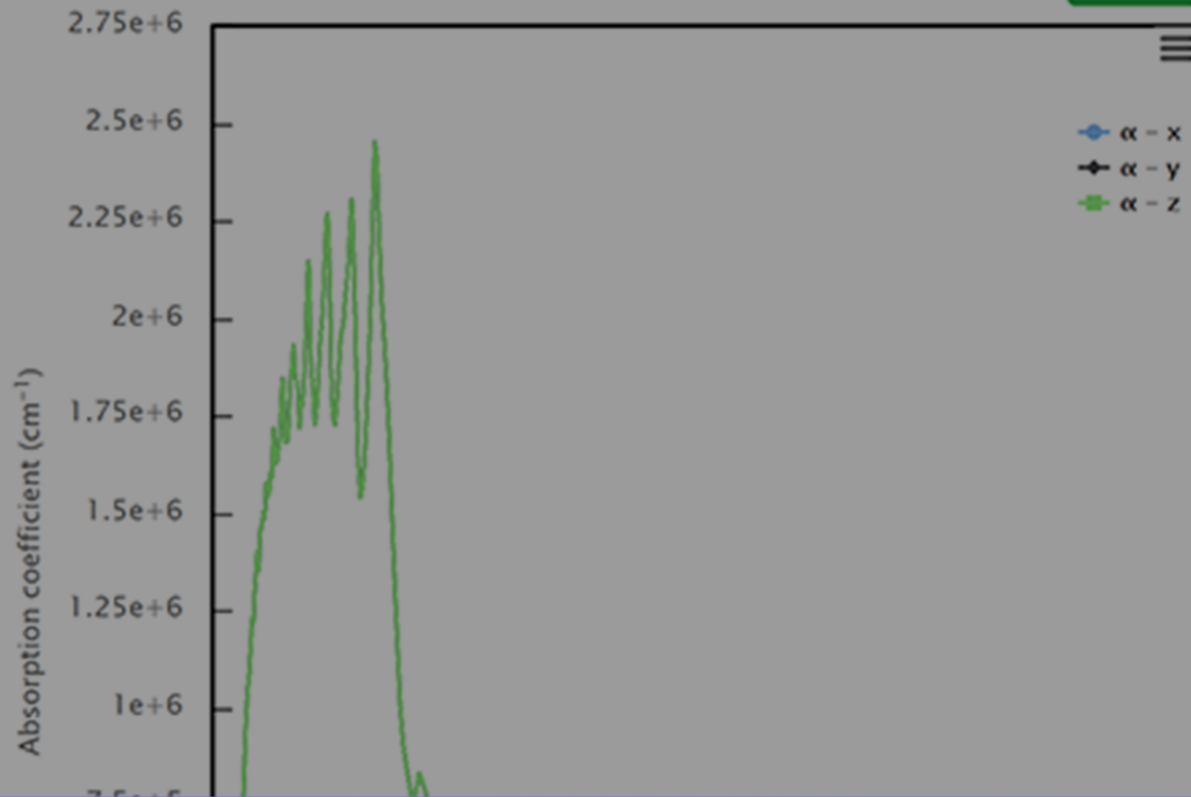
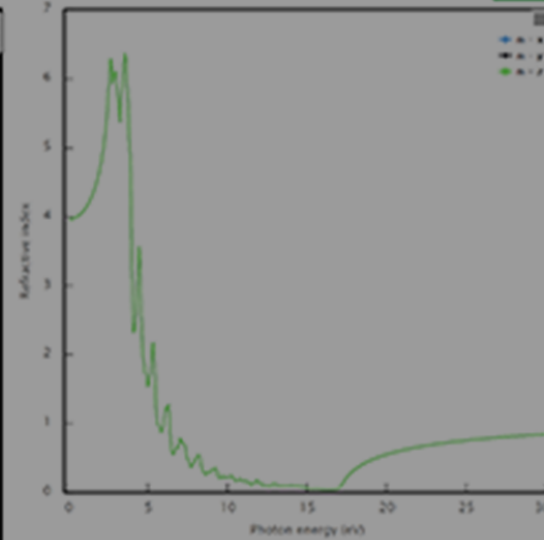


Absorption coefficient



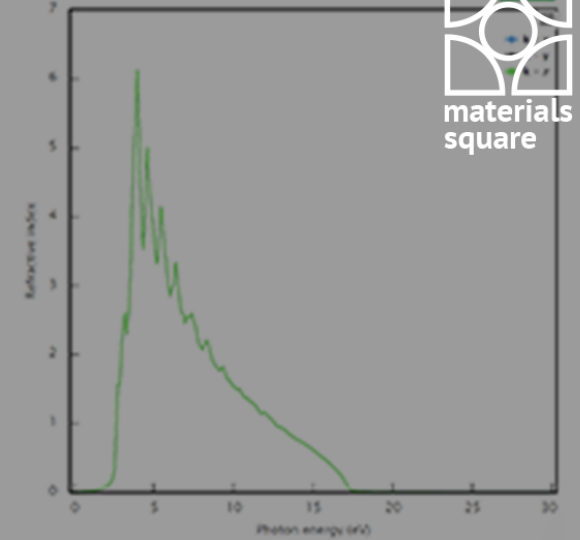
CSV

Refractive index (real)

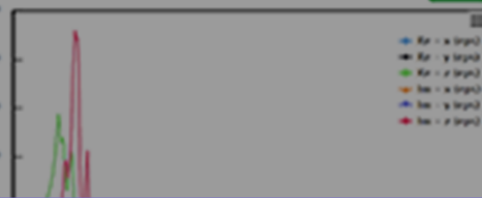


CSV

Refractive index (imaginary)

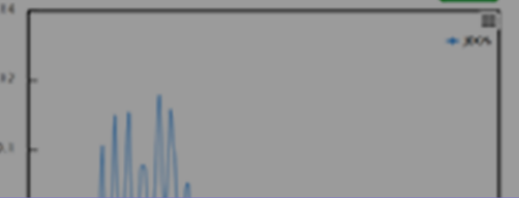


Dielectric function



CSV

JDOS



WEBINAR : Optical Property Calculations on MatSQ

October 27th, 2020, 2:00 PM (GMT+9)

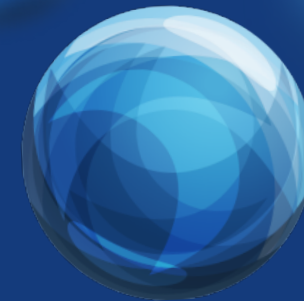
Contents

1 Introduction to Optical Processes

2 Optical property calculation on MatSQ

- Optical Property Calculations for Si
- Optical Property Calculations for GaAs

3 Summary / Q & A



Previous Webinar on MatSQ



WEBINAR : Introduction to Materials Square
Wed, March 18 @ 6PM PST | Thu, March 19 @ 10AM KST



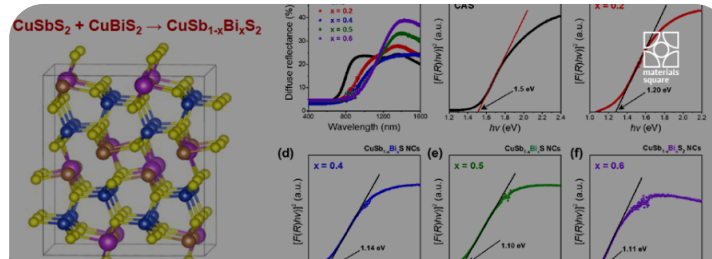
WEBINAR : Phonon Calculation
Wed, April 7 @ 11PM PST | Thu, April 8 @ 3PM KST



WEBINAR : Calphad with Materials Square
Fri, May 8 @ 1AM PST | Fri, May 8 @ 5 PM KST



WEBINAR : Lattice Thermal Conductivity Calculation with MatSQ
Thu, June 4 @ 11AM, KST | Wed, June 3 @ 7PM, PST



WEBINAR : DFT energy calculations for mixed semiconductor systems
Thu, Aug 6 @ 4 PM, CEST | Thu, Aug 6 @ 11 PM, KST

TODAY : “Optical Properties”

Previous Webinar on MatSQ

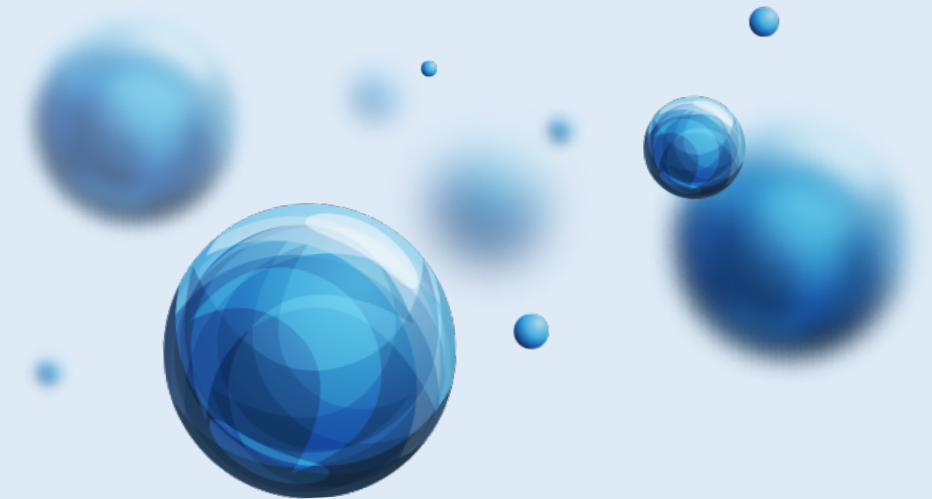
More Details, Visit here

<https://www.matsq.com>

1 Introduction to Optical Processes

Optical Process

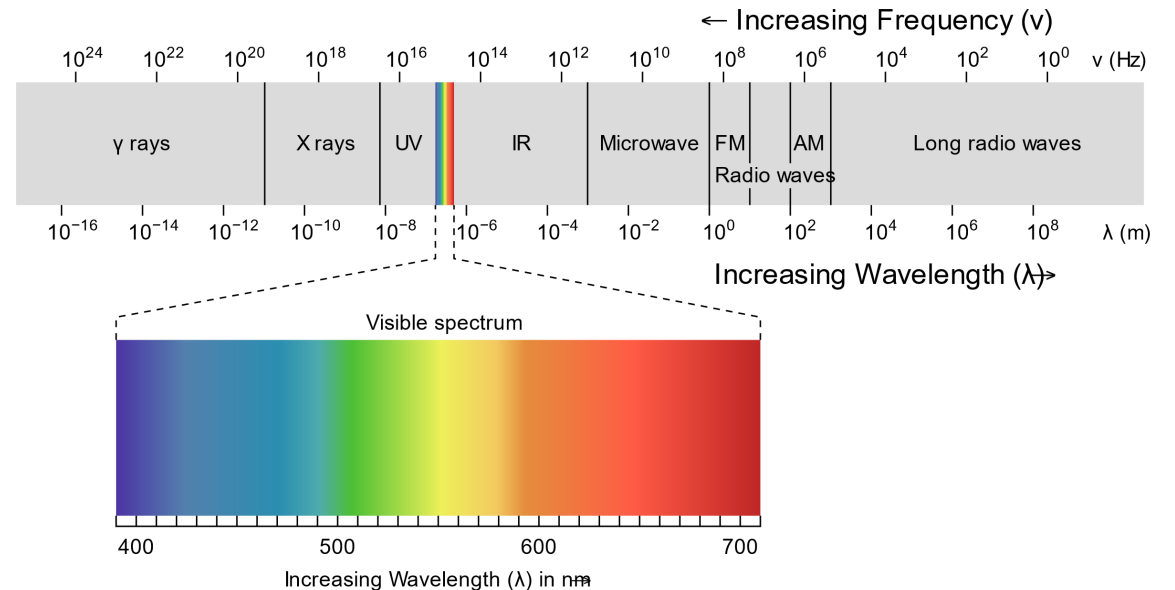
Optical Properties



Optical Processes

What is **Light** ??

- Generally, All kinds of electromagnetic waves
- In the quantum mechanics :
 - Not only considered “*waves*” but also “*particles*” (*Duality of light*)
 - The energy of an electromagnetic wave is quantized.
 - The basic unit of electromagnetic wave energy : “**Photon**”



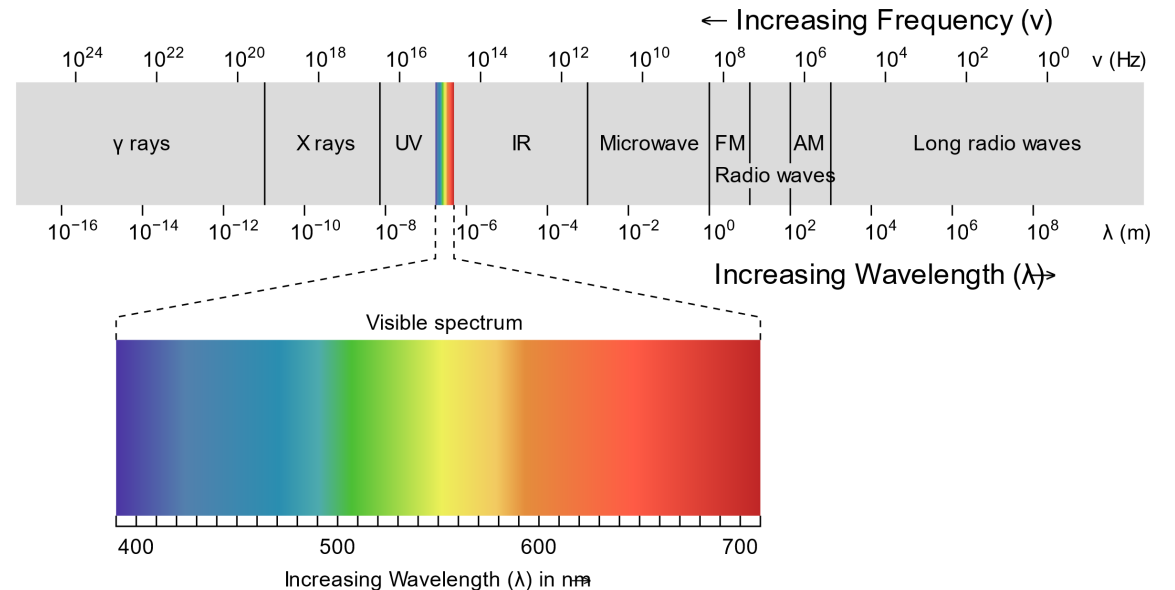
Source: Wikipedia

Optical Processes

Light is "continuous" AND "discontinuous" (quantized/discrete)

- Planck-Einstein Relation : $E = h\nu$
(originated from black body radiation,
E=Photon E, h = Planck constant, ν = frequency)

- It can be also expressed by $E = \frac{hc}{\lambda}$
(\because photon always follows the speed of light.
 λ = Wavelength, c = speed of light)



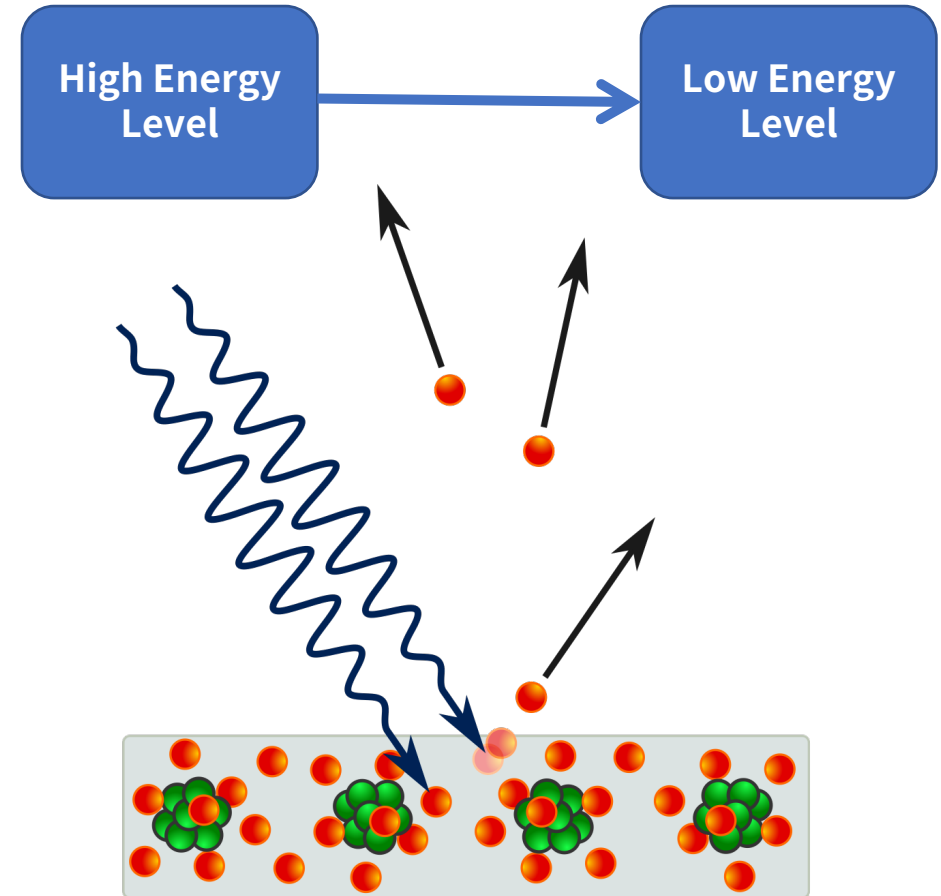
Source: Wikipedia

Optical Processes - Optical Property

- Optical Property : It is determined by interactions between “**electromagnetic wave**” and “**materials**”.

- Metal** : Mostly reflected (“Opaque”)
(General reflectance of metal, 90~95%)

Because, the absorption of light occurs at the highest energy level and photons are emitted directly from high energy to low energy levels.



Absorption and Emission on Metal

[Source : Wikipedia]

Optical Processes - Optical Property

II. Semiconductor :

Transmission, Reflection, Refraction,
Diffraction, adsorption and Scattering.

Transmission : When photon $E <$ bandgap energy, passing through the medium

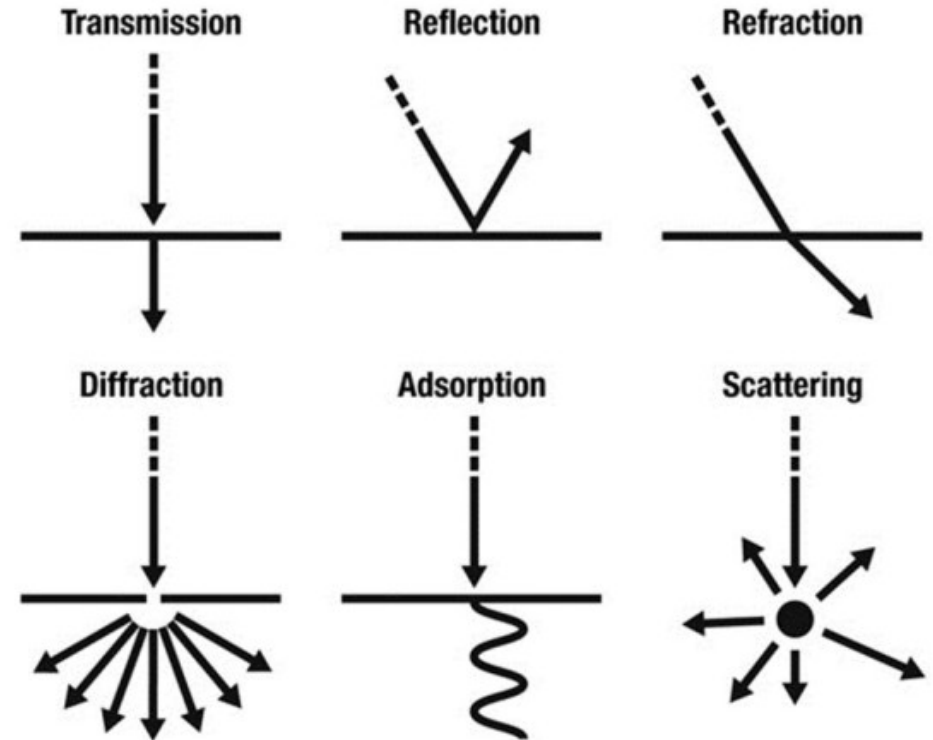
Adsorption : When photon $E \geq$ bandgap energy

Reflection : Light traveling in opposite directions on the surface of a material

Refraction : Changing the speed through which a medium passes through another substance

Diffraction : When the light of a wave passes through a slit

Scattering : Light propagating in various directions on the surface of a medium



Interactions between semiconductor and light

[Source : <https://blog.naver.com/namgoocha>]

Optical Processes - Optical Property

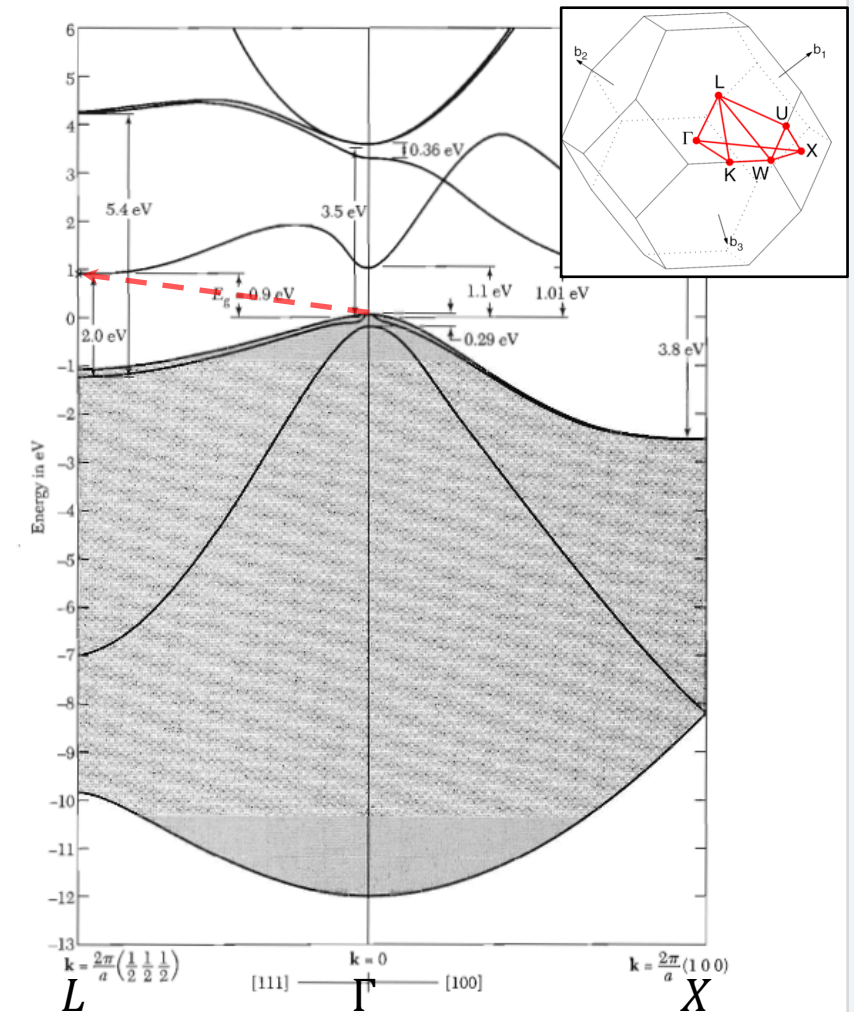
II. Semiconductor :

Semiconductor have “band gap”

Band gap, $E_g = CBM - VBM$ (distance between the valence **band** of electrons and the conduction **band**)

Material	Symbol	Band Gap [eV] at RT
Silicon	Si	1.1
Germanium	Ge	0.7
Gallium Nitride	GaN	3.4
Tungsten Selenide	WSe ₂	1.2
TiO ₂ (Anatase)	TiO ₂	3.2

Bandgap Table for semiconductors



[Source : “Introduction to Solid State Physics”, Kittel]

Optical Processes - Optical Property

II. Semiconductor :

Dominant interactions between UV (10~400 nm) and VL (380~740 nm) and material :

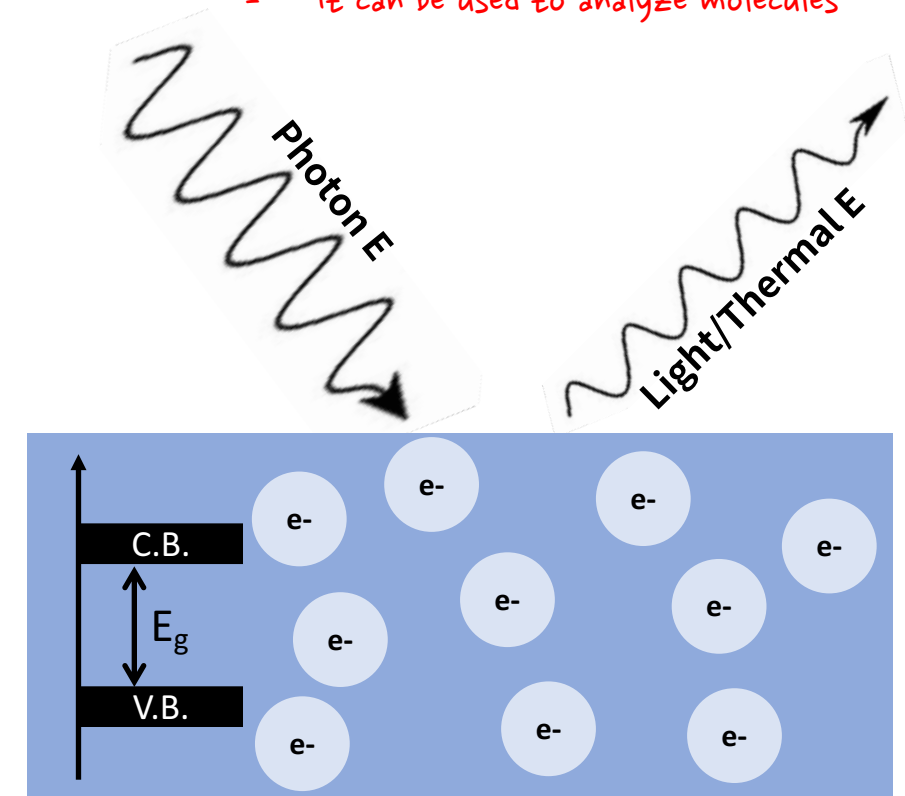
“**Absorption**” and “**Emission**”

i. Photon $E >$ Band gap :

- e^- are excited \rightarrow Excited e^- returns to the ground states (ΔE) \rightarrow Light/thermal E
- ΔE : depending on the band gap !! \rightarrow Can be used analyzing materials properties

How about IR ?

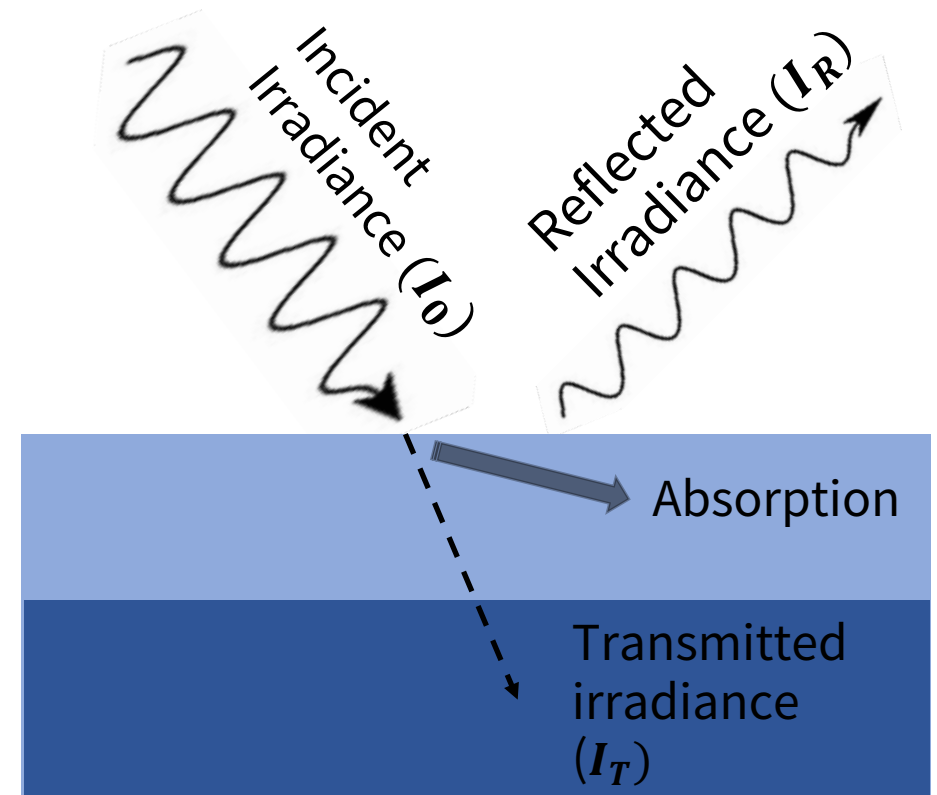
- It has small E (can't excited e^-)
- But, it may affect to atomic vibration
- It can be used to analyze molecules



Optical Processes - Optical Property

III. Reflectance, Transmittance, Absorbance

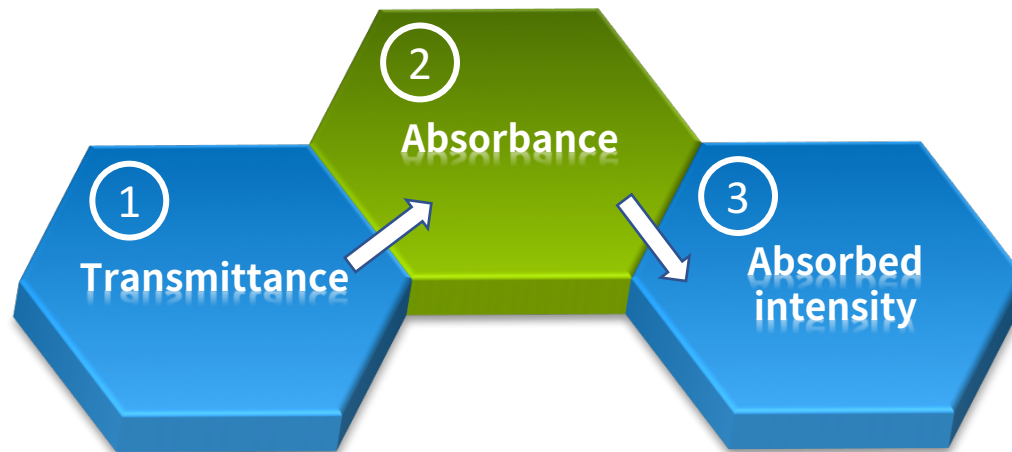
- Reflectance (**R**) can be expressed by, $R = I_R/I_0$ with I_R = Reflected irradiance, I_0 = Incident irradiance (W/cm^2)
- Transmittance (**T**), $T = I_T/I_0$, I_T = Transmitted irradiance
- According to the Energy conservation, $T + R = 1$



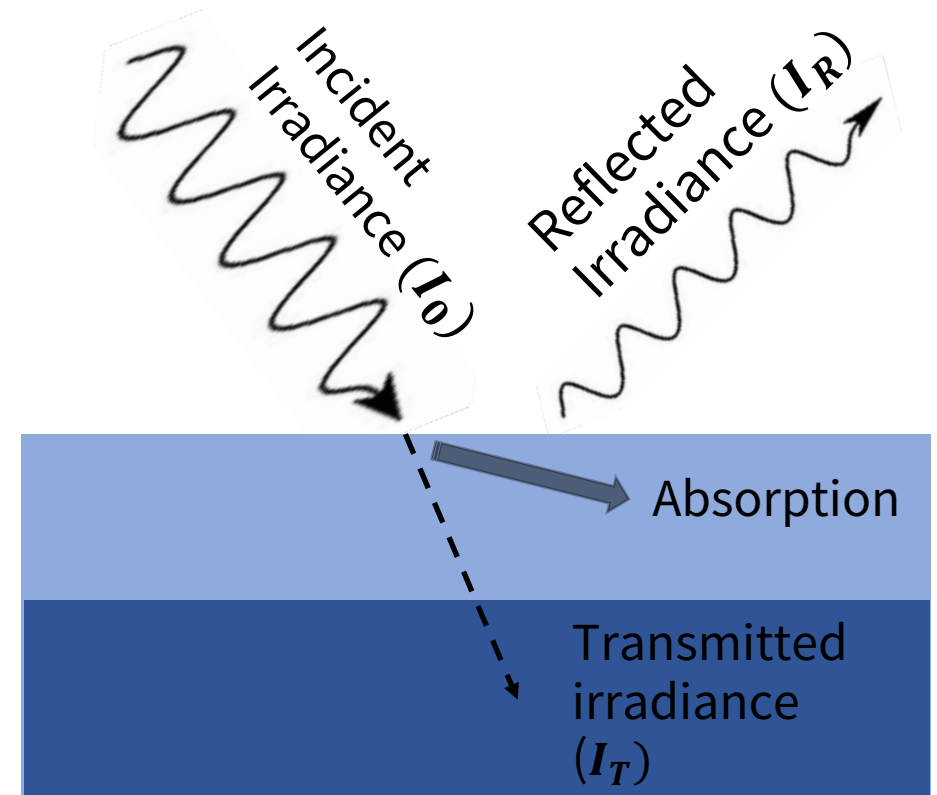
Optical Processes - Optical Property

III. Reflectance, Transmittance, Absorbance

- We can't measure the intensity of the absorbed light directly, but we can calculate indirect way.



- Absorbance (A), $A = \log_{10}(I_0/I_T) = -\log_{10}T$



Optical Processes - Optical Property

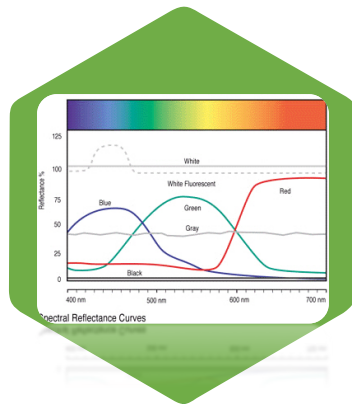
What are the measurable optical properties in experiments, directly ?

[Image Sources]

1. https://www.sabic-ip.com/cxp/jsp/user/LearnAboutColor/ColorBasicsDetail/reflectance_curves.jsp

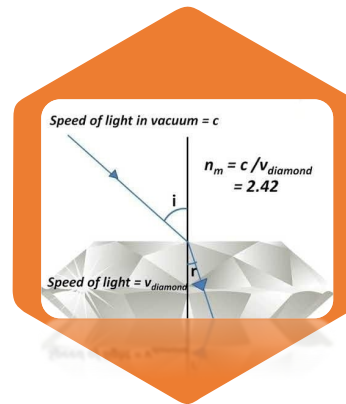
2. <https://www.villarrealjewelers.com/refractive-index-diamond-2>

3. Preparation, Characterization, Properties and Application of Nanofluid



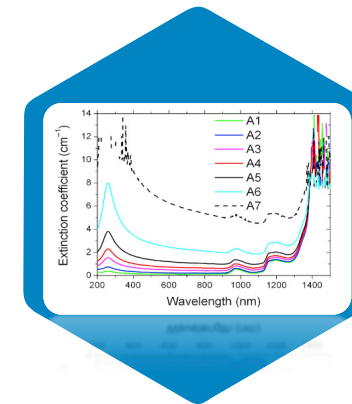
Reflectance, $R(\omega)$

- $R = I_R/I_0$
- Refer to the previous slide



Refractive Index, $n(\omega)$

- $n = C/C_m$
- C = speed of light in vacuum,
 C_m = speed of light in the medium
(phase velocity)



Extinction coefficient, $K(\omega)$

- It describe attenuated light when passing through a medium
- Mass attenuation coefficient
- Imaginary part of $n(\omega)$

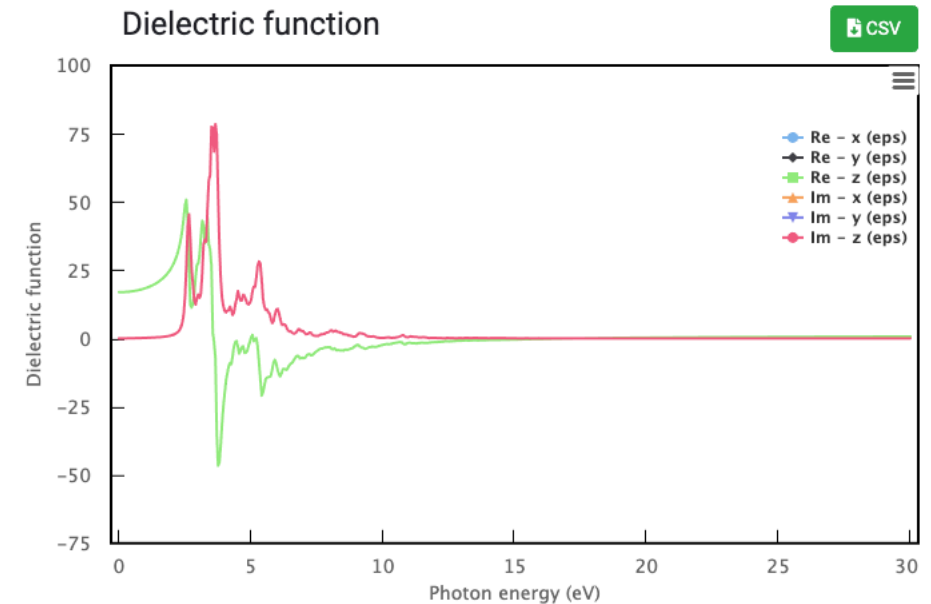
Optical Processes - Optical Property

- Dielectric Function / Refractive index / Absorption coefficient

I. Dielectric Function / Refractive index

The dielectric function describes the linear relation between electrical displacement and the macroscopic electric field.

$$\epsilon(\omega) = \underbrace{\epsilon_1(\omega)}_{\text{Real Part}} + i \underbrace{\epsilon_2(\omega)}_{\text{Imaginary Part}}$$



Refer to Open Research on MatSQ !!

Optical Processes - Optical Property

- Dielectric Function / Refractive index / Absorption coefficient

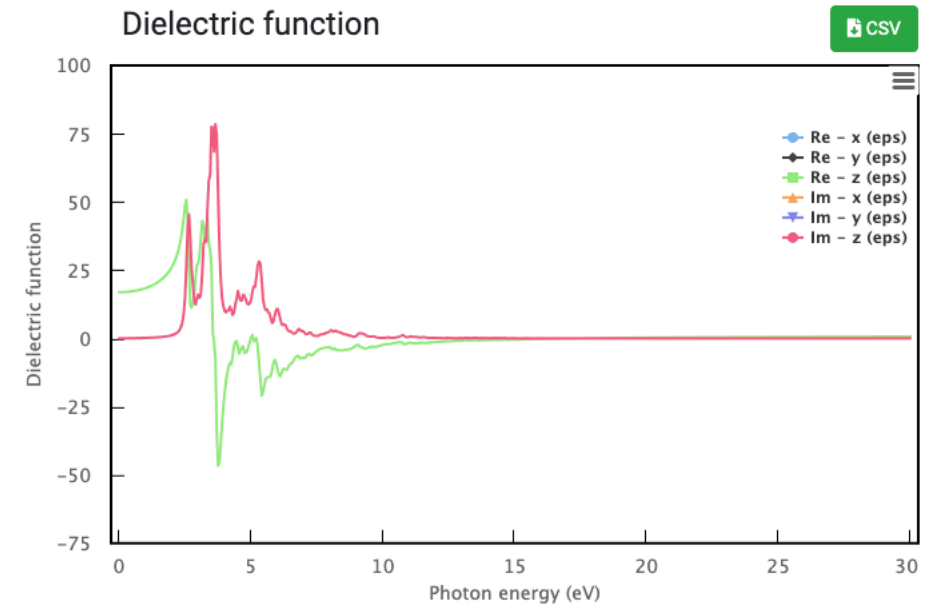
I. Dielectric Function / Refractive index

By definition, Refractive index $n(\omega)$ and Extinction coefficient $K(\omega)$ are related to the dielectric function $\epsilon(\omega)$ by,

$$\sqrt{\epsilon(\omega)} = \underbrace{n(\omega)}_{\text{Complex Refractive Index}} + i \underbrace{K(\omega)}_{\text{Extinction coefficient}}$$

More details, please refer to the textbook :)

(Solid state physics by Kittel or Ashcroft & Mermin)



Refer to Open Research on MatSQ !!

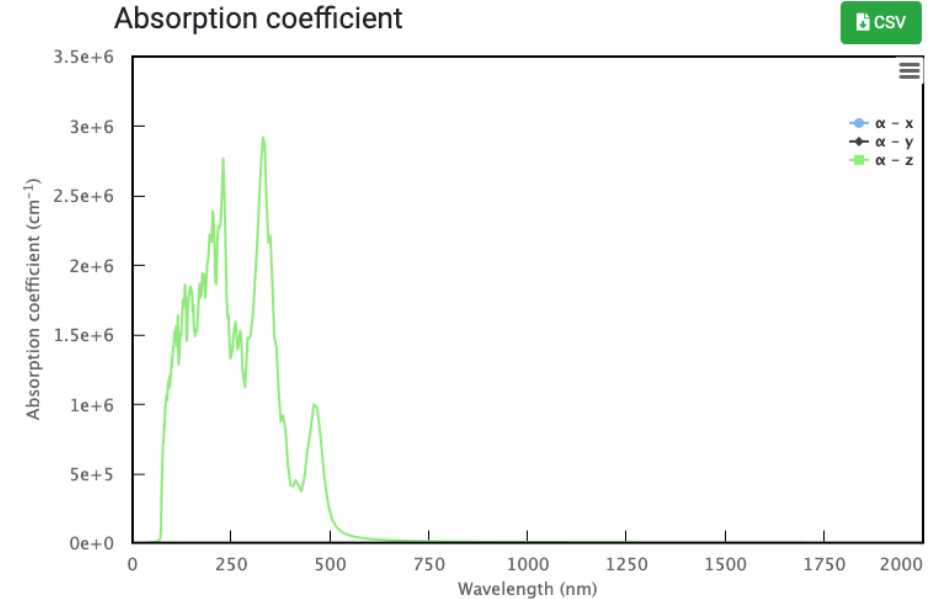
Optical Processes - Optical Property

- Dielectric Function / Refractive index / Absorption coefficient

II. Absorption coefficient (α)

The absorption coefficient is described as the reciprocal of the depth of penetration of radiation into a bulk solid.
(commonly used unit, cm^{-1})

$$\alpha(\omega) = \frac{\text{Extinction coefficient } 4\pi K(\omega)}{\text{Speed of light } c}$$



Refer to Open Research on MatSQ !!

Optical Processes - Optical Property

- Dielectric Function / Refractive index / Absorption coefficient

III. Wrap-up

$$\epsilon(\omega) = \underbrace{\epsilon_1(\omega)}_{\text{Real Part}} + i \underbrace{\epsilon_2(\omega)}_{\text{Imaginary Part}}$$

$$\sqrt{\epsilon(\omega)} = \underbrace{n(\omega)}_{\text{Complex Refractive Index}} + i \underbrace{K(\omega)}_{\text{Extinction coefficient}}$$

$$\alpha(\omega) = \frac{4\pi \underbrace{K(\omega)}_{\text{Extinction coefficient}}}{\underbrace{c}_{\text{Speed of light}}}$$

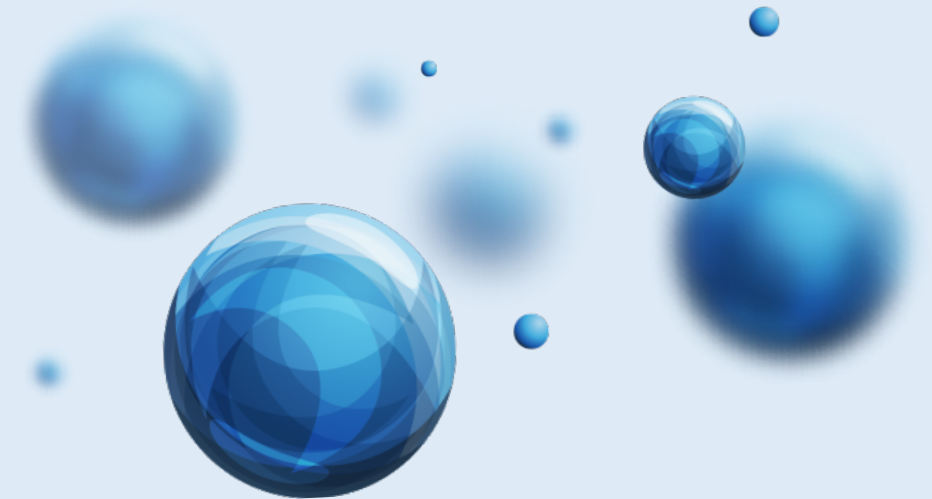
$$n(\omega) = \left[\frac{1}{2} ((\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2) + \epsilon_1(\omega)) \right]^{1/2}$$

$$K(\omega) = \left[\frac{1}{2} ((\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2) - \epsilon_1(\omega)) \right]^{1/2}$$

2 Tutorials

Optical Property Calculations for Si

Optical Property Calculations for GaAs



Tutorial Session

- 1) Please open your browser (chrome/safari recommended)
- 2) Go to <https://www.matsq.com> and log-in
- 3) Click Work-New work
- 4) Wait !!

Overview (Optical Property Calculation on MatSQ)

I. Main Calculation

1. Modeling the structure.
2. Perform relaxation calculation.
Set the input script as follows:
Data to get: Optical property
Precision: High (long time)
Model type: Bulk
Structure optimization
: Ionic+cell optimization
3. When the calculation is finished, press 'Update Status' to update the status bar.

II. Post-process

4. Perform NSCF calculation
Check the input script as follows:
Data to get: Optical property (nscf)
Precision: High (long time)
Model type: Bulk
Structure optimization
: No optimization
5. Also, the 'Optical property' tab added. In the tab, you can set the input for post-processing calculation.
6. When the calculation is finished, press 'Update Status' to update the status bar.

III. Analysis

7. Add the 'Optical Property' module, and connect that to the Quantum Espresso module with the 'Optical property' tab.

Step 1. Simulation Modeling

The screenshot shows the 'materials square' software interface. At the top, there is a navigation bar with 'Account', 'Work', 'Data', 'Blog', 'Docs', and 'Open Research'. The main workspace is titled 'Step 1 : Modeling' and contains a toolbar with icons for 'STRAIN', 'CLONE', 'VACUUM', 'CLEAVE', 'MERGE', 'PRIMITIVE', and 'CONVENTIONAL'. The central 3D view displays a silicon unit cell with two yellow spheres representing atoms. A 'HISTORY' panel on the right shows 'Preset Str.' and 'Primitive'. Below the 3D view, material properties are listed: Si: 2, a,b,c (Å): 3.54, 3.54, 3.54, a,b,c (°): 60.00, 60.00, 60.00, Density: 2.3292 g/cm³, and Volume: 40.046 Å³. The bottom of the interface features a 'Import Module' dropdown, buttons for 'Modeling', 'Simulation', 'Analyzer', and 'Etc.', and a status bar with 'Last save: None', 'Webinar 106 | How to Calc', and 'Save' and 'Settings' buttons.

Step 2. Structural Relaxation

The screenshot shows the Quantum Espresso interface. The 'Data to get' dropdown menu is open, showing 'Optical property' selected. The 'nosym' parameter in the input file is set to '.TRUE.'. The 'Job Submit' section is visible at the bottom right.

Input File Parameters:

Parameter	Value
vc-relax	vc-relax
200	200
Information amount	high
Force threshold (Ry/bohr)	0.00038
Ion dynamics	bfgs
Upscale	100
E _{cut} (wfc)(Ry)	30
E _{cut} (rho)(Ry)	180
Occupations	smearing
Gaussian broadening (Ry)	0.002
noinv	.TRUE.
nosym	.TRUE.
Cell dynamics	bfgs
Cell factor	2
Pressure threshold (Kbar)	0.2
Cell relax type	all
Max iteration step	200
SCF must converge	True
Mixing mode	plain
Mixing beta	0.5
Convergence threshold (Ry)	0.000001
Starting wavefunction	random
Sampling	Monkhorst-Pack
Grid	8 8 8
Shift	0 0 0

Job Submit:

Resource: On-Demand 48
Job Name: [Empty]

If you change the 'Data to get' option to 'Optical property', you can set the input more conveniently.

Step 3. When the calculation is finished, press 'Update Status' to update the status bar.

The screenshot displays the MatSQ interface for a Quantum Espresso calculation. The top navigation bar includes 'materials square', 'Account', 'Work', 'Data', 'Blog', 'Docs', 'Open Research', '\$ 4661.63', '1', and 'Log out'. The main area is divided into several sections:

- &CONTROL:** Calculation type (vc-relax), Max SCF steps (200), Information amount (high), Force threshold (Ry/bohr) (0.00038).
- &SYSTEM:** E_{cut}(wfc)(Ry) (30), E_{cut}(rho)(Ry) (180), Occupations (smearing), Gaussian broadening (Ry) (0.002), noinv (.TRUE.), nosym (.TRUE.).
- &IONS:** Ion dynamics (bfgs), Upscale (100).
- &CELL:** Cell dynamics (bfgs), Cell factor (2), Pressure threshold (Kbar) (0.2), Cell relax type (all).
- SCF Parameters:** SCF must converge (True), Mixing mode (plain), Mixing beta (0.5), Convergence threshold (Ry) (0.000001), Starting wavefunction (random).
- KPOINTS:** Sampling (Monkhorst-Pack), Grid (7 7 7), Shift (0 0 0).

A 'Job Submit' section is visible, showing:

- Resource: On-Demand, 48
- Job Name: GaAs.vcrlx
- Version: 6.4
- Finish Notice: E-mail

At the bottom right, there is a green 'Update Status' button next to a 'Running' status indicator. A code editor at the bottom left shows the input file content:

```

input.pw.x Potential
&CONTROL
calculation = 'vc-relax'
forc_conv_thr = 0.00038
nstep = 200
outdir = './output/'
prefix = 'VLAB'
pseudo_dir = './'
restart_mode = 'from_scratch'
tpnfor = .TRUE.
verbosity = 'high'
wf_collect = .TRUE.
/
  
```

The bottom status bar includes 'Import Module', 'Modeling', 'Simulation', 'Analyzer', 'Etc.', 'Last save: 2020-10-26 14:47:09', 'Webinar 106 | How to Calc', 'Save', and a chat icon.

Step 4. NSCF Calculation

When connecting to the Quantum Espresso module calculated with the 'Optical property', the 'Optical property (restart)' option is automatically selected.

The screenshot shows the Quantum Espresso interface with the following settings:

- Scripting Option:** Template
- Update Structure:**
- Data to get:** Optical property (nscf)
- Precision:** High (long time)
- Model type:** Bulk
- Structure optimization:** No optimization
- Option:** Spin polarization, Electric field, DFT+U
- Information amount:** high
- Force threshold (Ry/bohr):** 0.00038
- &SYSTEM:** E_{cut}(wfc)(Ry) 30, E_{cut}(rho)(Ry) 180, Occupations smearing, Gaussian broadening (Ry) 0.002, noinv .TRUE., nosym .TRUE.
- &ELECTRONS:** Max iteration step 200, SCF must converge True, Mixing mode plain, Mixing beta 0.5, Convergence threshold (Ry) 0.000001, Starting wavefunction random
- KPOINTS:** Sampling Monkhorst-Pack, Grid 16 16 16, Shift 0 0 0
- Job Submit:** Resource: On-Demand 48, Job Name: [empty]

Step 5. Also, the 'Optical property' tab added.
In the 'Optical property' tab, you can set the input for epsilon.x calculation.

The screenshot displays the MatSQ web interface for configuring a Quantum Espresso calculation. The main panel is titled 'Quantum Espresso' and shows the 'Optical property' tab selected. A dropdown menu is open, showing options: DOS, DOS, Band Structure, Charge density, Epsilon (highlighted), and Intra-band Broadening (eV). The 'Epsilon' option is selected, and the input field for 'epsilon.x' is visible. The 'Job Submit' section shows 'Resource' set to 'On-Demand' (48), 'Job Name' as an empty field, 'Version' set to '6.4', and 'Finish Notice' checked for 'E-mail'. A green 'Start Job!' button is at the bottom right. The footer includes the MatSQ logo, contact information, and navigation links for Simulation, Plans & Pricing, Resources, and Social.

You can also add the 'Optical property' tab.

Step 6. When the calculation is finished, press 'Update Status' to update the status bar.

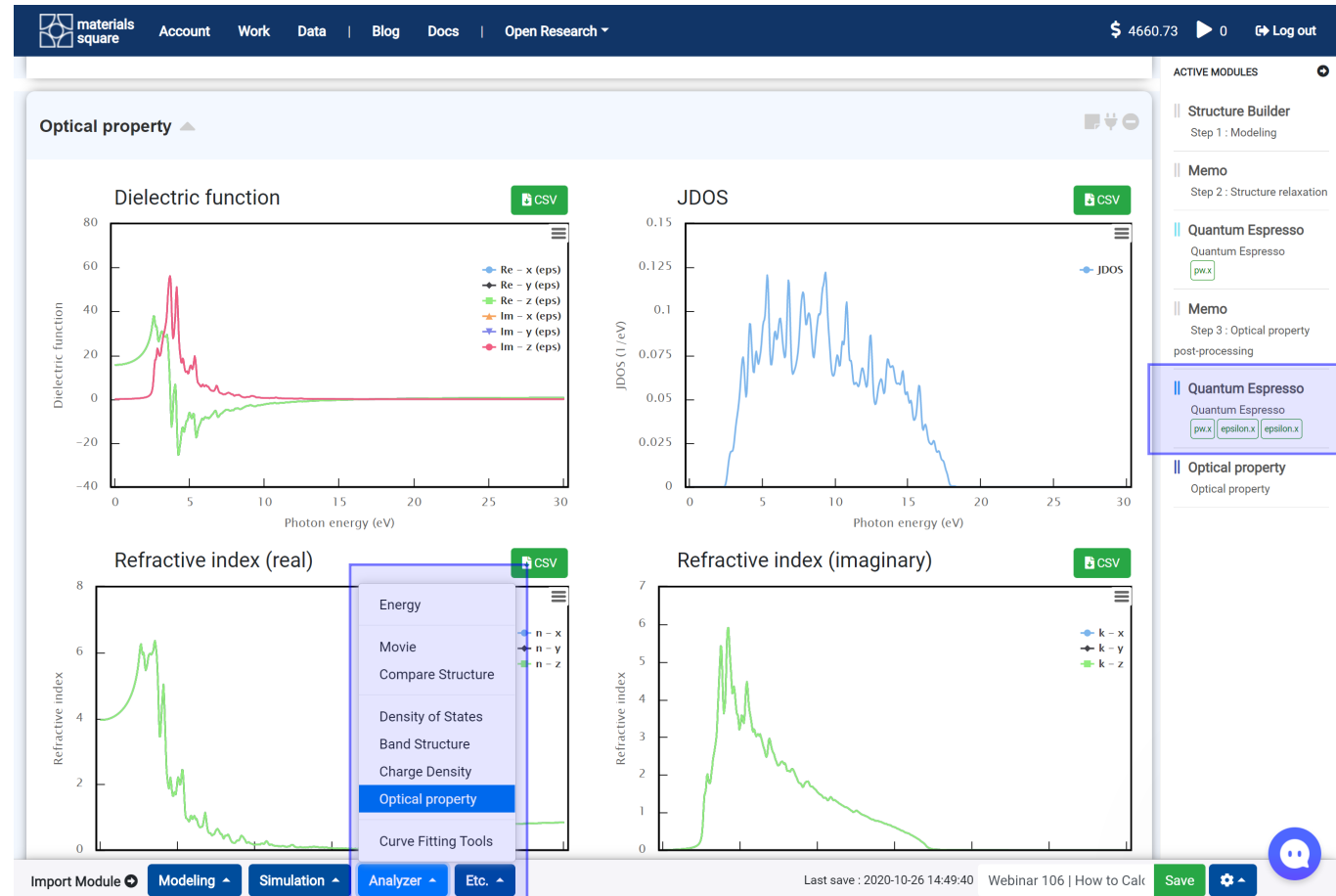
The screenshot displays the MatSQ web interface for a calculation. The top navigation bar includes 'materials square', 'Account', 'Work', 'Data', 'Blog', 'Docs', and 'Open Research'. The user's account balance is \$4660.73, and there are 0 credits. A 'Log out' button is visible.

The main interface is divided into several sections:

- Configuration:** Includes dropdowns for 'Data to get' (Optical property (nscf)), 'Precision' (High (long time)), 'Model type' (Bulk), and 'Structure optimization' (No optimization). There are also checkboxes for 'Option' settings: Spin polarization, Van der Waals, Electric field, Spin Orbit Coupling, and DFT+U.
- Parameters:** Organized into sections:
 - &CONTROL:** Calculation type (nscf), Information amount (high), Force threshold (Ry/bohr) (0.00038).
 - &SYSTEM:** $E_{cut}(wfc)(Ry)$ (30), $E_{cut}(\rho)(Ry)$ (180), Occupations (smearing), Gaussian broadening (Ry) (0.002), noinv, nosym.
 - &ELECTRONS:** Max iteration step (200), SCF must converge (True), Mixing mode (plain), Mixing beta (0.5), Convergence threshold (Ry) (0.000001), Starting wavefunction (random).
 - KPOINTS:** Sampling (Monkhorst-Pack), Grid (16 16 16), Shift (0 0 0).
- Job Submit:** A table for element and filename, and submission options: Resource (On-Demand, 48), Job Name (si.nscf), Version (6.4), and Finish Notice (E-mail checked).
- ACTIVE MODULES:** A sidebar on the right showing the workflow: Structure Builder (Step 1: Modeling), Memo (Step 2: Structure relaxation), Quantum Espresso (pw.x), Memo (Step 3: Optical property post-processing), and Quantum Espresso (pw.x, epsilon.x, epsilon.x).

At the bottom, there is a 'Job Submit' section with a blue 'Potential' button and a 'Job Submit' section with a 'Resource' dropdown set to 'On-Demand' and '48', 'Job Name' set to 'si.nscf', 'Version' set to '6.4', and 'Finish Notice' checked for 'E-mail'. A green 'Update Status' button is highlighted, and a 'Running' status indicator is visible. The bottom status bar shows 'Last save: 2020-10-26 14:49:40', 'Webinar 106 | How to Calc', and 'Save' and 'Settings' buttons.

Step 7. Add the 'Optical Property' module, and connect that to the Quantum Espresso module with the 'Optical property' tab.



Step 1. Simulation Modeling

materials square Account Work Data | Blog Docs | Open Research 2534 1/1

Step 1 : Modeling

Modeling Cell Atom Extension

DATABASE JOBS MODULE FILE CRYSTAL PRESET EDIT

Search Structure from Open DB

Formula : GaAs

mp-12452/4	GaAs	P1	100	234b.231
mp-15619	GaAs	Pa-3	16	350.867
mp-2534	GaAs	F-43m	2	47.532
mp-1232355	GaAs	Cm	16	691.114
mp-10048	GaAs	P4/mmm	2	40.277

ACTIVE MODULES

Structure Builder

Step 1 : Modeling

HISTORY

OpenDB

Ga : 1, As : 1
a,b,c (Å) : 4.07, 4.07, 4.07
α,β,γ (°) : 60.00, 60.00, 60.00
Density : 5.0531 g/cm³
Volume : 47.532 Å³

Import Module Modeling Simulation Analyzer Etc.

Last save : 2020-10-26 15:09:13 Webinar 106 | How to Calc Save

Step 2. Structural Relaxation

The screenshot shows the MatSQ interface for a Quantum Espresso calculation. The 'Data to get' dropdown menu is open, showing 'Optical property' selected. The 'Job Submit' section is visible at the bottom right, showing resource allocation and job name fields.

ACTIVE MODULES

- Structure Builder
 - Step 1 : Modeling
- Memo
 - Step 2 : Structural relaxation
- Quantum Espresso
 - Quantum Espresso
 - pw.x

Scripting Option : Template Update Structure

Data to get (Dropdown): Optical property, Energy / Structure, DOS, Charge Density, Optical property

Option

- Spin polarization
- Van der Waals
- Electric field
- Spin Orbit Coupling
- DFT+U

&CONTROL

- Calculation type: vc-relax
- Max step: 200
- Information amount: high
- Force threshold (Ry/bohr): 0.00038

&SYSTEM

- $E_{cut}(wfc)(Ry)$: 50
- $E_{cut}(\rho)(Ry)$: 400
- Occupations: smearing
- Gaussian broadening (Ry): 0.002
- noinv: .TRUE.
- nosym: .TRUE.

&ELECTRONS

- Max iteration step: 200
- SCF must converge: True
- Mixing mode: plain
- Mixing beta: 0.5
- Convergence threshold (Ry): 0.000001
- Starting wavefunction: random

&IONS

- Ion dynamics: bfgs
- Upscale: 100

&CELL

- Cell dynamics: bfgs
- Cell factor: 2
- Pressure threshold (Kbar): 0.2
- Cell relax type: all

KPOINTS

- Sampling: Monkhorst-Pack
- Grid: 7 7 7
- Shift: 0 0 0

Job Submit

- Resource: On-Demand 48
- Job Name: [Empty]
- Version: 6.4

input.pw.x

Element	Filename
Ga	Ga_ONCV_PBE-1.2.upf
As	As_ONCV_PBE-1.2.upf

Buttons: Import Module, Modeling, Simulation, Analyzer, Etc.

Footer: Last save : 2020-10-26 15:09:13 Webinar 106 | How to Calc Save

If you change the 'Data to get' option to 'Optical property', you can set the input more conveniently.

Step 3. When the calculation is finished, press 'Update Status' to update the status bar.

The screenshot displays the MatSQ interface for a Quantum Espresso calculation. The main area is divided into several sections for parameter configuration:

- &CONTROL:** Calculation type (vc-relax), Max SCF steps (200), Information amount (high), Force threshold (0.00038 Ry/bohr).
- &SYSTEM:** E_{cut}(wfc)(Ry) (50), E_{cut}(rho)(Ry) (400), Occupations (smearing), Gaussian broadening (0.002), noinv (.TRUE.), nosym (.TRUE.).
- &IONS:** Ion dynamics (bfgs), Upscale (100).
- &CELL:** Cell dynamics (bfgs), Cell factor (2), Pressure threshold (0.2 Kbar), Cell relax type (all).
- SCF Parameters:** SCF must converge (True), Mixing mode (plain), Mixing beta (0.5), Convergence threshold (0.000001), Starting wavefunction (random).
- KPOINTS:** Sampling (Monkhorst-Pack), Grid (7 7 7), Shift (0 0 0).

At the bottom, the **Job Submit** section includes:

- Resource: On-Demand, 48
- Job Name: GaAs.vcrlx
- Version: 6.4
- Finish Notice: E-mail

A green **Update Status** button is highlighted with a red box, and a green **Running** status indicator is visible next to it. A code editor at the bottom left shows the input file content:

```
&CONTROL
calculation = 'vc-relax'
forc_conv_thr = 0.00038
nstep = 200
outdir = './output/'
prefix = 'VLAB'
pseudo_dir = './'
restart_mode = 'from_scratch'
tpmfor = .TRUE.
verbosity = 'high'
wf_collect = .TRUE.
/
```

Step 4. NSCF Calculation

When connecting to the Quantum Espresso module calculated with the 'Optical property', the 'Optical property (restart)' option is automatically selected.

ACTIVE MODULES

- Structure Builder
 - Step 1 : Modeling
- Memo
 - Step 2 : Structural relaxation
- Quantum Espresso
 - Quantum Espresso [pw.x]
- Memo
 - Step 3 : Optical property post-processing
- Quantum Espresso
 - Quantum Espresso [pw.x] [epsilon.x] [epsilon.x]

Scripting Option : Template Update Structure Keyword information

Data to get

- Optical property (nscf)
- Energy / Structure
- DOS
- Charge Density
- Band Structure
- Optical property
- Optical property (nscf)

Information amount high

Force threshold (Ry/bohr) 0.00038

Precision High (long time)

Model type Bulk

Structure optimization No optimization

Option

- Spin polarization
- Van der Waals
- Electric field
- Spin-orbit coupling
- DFT+U

&SYSTEM

E _{cut} (wfc)(Ry)	50
E _{cut} (rho)(Ry)	400
Occupations	smearing
Gaussian broadening (Ry)	0.002
noinv	.TRUE.
nosym	.TRUE.

&ELECTRONS

Max iteration step	200
SCF must converge	True
Mixing mode	plain
Mixing beta	0.5
Convergence threshold (Ry)	0.000001
Starting wavefunction	random

KPOINTS

Sampling: Monkhorst-Pack

Grid	21	21	21
Shift	0	0	0

Job Submit

Resource : On-Demand 48

Job Name : GaAs.nscf

Version : 6.4

Element **Filename**

Ga	Ga_ONCV_PBE-1.2.upf
As	As_ONCV_PBE-1.2.upf

Import Module Modeling Simulation Analyzer Etc.

Last save : 2020-10-26 15:39:33 Webinar 106 | How to Calc Save

Step 5. Also, the 'Optical property' tab added.
In the 'Optical property' tab, you can set the input for epsilon.x calculation.

The screenshot displays the MatSQ Quantum Espresso interface. The main panel is titled 'Quantum Espresso' and shows the 'Optical property' tab selected. A dropdown menu is open, showing options: Epsilon, DOS, Band Structure, Charge density, and Epsilon. The 'Epsilon' option is highlighted. Below the dropdown, there are input fields for 'Epsilon' (0.136), 'Frequency Range (eV)' (0 - 30), 'Frequency Mesh' (600), and 'Optional Rigid Shift' (0). A 'Job Submit' section is visible on the right, with 'Resource' set to 'On-Demand' (48), 'Job Name' field, 'Version' set to '6.4', and 'Finish Notice' checked for 'E-mail'. A 'Start Job!' button is at the bottom right. The interface also shows a 'Memo' section on the right with 'Step 3 : Optical property post-processing' and 'Quantum Espresso' tabs. The bottom navigation bar includes 'Import Module', 'Modeling', 'Simulation', 'Analyzer', and 'Etc.' buttons. The footer contains the MatSQ logo, contact information, and navigation links for Simulation, Plans & Pricing, Resources, and Social media.

You can also add the 'Optical property' tab.

Step 6. When the calculation is finished, press 'Update Status' to update the status bar.

The screenshot displays the MatSQ interface for a calculation. The top navigation bar includes 'materials square', 'Account', 'Work', 'Data', 'Blog', 'Docs', and 'Open Research'. The user's account balance is \$ 4658.87, and there is a 'Log out' button. The main interface is divided into several sections:

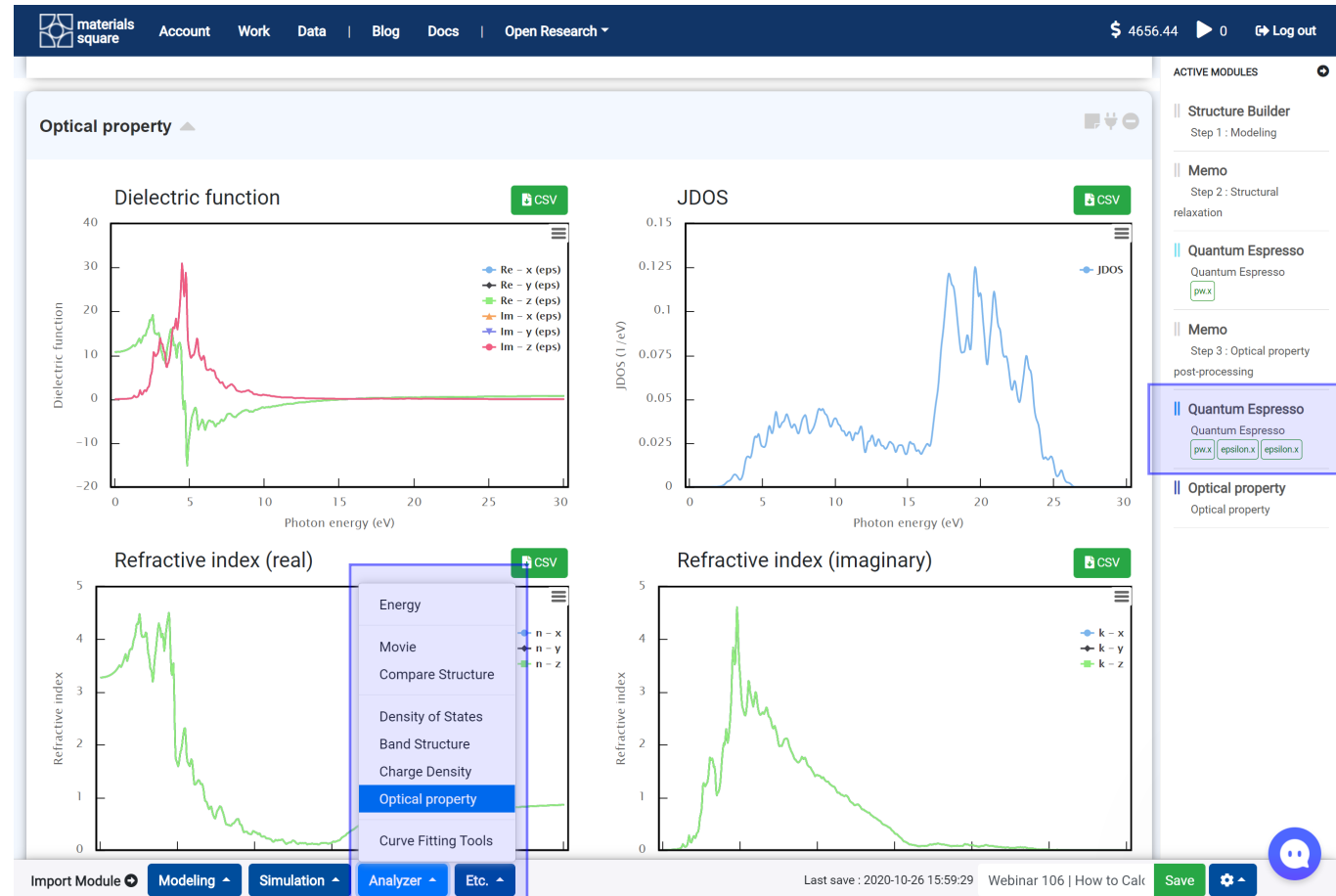
- Data to get:** Includes dropdowns for 'Optical property (nscf)', 'Precision' (High (long time)), 'Model type' (Bulk), and 'Structure optimization' (No optimization).
- Option:** A list of checkboxes for 'Spin polarization', 'Van der Waals', 'Electric field', 'Spin Orbit Coupling', and 'DFT+U'.
- &CONTROL:** Includes 'Calculation type' (nscf), 'Information amount' (high), and 'Force threshold (Ry/bohr)' (0.00038).
- &SYSTEM:** Includes 'E_{cut}(wfc)(Ry)' (50), 'E_{cut}(rho)(Ry)' (400), 'Occupations' (smearing), 'Gaussian broadening (Ry)' (0.002), 'noinv' (.TRUE.), and 'nosym' (.TRUE.).
- &ELECTRONS:** Includes 'Max iteration step' (200), 'SCF must converge' (True), 'Mixing mode' (plain), 'Mixing beta' (0.5), 'Convergence threshold (Ry)' (0.000001), and 'Starting wavefunction' (random).
- KPOINTS:** Includes 'Sampling' (Monkhorst-Pack) and 'Grid' (21 21 21, 0 0 0).
- Job Submit:** Includes 'Resource' (On-Demand, 48), 'Job Name' (GaAs.nscf), 'Version' (6.4), and 'Finish Notice' (E-mail).
- ACTIVE MODULES:** A sidebar on the right showing 'Structure Builder' (Step 1: Modeling), 'Memo' (Step 2: Structural relaxation), 'Quantum Espresso' (Quantum Espresso, pw.x), 'Memo' (Step 3: Optical property post-processing), and another 'Quantum Espresso' (Quantum Espresso, pw.x, epsilon.x, epsilon.x).

At the bottom, there is a 'Job Submit' section with a 'Potential' button and a table of elements:

Element	Filename
Ga	Ga_ONCV_PBE-1.2.upf
As	As_ONCV_PBE-1.2.upf

Below the table, there is a 'Job Submit' section with a 'Resource' dropdown (On-Demand, 48), 'Job Name' (GaAs.nscf), 'Version' (6.4), and 'Finish Notice' (E-mail). A blue 'Update Status' button is highlighted, and a green 'Running' button is visible. The bottom status bar shows 'Import Module', 'Modeling', 'Simulation', 'Analyzer', 'Etc.', 'Last save: 2020-10-26 15:59:29', 'Webinar 106 | How to Calc', 'Save', and a chat icon.

Step 7. Add the 'Optical Property' module, and connect that to the Quantum Espresso module with the 'Optical property' tab.



Please leave comments/questions on matsq.com or **YouTube** channel

Materials Square YouTube Channel !!

Materials Square
구독자 336명

홈 동영상 재생목록 채널 토론 정보

업로드한 동영상 ▶ 모두 재생

- Antiphase Boundary Energy**
with MatSQ CALPHAD
1:43
[Materials Square] Antiphase Boundary Energy for Ni-Bas...
조회수 34회 · 6일 전
자막
- Stacking Fault Energy**
with MatSQ CALPHAD
1:30
[Materials Square] How to Obtain Stacking Fault Energ...
- How to Optain Optical Property**
with MatSQ Quantum Espresso
4:14
[Materials Square] Optical Property Calculation for...
- Optical Property**
MatSQ UPDATE!
1:05:11
[Materials Square] 웨비나- MatSQ 203: 최신 MatSQ...
조회수 53회 · 3주 전
- Driving Force**
with MatSQ CALPHAD
0:39
[Materials Square] NEW UPDATE! Optical Property
조회수 99회 · 4주 전
- Driving Force**
with MatSQ CALPHAD
2:47
[Materials Square] How to Obtain Driving Force with...

+

Any Questions

Thank You



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