical Radiation Pattern in Homogeneous Material**



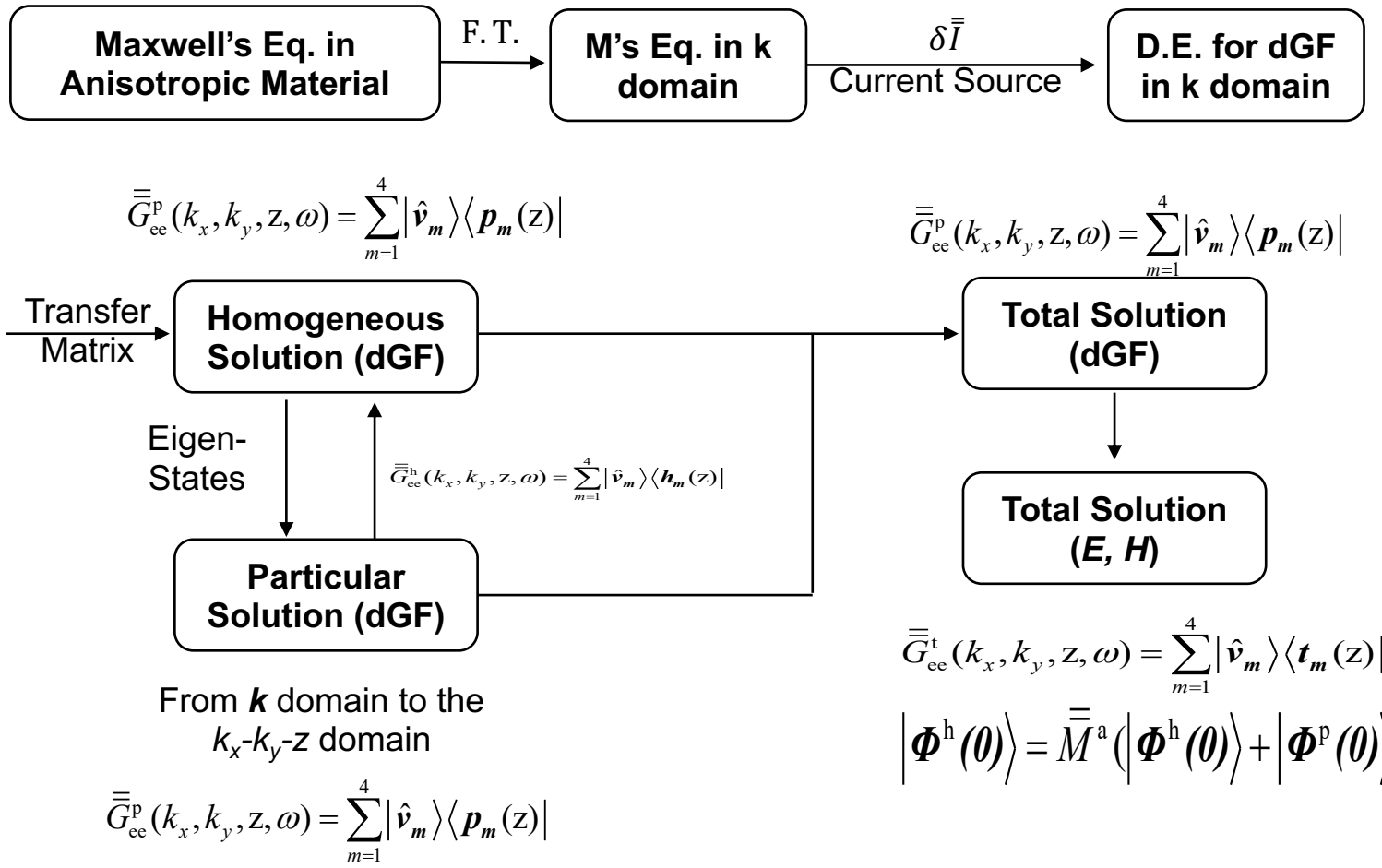
1, Special Relativity

2. Ampere's Right Hand Rule

→ Hertizan Dipole

$$I_{Hertzian}(\Omega) = \frac{3}{8\pi} \sin^2\theta$$

Solve Procedure-1



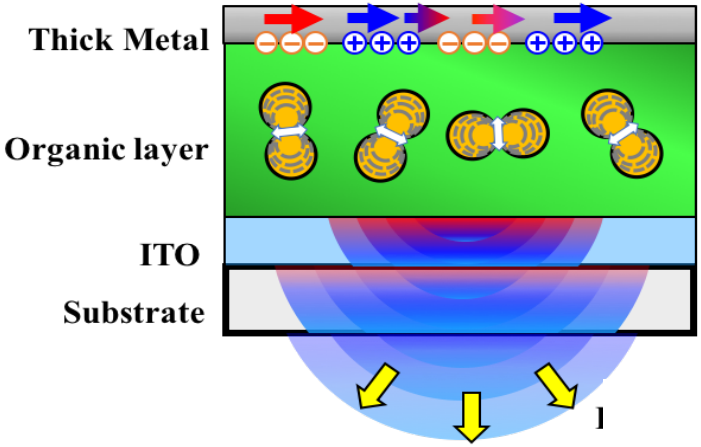
Dipole Orientation Distribution

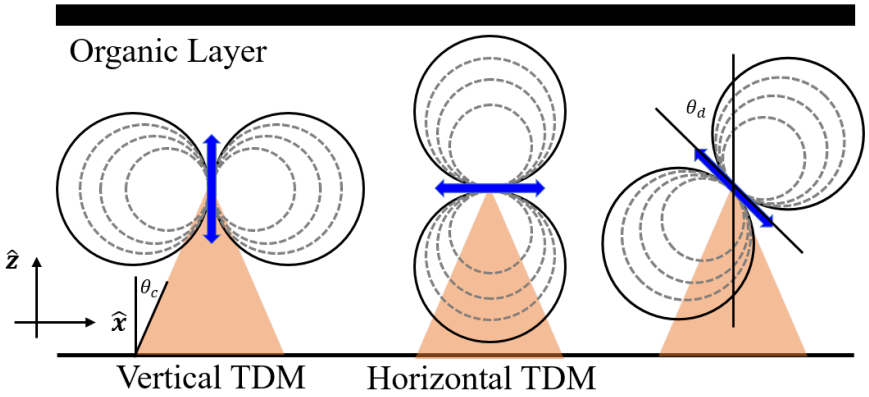
對於一般的有機發光體來說，不同分子的發光偶極矩的振盪方向可能並不相同，為了要能模擬這種現象，在此我們引入了dipole orientation distribution function來模擬這種情形。

$$< P_z(k_x,k_y,z,\omega) >=< \left\langle \boldsymbol{J}(k_x,k_y,z,\omega;\boldsymbol{\alpha}) \middle| \bar{\bar{P}}_z(k_x,k_y,z,\omega) \middle| \boldsymbol{J}(k_x,k_y,z,\omega;\boldsymbol{\alpha}) \right\rangle >$$

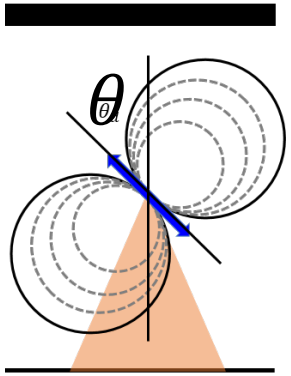
$$< P_z >= \sum_{i,j=x,y,z} \bar{\bar{P}}_{z,ij} < J_i^*(\boldsymbol{\alpha}) J_j(\boldsymbol{\alpha}) >$$

α : random variables about emitting dipoles
e.x. orientation, phase





Dipole Orientation Distribution



$$\begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} = -i\omega d \begin{bmatrix} e^{i\alpha_x} \sin\theta\cos\phi \\ e^{i\alpha_y} \sin\theta\sin\phi \\ e^{i\alpha_z} \cos\theta \end{bmatrix}$$

$$<J^2> = <J^* J> \equiv <J_x^* J_x + J_y^* J_y + J_z^* J_z> = <\omega^2 d^2>$$

Dipole Orientation Factor

$$\eta_1 = <\frac{1}{2}(1-\cos^2\theta)> = <\frac{1}{2}\sin^2\theta>$$

$$\eta_2 = <\frac{1}{2}\sin^2\theta(\cos^2\phi - \sin^2\phi)>$$

$$\eta_3 = <\sin^2\theta\cos\phi\sin\phi>$$

$$\eta_4 = <\cos\theta\sin\theta\cos\phi>$$

$$\eta_5 = <\cos\theta\sin\theta\sin\phi>$$

$$<J_x^* J_x> = (\eta_1+\eta_2)<J^2>$$

$$<J_y^* J_y> = (\eta_1-\eta_2)<J^2>$$

$$<J_z^* J_z> = (1-2\eta_1)<J^2>$$

$$<J_x^* J_y> = \eta_3 <e^{i(\alpha_y-\alpha_x)}><J^2>$$

$$<J_x^* J_z> = \eta_4 <e^{i(\alpha_z-\alpha_x)}><J^2>$$

$$<J_y^* J_z> = \eta_5 <e^{i(\alpha_z-\alpha_y)}><J^2>$$

How to execute the calculator

python: windows
python3: mac, linux

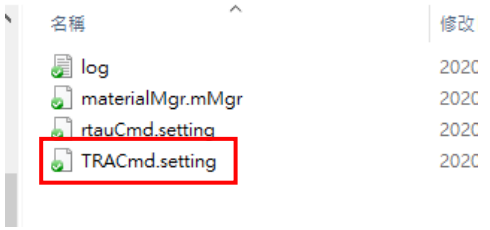
```
>python DeviceFeildCmd.pyc
```

Execution file

```
>>> Please insert username : user-1
```

Type user name

```
TRA Setting is not built in ../../SETTING/user-1
Now saving the default TRA setting.
```



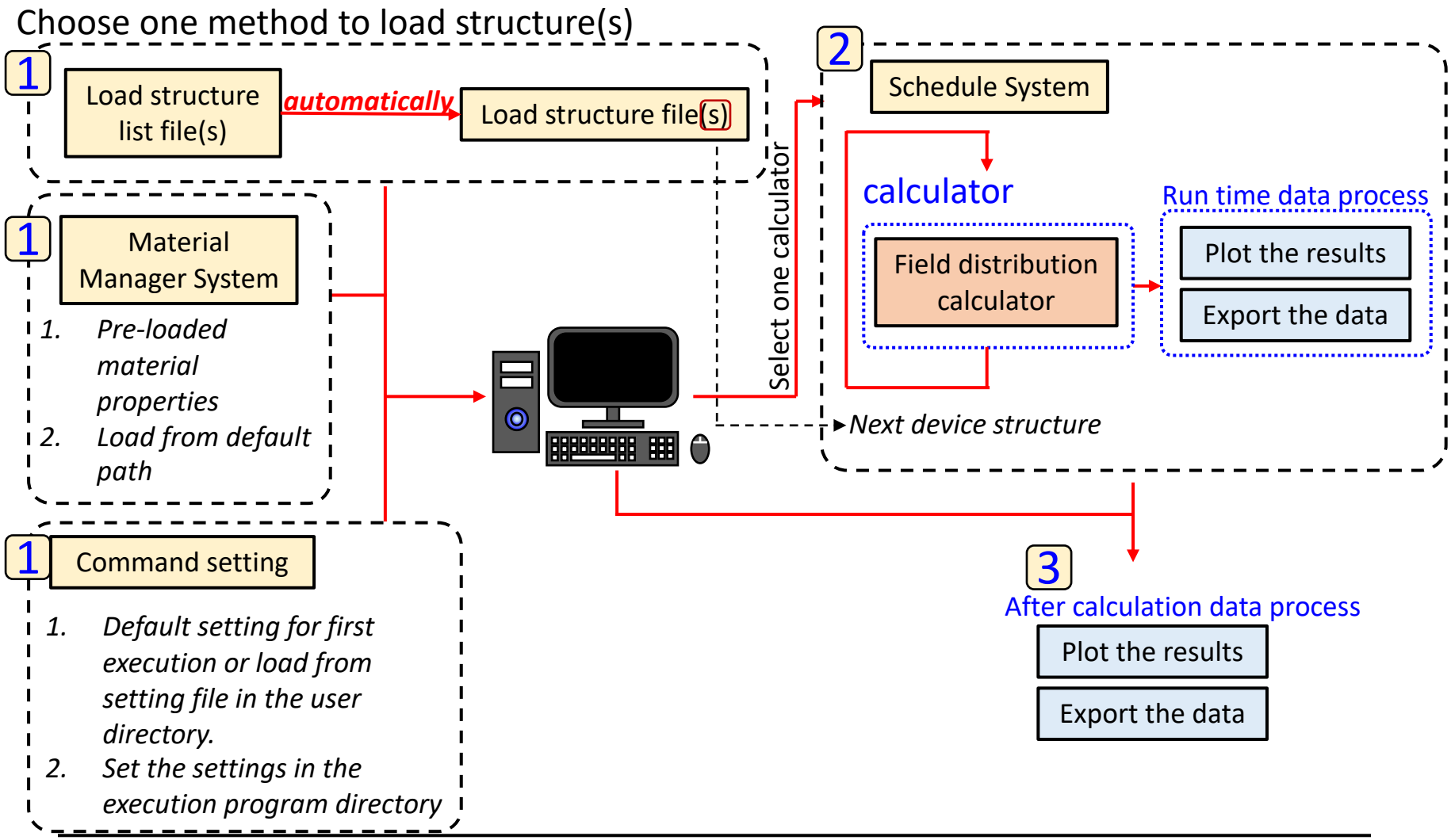
Help

```
>>> ?

User Control Command
========================================
1. Settting Command:
changeUser              exit

Material Manager Command
========================================
1. Settting Command:
printMgr                saveMgr

Structure/Structure List Command
========================================
1. Structure List Command:
ReadStructListPath      ReadStructListName
SaveStructListPath      SaveStructListName
readStructList          saveStructList

2. Structure Command:
ReadStructPath          ReadStructName
SaveFilePath            SaveFileName
readStruct              deleteStruct

3. Print Information Command:
printStructInfo         printStructSettingInfo
printListInfo

4. Result Command:
ResultFilePath          ResultFileName
deleteResult
save_run_time_result_Bool
resetSN
```

Help

```
Device Field Command (Calculate the electric/magnetic field in the deice.)
=======================================
1. Settting Command:
SettingFilePath      SettingFileName
setDefaultSetting    printDFInfo
loadDFSETTING        saveDFSETTING

2. Command in kxky domain:
kxko                 kyko                z                    ----Parameter
runDFz_kxky          plotDFzvskxky

3. Command in k polar domain:
ktko                 Thetakt             z                    ----Parameter
runDFz_PolarInK      plotDFzvskPolar

4. Write Bool:
write_EBool          write_HBool
write_TotalFieldBool
write_ForwardFieldBool write_BackwardFieldBool
write_M1M3FieldBool  write_M2M4FieldBool
write_M1FieldBool    write_M2FieldBool
write_M3FieldBool    write_M4FieldBool

5. Plot Bool:
changefigshowBool
plot_EBool           plot_HBool
plot_TotalFieldBool
plot_ForwardFieldBool plot_BackwardFieldBool
plot_M1M3FieldBool   plot_M2M4FieldBool
plot_M1FieldBool     plot_M2FieldBool
plot_M3FieldBool     plot_M4FieldBool

5. Run Time Bool:
runtime_plot
```

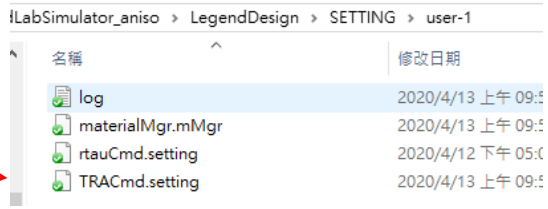
Calculating Workflow



Default Setting

Print setting

```
>>> printDFInfo

Setting file path : ../../SETTING/user-1
Setting file name : DFCmd.setting
kt/ko : 0.00000:0.10000:1.00000
Theta in kt/ko domain : 0.00000:10.00000:360.00000
kx/ko : -1.00000:0.10000:1.00000
ky/ko : -1.00000:0.10000:1.00000
z(nm) : -50.00000:1.00000:50.00000
Save Run Time Result  : True
Run Time Plot         : False

Plot Mode Bool:
     True_E               : True
     True_H               : True
     Total (M1+M2+M3+M4)  : True
     +z    (M1+M2)        : False
     -z    (M3+M4)        : False
     M1                   : False
     M2                   : False
     M3                   : False
     M4                   : False
Write Mode Bool:
     True_E               : True
     True_H               : True
     Total (M1+M2+M3+M4)  : True
     +z    (M1+M2)        : True
     -z    (M3+M4)        : True
     M1                   : True
     M2                   : True
     M3                   : True
     M4                   : True
Figure Show Bool : True
```



All the setting would **automatically** saved into the setting file when the program **finished**. The user can set the setting at first or share the setting files with others.

Setting

```
kt/ko : 0.00000:0.10000:1.00000
Theta in kt/ko domain : 0.00000:10.00000:360.00000
```

kt/ko and θ_{kt}setting method

```
<DFCmd> help ktko
Set the kt/ko. (Empty for delete setting)
[Usage] ktko [ktko] - single value, start:spacing:end, (v1,v2,v3,v4)

<DFCmd> help Thetakt
Set the polar angle in kx ky domain.
[Usage] Thetakt [theta] - single value, start:spacing:end, (v1,v2,v3,v4)
```

```
kx/ko : -1.00000:0.10000:1.00000
ky/ko : -1.00000:0.10000:1.00000
```

kx/ko and ky/ko setting method

```
<DFCmd> help kxko
Set the kx/ko. (Empty for delete setting)
[Usage] kxko [kxko] - single value, start:spacing:end, (v1,v2,v3,v4)

<DFCmd> help kyko
Set the ky/ko. (Empty for delete setting)
[Usage] kyko [kyko] - single value, start:spacing:end, (v1,v2,v3,v4)
```

Setting

```
z(nm) : -50.00000:1.00000:50.00000
```

z setting method

```
<DFCmd> help z
Set the simulation position z. (Empty for delete setting)
[Usage] z [z] - single value, start:spacing:end, (v1,v2,v3,v4)
```

Run-Time Setting

```
Save Run Time Result   : True
```

Whether to save the data in the memory after the calculation. If the user would like to execute plot or other data manipulation commands, the save-run-time-result bool should be “True”. However, the user should notice the memory usage when scanning a lot of parameters.

```
Run Time Plot          : False
```

Whether to plot the results when calculation.

Setting

```
Plot Mode Bool:
     True_E                 : True
     True_H                 : True
     Total (M1+M2+M3+M4)    : True
     +z    (M1+M2)          : False
     -z    (M3+M4)          : False
     M1                     : False
     M2                     : False
     M3                     : False
     M4                     : False
```

Check whether the corresponding mode would be plot or not.

```
Write Mode Bool:
     True_E                 : True
     True_H                 : True
     Total (M1+M2+M3+M4)    : True
     +z    (M1+M2)          : True
     -z    (M3+M4)          : True
     M1                     : True
     M2                     : True
     M3                     : True
     M4                     : True
```

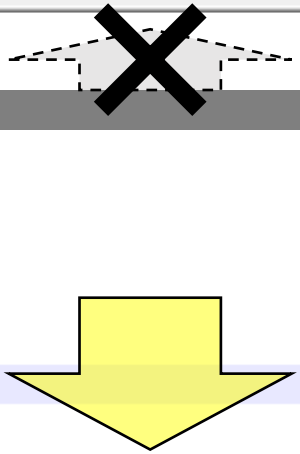
Check whether the corresponding mode would be written into a txt file or not.

Calculate Device Distribution

Bottom-emitting OLED

sfile-1.txt

	MATERIAL	THICKNESS(nm)
1		
2	air	X
3	Al	120.000000
4	LiF	1.000000
5	B3PYMPM	50
6	CBP	20.000000
7	TAPC	50
8	cito	80
9	glass	X
10		
11		
12		
13		
14	wavelength(nm) : 480.0:10.0:600.0	
15	EML :	
16	Layerno	: 5
17	Position(nm)	: 10.000000
18	ratio	: 1.000000
19	QY	: 1.000000
20	Fluorescence	: cbp_irppy2acac
21	DOF	: cbp_irppy2acac
22		



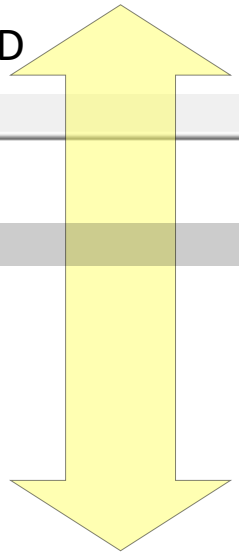
Thick metal

structureList-DFzCmd.txt

Name	readfilename	readfilepath	savefilename	
#Ts1	sfile-1.txt	./Example/structure/Transparent	sfile-1	../../Examp

Calculate Device Distribution

Transparent/ Double-emitting OLED



sfile-1.txt

	MATERIAL	THICKNESS(nm)	
1			
2	air	X	
3	Al	10:5:20	Thin metal
4	LiF	1.000000	
5	B3PYMPM	50	
6	CBP	20.000000	
7	TAPC	20	
8	cito	50	
9	glass	X	
10			
11			
12			
13	wavelength(nm) : 450:10:650.0		
14	EML :		
15	Layerno	: 5	
16	Position(nm)	: 10.000000	
17	ratio	: 1.000000	
18	QY	: 1.000000	
19	Fluorescence	: cbp_irppy2acac	
20	DOF	: cbp_irppy2acac	

sfile-1.txt | structureList-DFzCmd.txt | structureList-DFzCmd.txt

	Name	readfilename	readfilepath	savefilename	
1					
2	#Cs1	sfile-1.txt	./Example/structure/Convention	sfile-1	../../Example/DFzC

Calculate Device Distribution

Bottom-emitting OLED

```
>>> changefigshowBool F

>>> save_run_time_result_Bool F

>>> ReadStructListPath  ./Example/structure/Convention

>>> ReadStructListName  structureList-DFzCmd.txt

>>> readStructList

Now reading structure list file ./Example/structure/Convention\structureList-DFzCmd.txt
  No./Name       filename       savefilename  CommandID  Check                  readfilepath
-------------------------------------------------------------------------------------------------------------------------
      #Cs1    sfile-1.txt            sfile-1       0.0      X  ./Example/structure/Convention  ../../Example/DFzCmd-1/Conv

Structure file reading...
-------------------------------------------------------------------------------------------
Now reading structure file ./Example/structure/Convention\sfile-1.txt
```

Transparent/ Double-emitting OLED

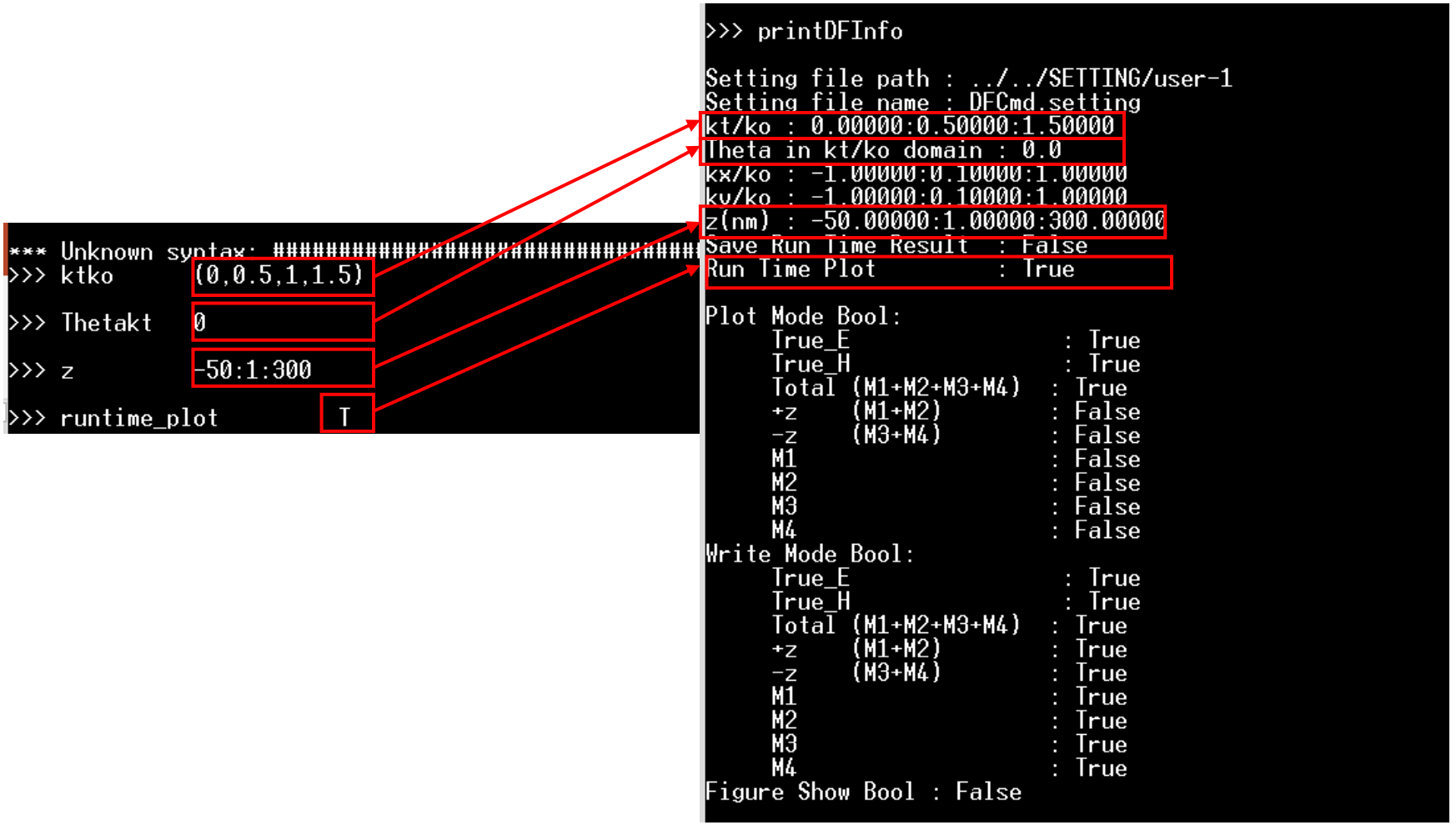
```
>>> ReadStructListPath  ./Example/structure/Transparent

>>> ReadStructListName  structureList-DFzCmd.txt

>>> readStructList

Now reading structure list file ./Example/structure/Transparent\structureList-DFzCmd.txt
  No./Name       filename       savefilename  CommandID  Check                  readfilepath
-------------------------------------------------------------------------------------------------------------------------
      #Ts1    sfile-1.txt            sfile-1       0.0      X  ./Example/structure/Transparent  ../../Example/DFzCmd-1/Transp

Structure file reading...
-------------------------------------------------------------------------------------------
Now reading structure file ./Example/structure/Transparent\sfile-1.txt
```

Calculate Device Distribution

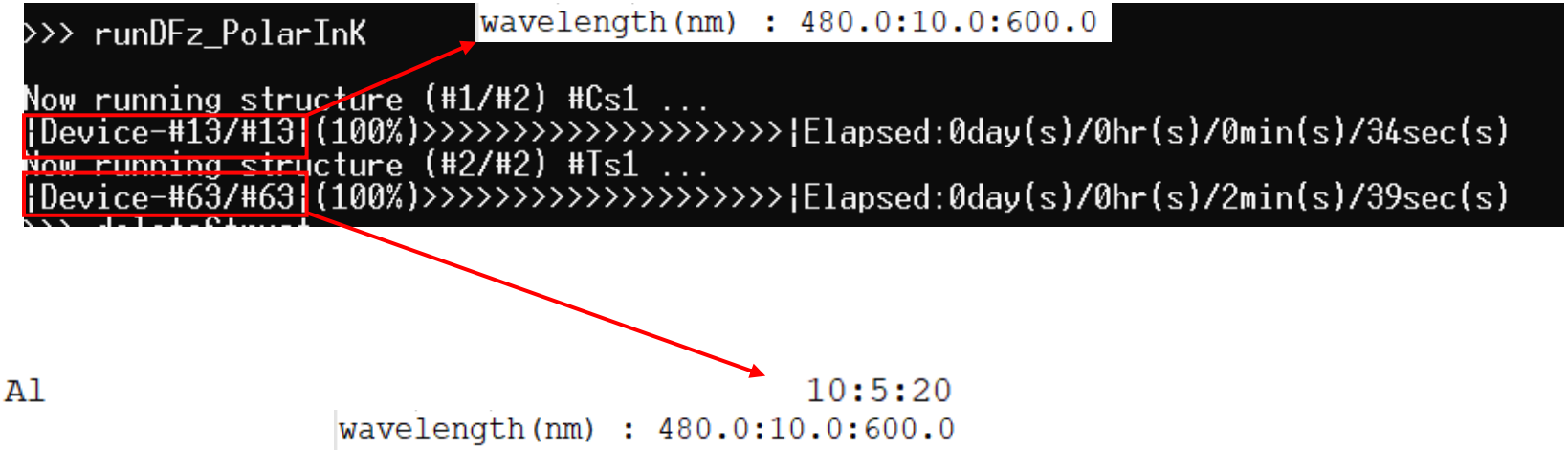
```
>>> printStructInfo

****************************************
Name: #Cs1
[#]   Material             Thickness(nm)
----------------------------------------
[1]   air                  X
[2]   Al                   120.0
[3]   LiF                  1.0
[4]   B3PYMPM              50.0
[5]   CBP                  20.0
[6]   TAPC                 50.0
[7]   cito                 80.0
[8]   glass                X

wavelength(nm) : 480.00000:10.00000:600.00000

EML   Fluorescence    DOF            Position(nm)    PLQY           Ratio
-------------------------------------------------------------------------------------------
[5]   cbp_irppy2acac  cbp_irppy2acac  10.0            1.0            1.0
Device number : 1
```

```
****************************************
Name: #Ts1
[#]   Material             Thickness(nm)
----------------------------------------
[1]   air                  X
[2]   Al                   10.00000:5.00000:20.00000
[3]   LiF                  1.0
[4]   B3PYMPM              50.0
[5]   CBP                  20.0
[6]   TAPC                 20.0
[7]   cito                 50.0
[8]   glass                X

wavelength(nm) : 450.00000:10.00000:650.00000

EML   Fluorescence    DOF            Position(nm)    PLQY           Ratio
-------------------------------------------------------------------------------------------
[5]   cbp_irppy2acac  cbp_irppy2acac  10.0            1.0            1.0
Device number : 3


>>> ########################################
```

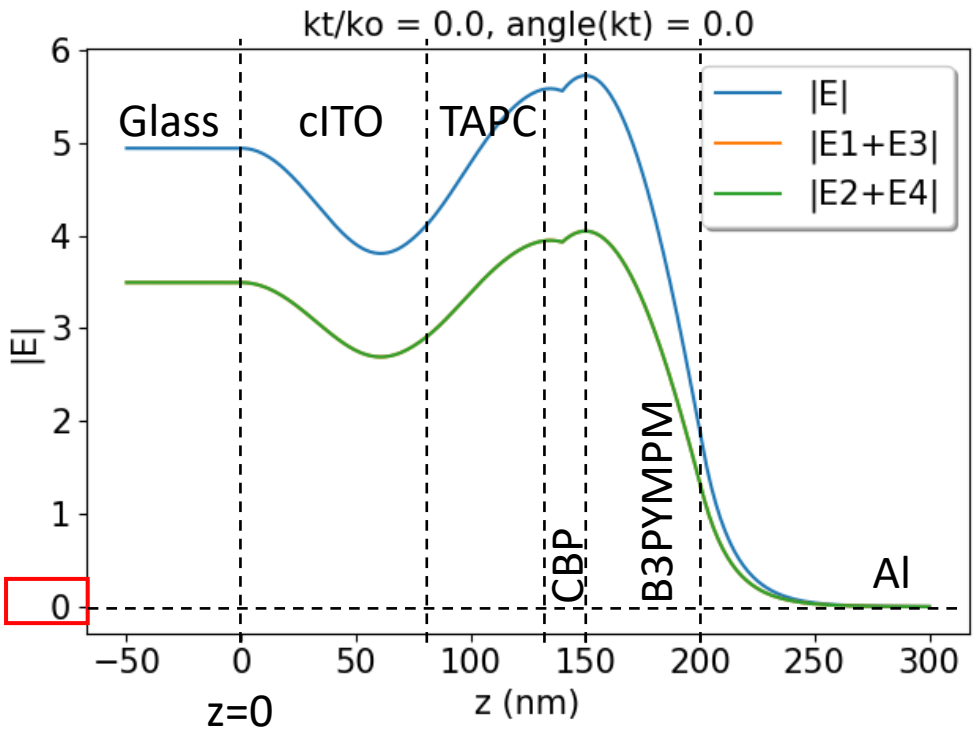
Calculate Device Distribution



Calculate Device Distribution



Data



Normal direction
TE=TM

TE
TM

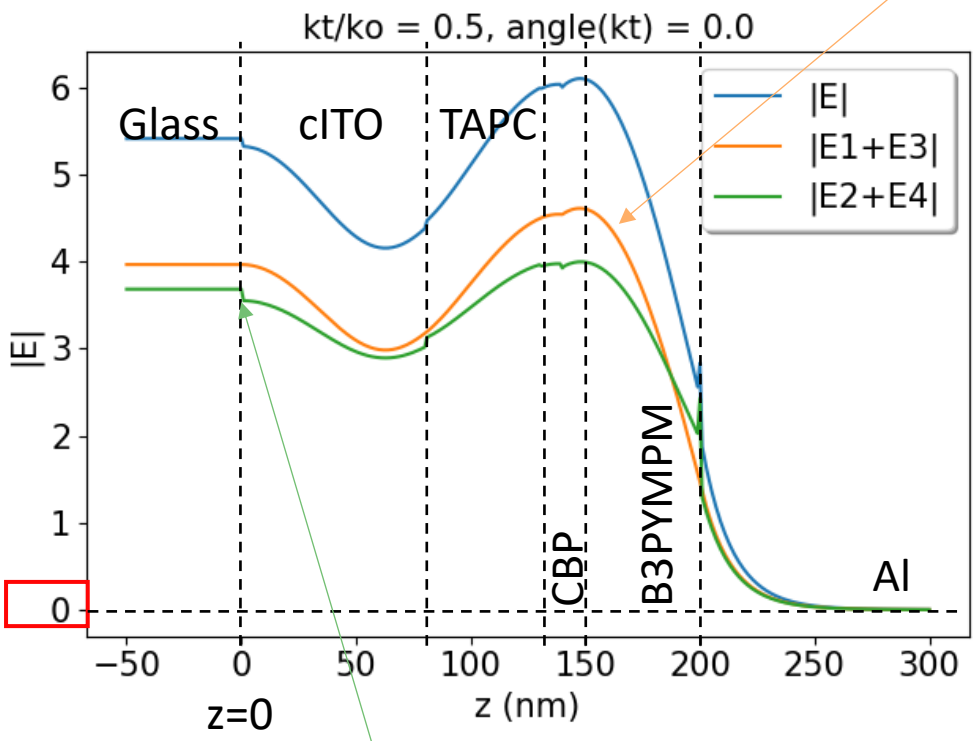
MATERIAL	THICKNESS(nm)
air	X
Al	120.000000
LiF	1.000000
B3PYMPM	50
CBP	20.000000
TAPC	50
cito	80
glass	X

z

z=0

Data

The electric field of TE mode is continuous on the interface.



TE

TM

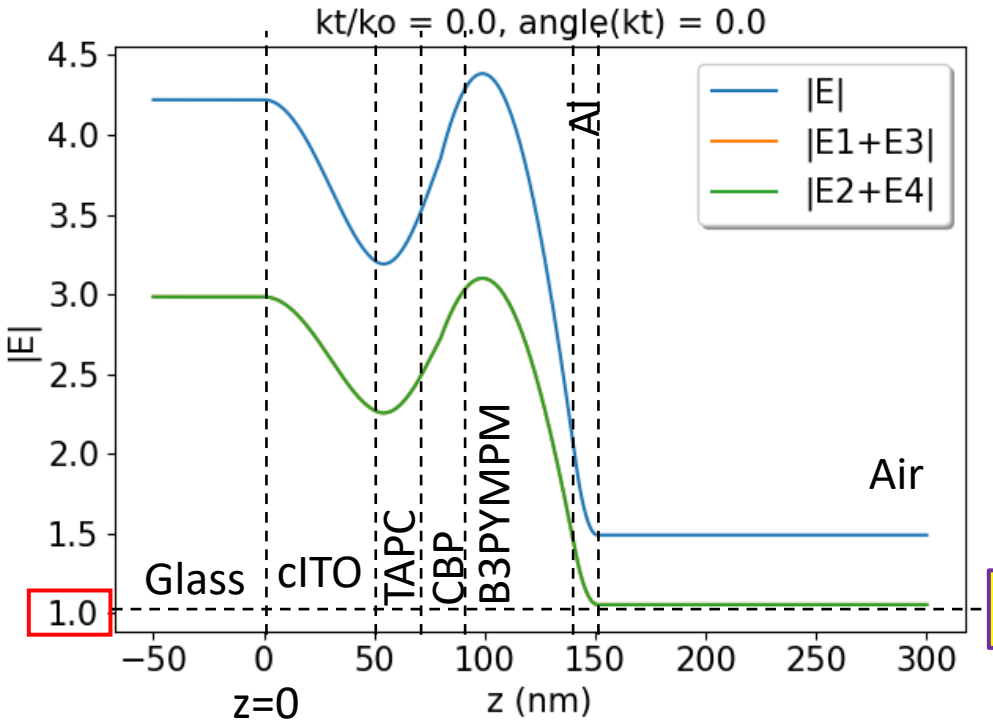
MATERIAL	THICKNESS(nm)
air	X
Al	120.000000
LiF	1.000000
B3PYMPM	50
CBP	20.000000
TAPC	50
cito	80
glass	X

z

z=0

The electric field of TM mode is discontinuous on the interface.

Data



Normal direction
TE=TM

TE
TM

MATERIAL	THICKNESS(nm)
air	X
Al	10
LiF	1.000000
B3PYMPM	50
CBP	20.000000
TAPC	20
cito	50
glass	X

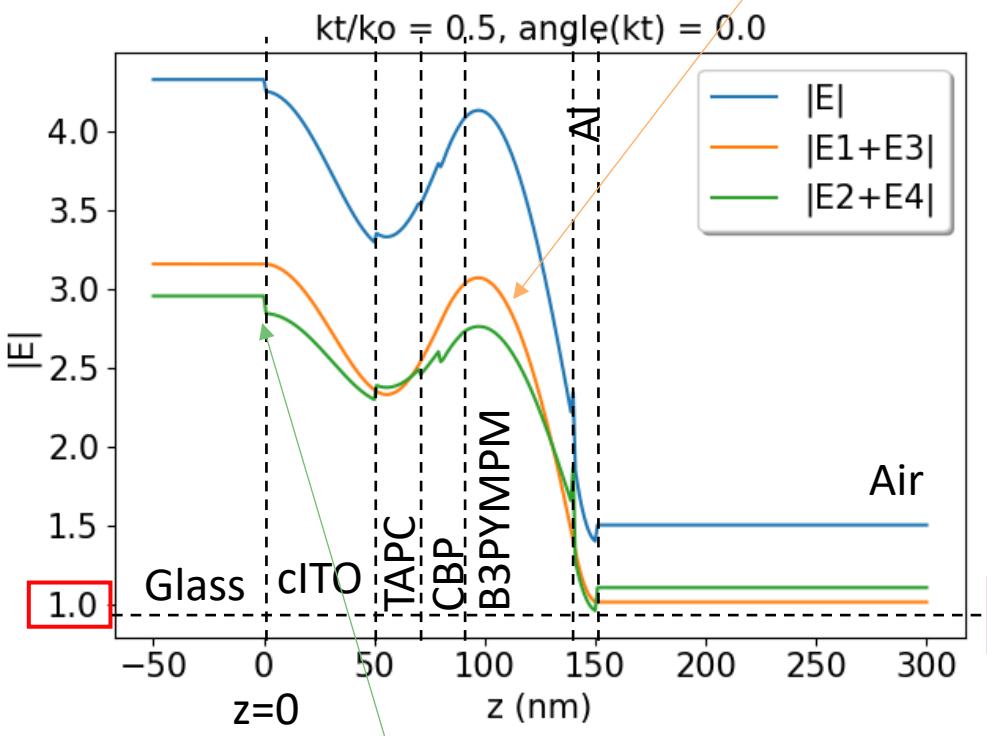
z

z=0

No zero.

Data

The electric field of TE mode is continuous on the interface.

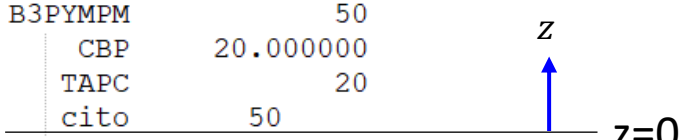


TE

TM

No zero.

MATERIAL	THICKNESS(nm)
air	X
Al	10
LiF	1.000000
B3PYMPM	50
CBP	20.000000
TAPC	20
cito	50
glass	X



The electric field of TM mode is discontinuous on the interface.

Calculate Device Distribution

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 Sun Apr 12 22:42:34 2020
Elapsed time : 0 day(s)/ 0 hr(s)/ 2 min(s)/ 28.69119143486023 sec(s)
------------------------------------------------------------------------------------------------------------
```