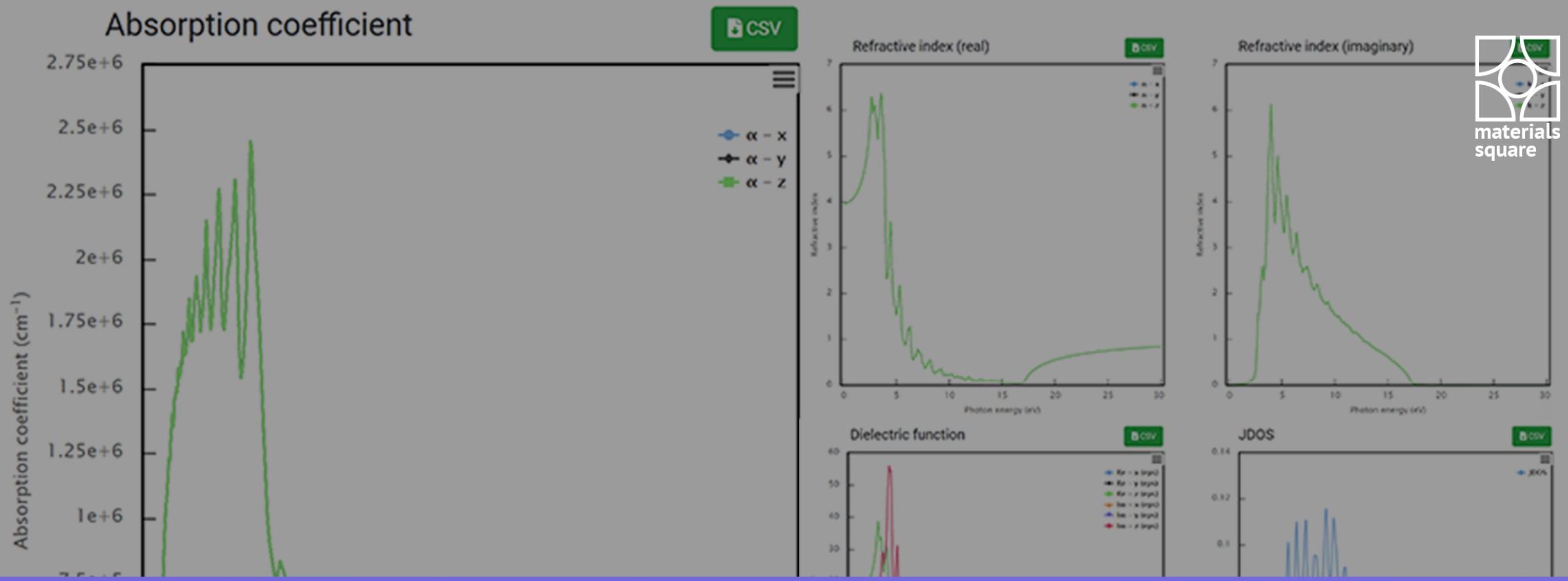


WEBINAR : Optical Property Calculations on MatSQ

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

Contents

Previous Webinar on MatSQ

WEBINAR : Introduction to Materials Square

Wed, March 18 @ 6PM PST | Thu, March 19 @ 10AM KST

WEBINAR : Phonon Calculation

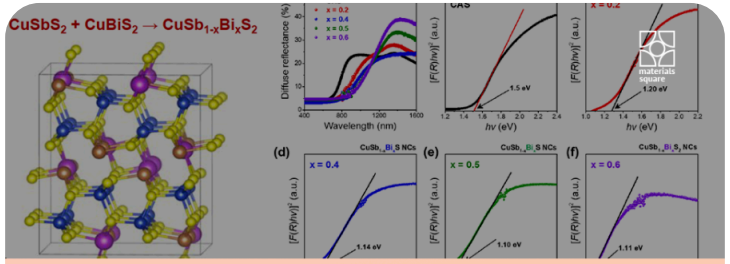
Wed, April 7 @ 11PM PST | Thu, April 8 @ 3PM KST

WEBINAR : Calphad with Materials Square

Fri, May 8 @ 1 AM PST | Fri, May 8 @ 5 PM KST

WEBINAR : Lattice Thermal Conductivity Calculation with MatSQ

Thu, June 4 @ 11AM, KST I Wed, June 3 @ 7PM, PST



WEBINAR : DFT energy calculations for mixed semiconductor systems

Thu, Aug 6 @ 4 PM, CEST I Thu, Aug 6 @ 11 PM, KST

TODAY : "Optical Properties"

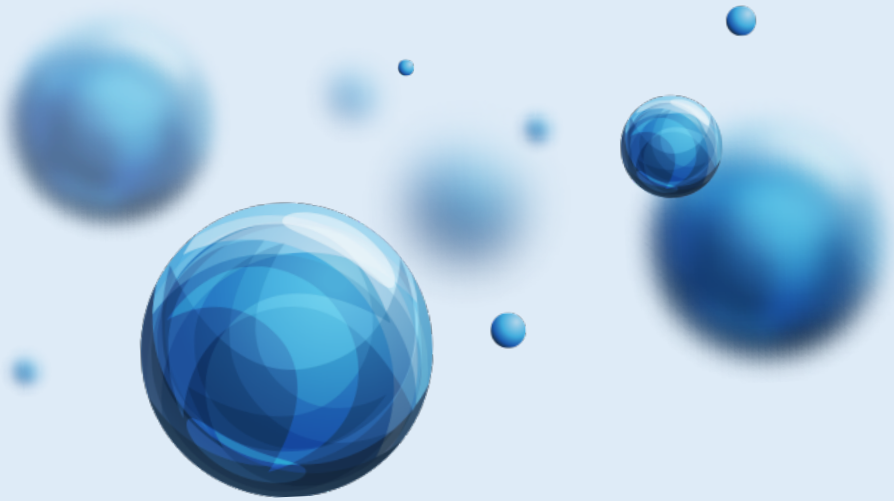
Previous Webinar on MatSQ

More Details, Visit here

https://www.matsq.com

1 Introduction to Optical Processes

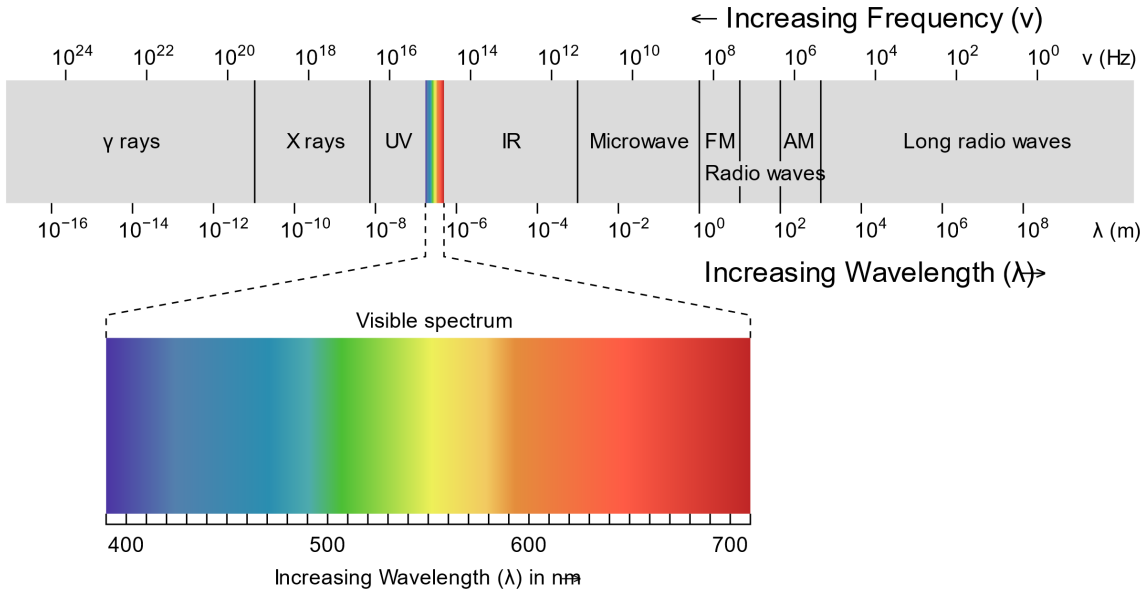
- Optical Process
- Optical Properties



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 : $E = h\nu$

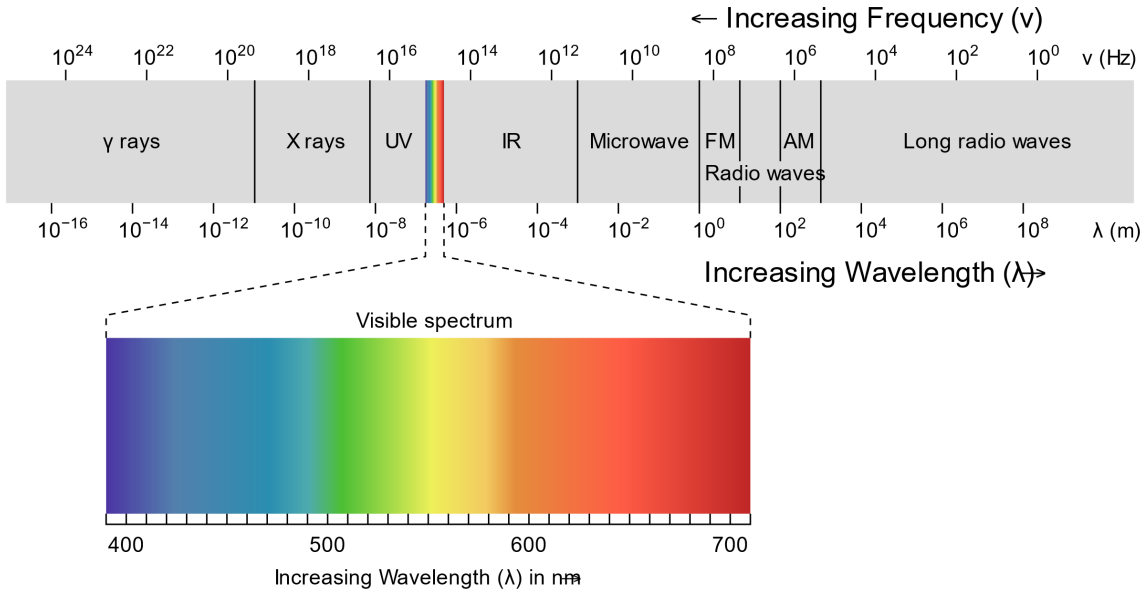
  (originated from black body radiation,

  E=Photon E, h = Planck constant, ν = frequency)

- It can be also expressed by $E = \frac{hc}{\lambda}$

  (∵ photon always follows the speed of light.

  λ = Wavelength, c = speed of light)



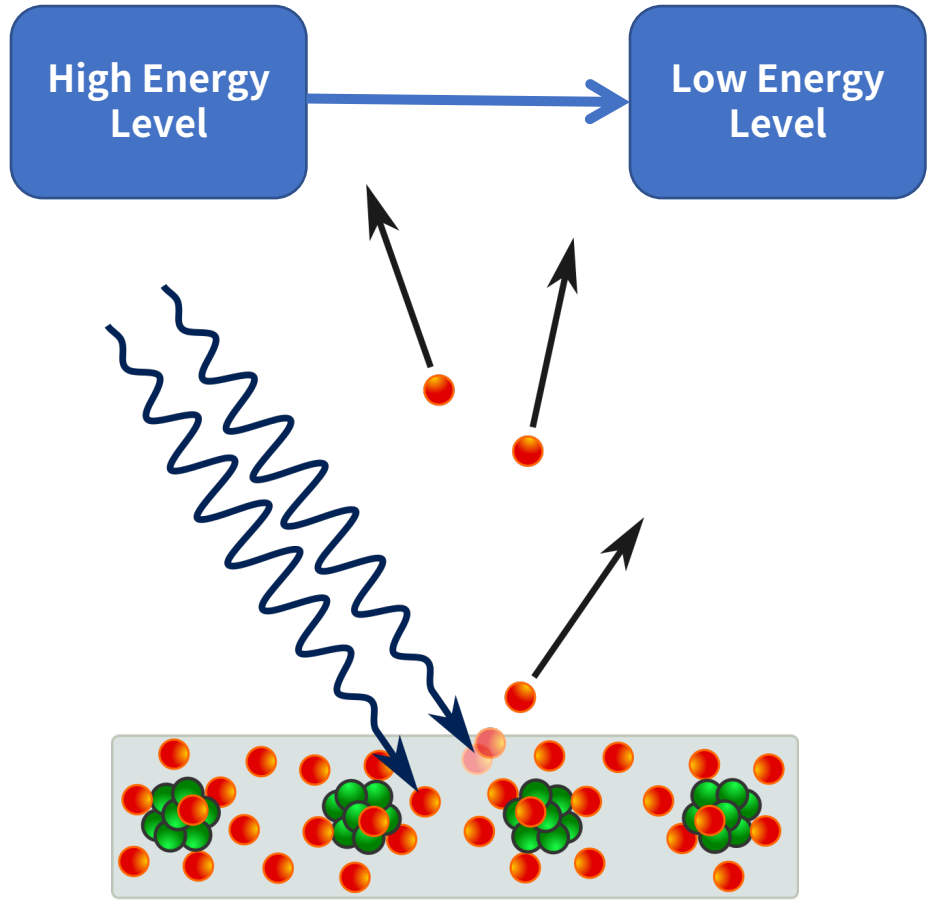
Source: Wikipedia

Optical Processes - Optical Property

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

  I. **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

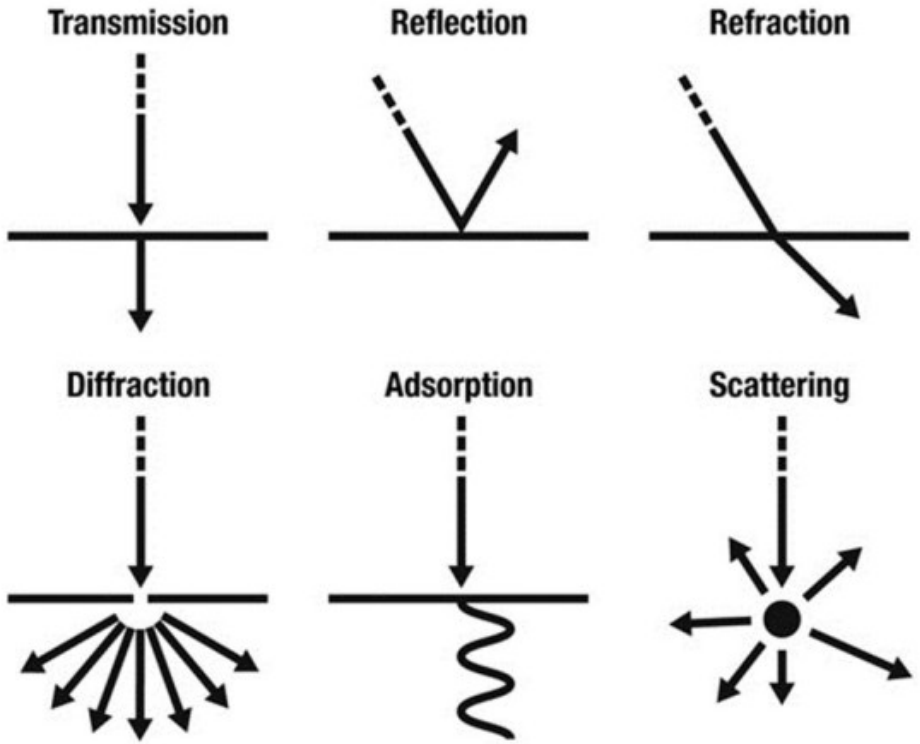
Adsorption : When photon E ≥ bandgap energy

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

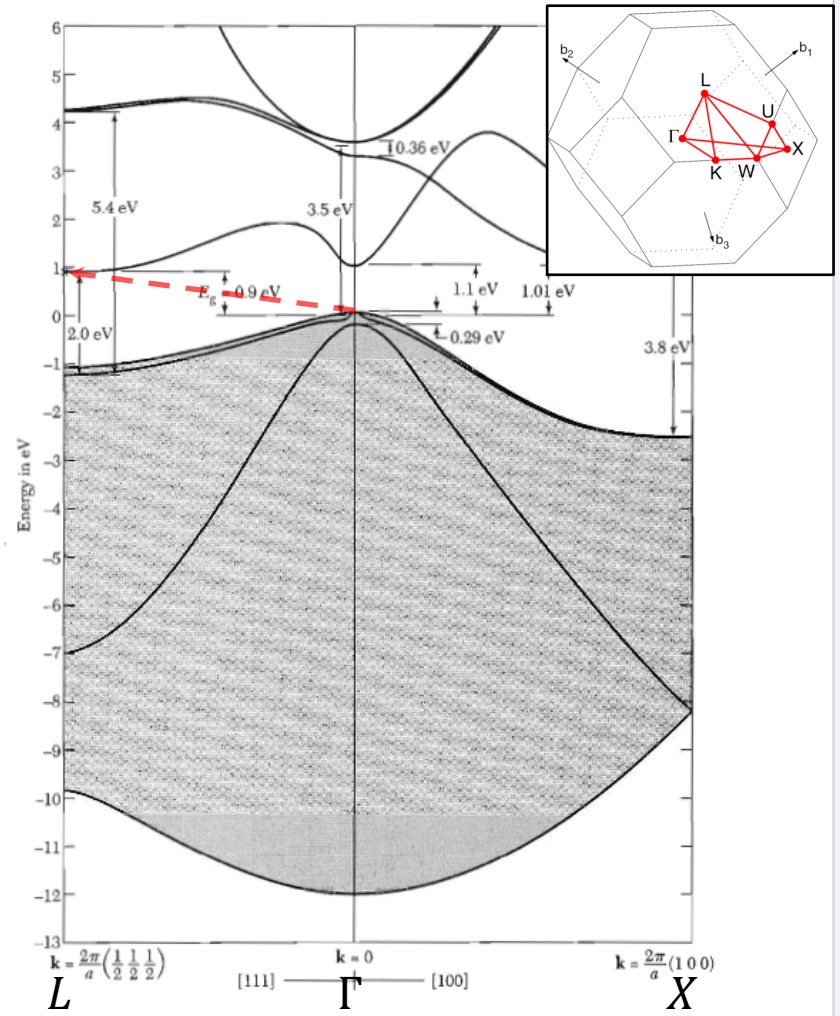
II. Semiconductor :

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

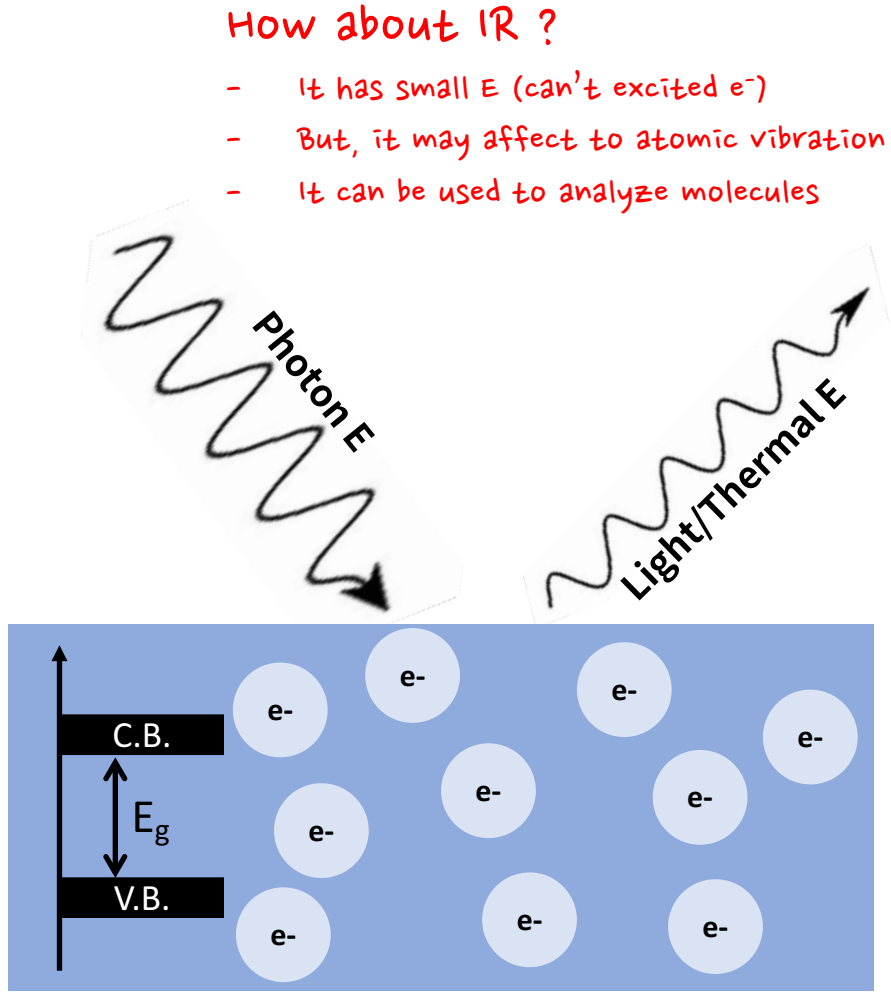
II. Semiconductor :

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

"**Absorption**" and "**Emission**"

i. Photon E > Band gap :

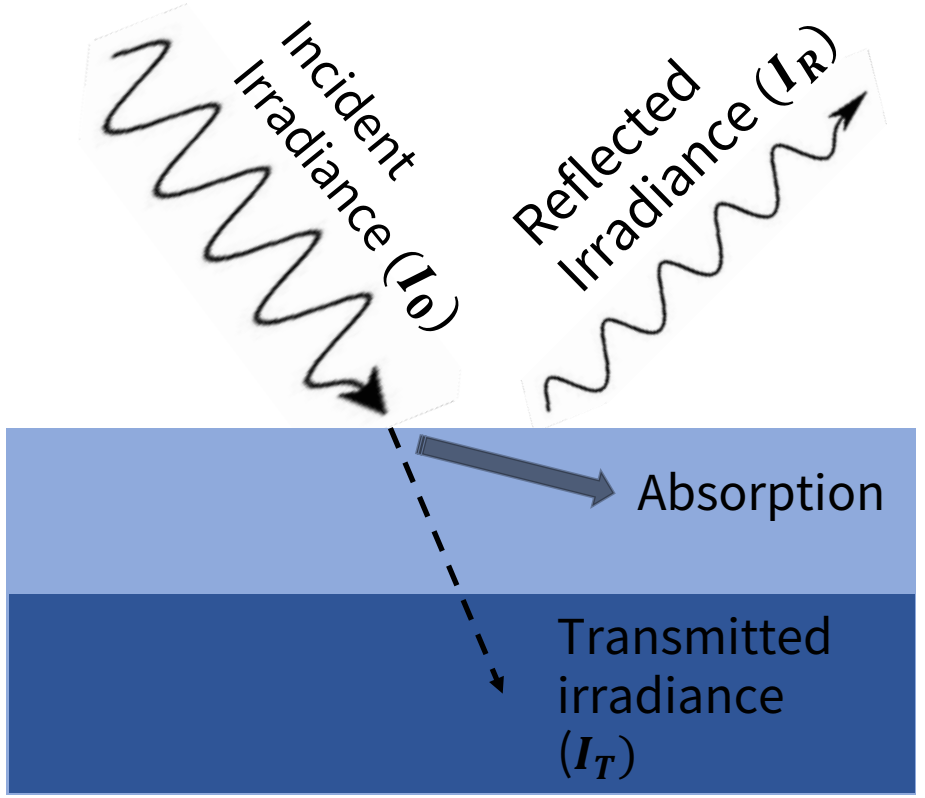
- e^- are excited → Excited e- returns to the ground states (ΔE) → Light/thermal E
- ΔE : depending on the band gap !! → Can be used analyzing materials properties



Optical Processes - Optical Property

III. Reflectance, Transmittance, Absorbance

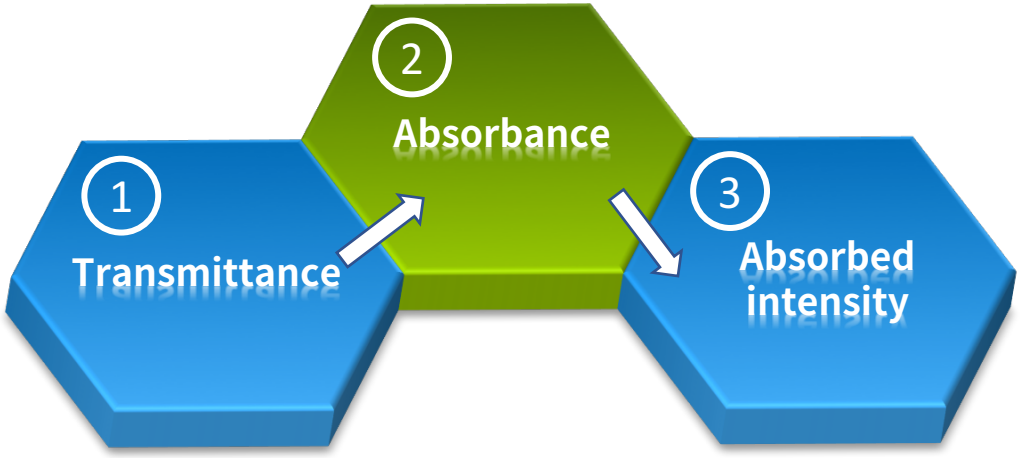
- Reflectance (**R**) can be expressed by, $\boldsymbol{R = I_R/I_0}$ with I_R = Reflected irradiance, I_0 = Incident irradiance (W/cm^2)
- Transmittance (**T**), $\boldsymbol{T = I_T/I_0}$, I_T = Transmitted irradiance
- According to the Energy conservation, $\boldsymbol{T + R = 1}$

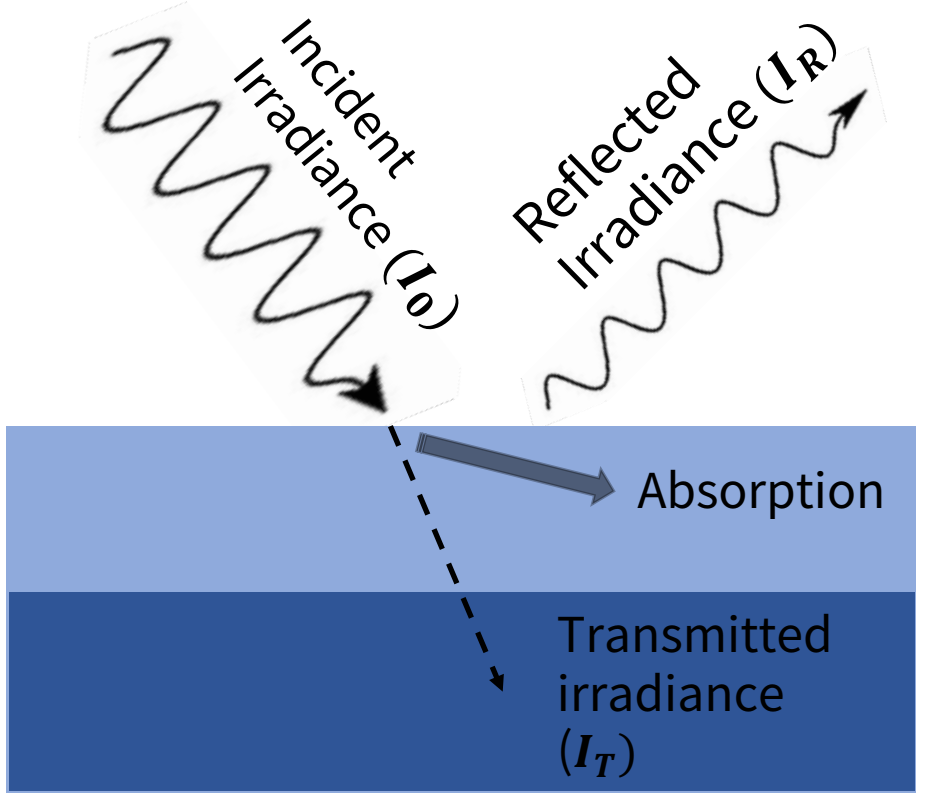


Optical Processes - Optical Property

III. Reflectance, Transmittance, Absorbance

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



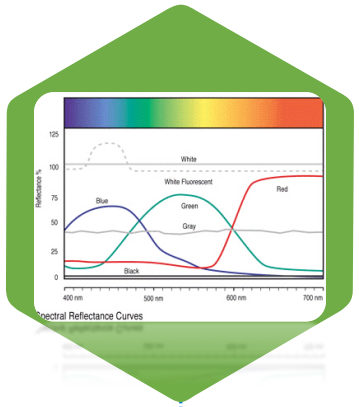


- Absorbance (A), $A = log_{10}(I_0/I_T) = -log_{10}T$

Optical Processes - Optical Property

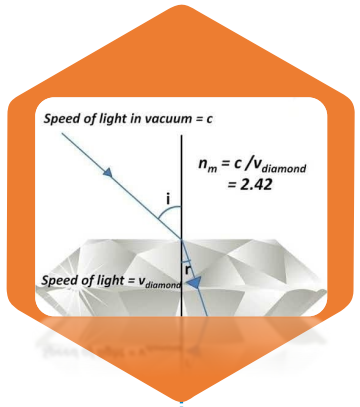
What are the measurable optical properties in experiments, directly ?

[Image Sources]
1. https://www.sabic-ip.com/cxp/jsp/user/LearnAboutColor/ColorBasicsDetail/reflectance_curves.jsp
2. ttps://www.villarrealjewelers.com/refractive-index-diamond-2
3. Preparation, Characterization, Properties and Application of Nanofluid



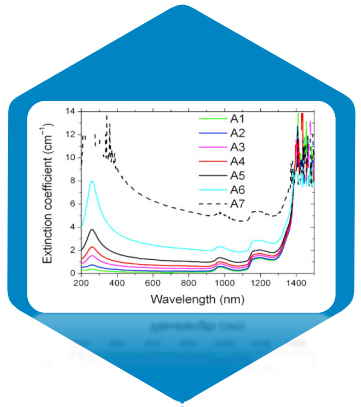
Reflectance, R(ω)

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



Refractive Index, *n*(ω)

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



Extinction coefficient, K(ω)

- It describe attenuated light when passing through a medium
- Mass attenuation coefficient
- Imaginary part of **n(ω)**

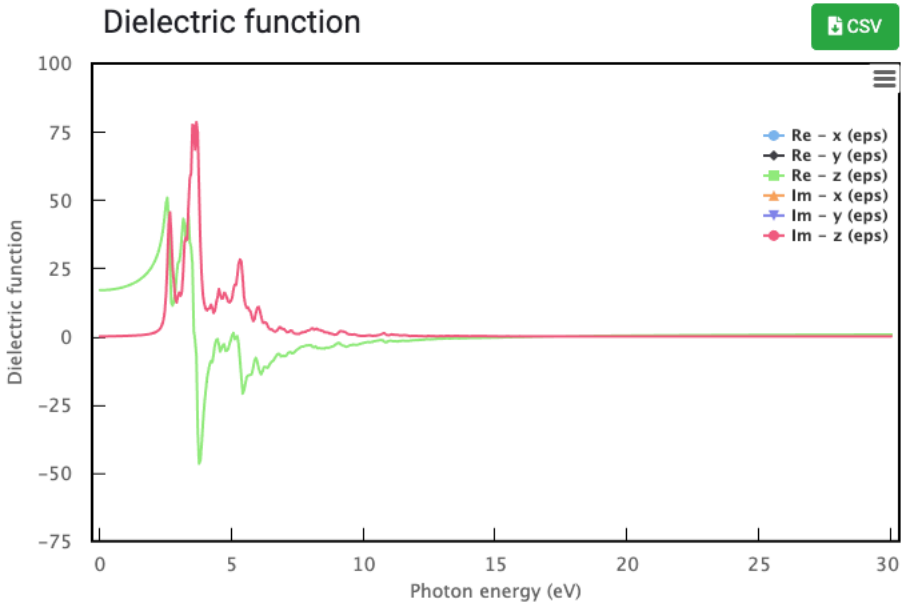
Optical Processes - Optical Property

- 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.

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



Refer to Open Research on MatSQ !!

Optical Processes - Optical Property

- Dielectric Function / Refractive index / Absorption coefficient

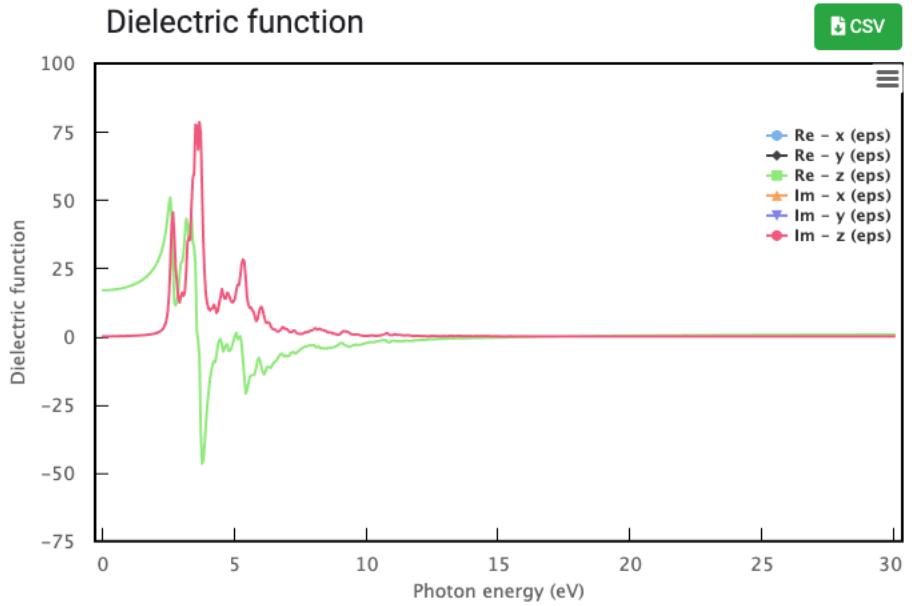
I. Dielectric Function / Refractive index

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

Extinction coefficient

$$\sqrt{\epsilon(\omega)} = n(\omega) + iK(\omega)$$

Complex Refractive Index



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

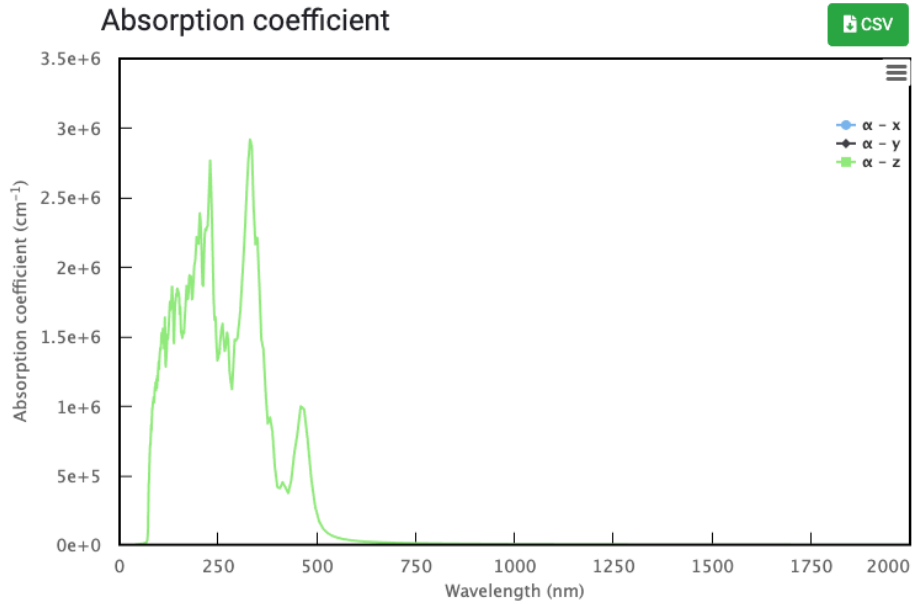
II. Absorption coefficient (α)

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

Extinction coefficient

$$\alpha(\omega) = \frac{4\pi K(\omega)}{C}$$

Speed of light



Refer to Open Research on MatSQ !!

Optical Processes - Optical Property

- Dielectric Function / Refractive index / Absorption coefficient

III. Wrap-up

Imaginary Part

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$$

Real Part

Extinction coefficient

$$\sqrt{\epsilon(\omega)} = n(\omega) + iK(\omega)$$

Complex Refractive Index

Extinction coefficient

$$\alpha(\omega) = \frac{4\pi K(\omega)}{C}$$

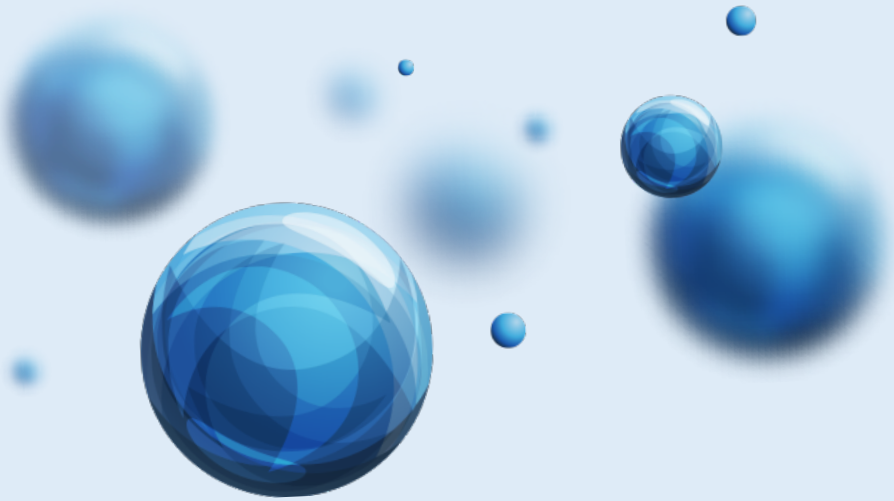
Speed of light

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

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

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.

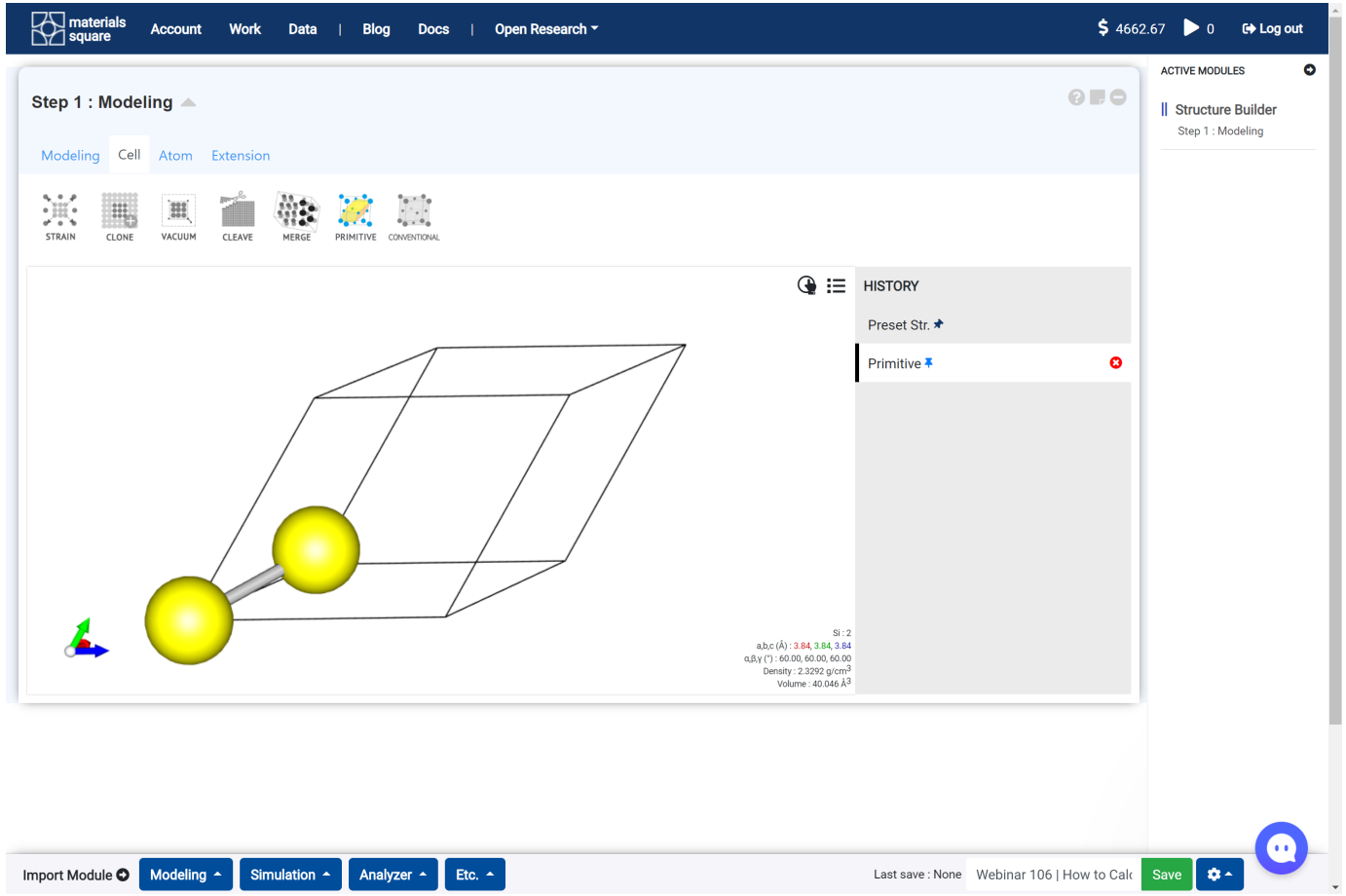
II. Post-process

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

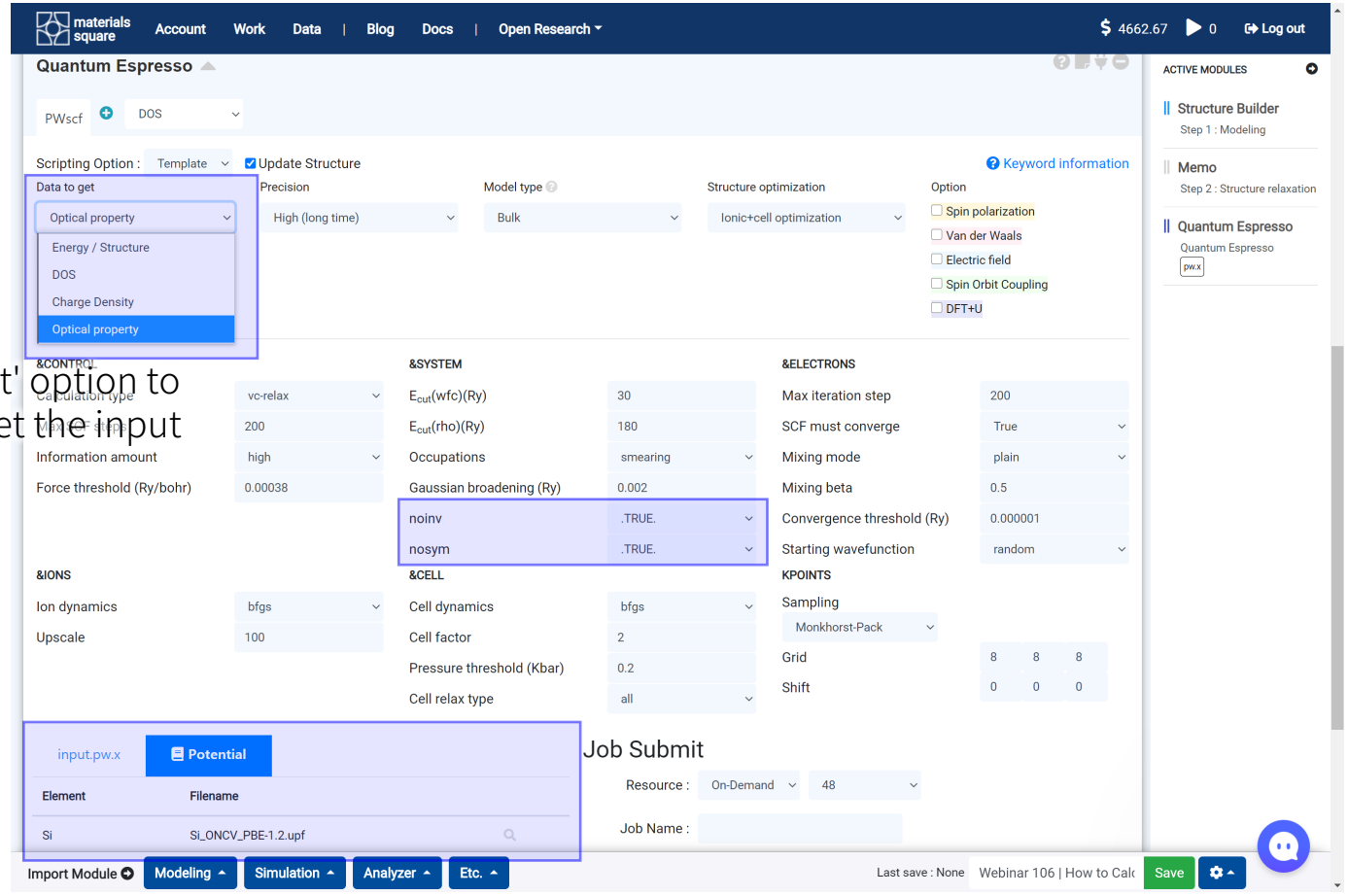
7. Add the 'Optical Property' module, and connect that to the Quantum Espresso module with the 'Optical property' tab.

Step 1. Simulation Modeling

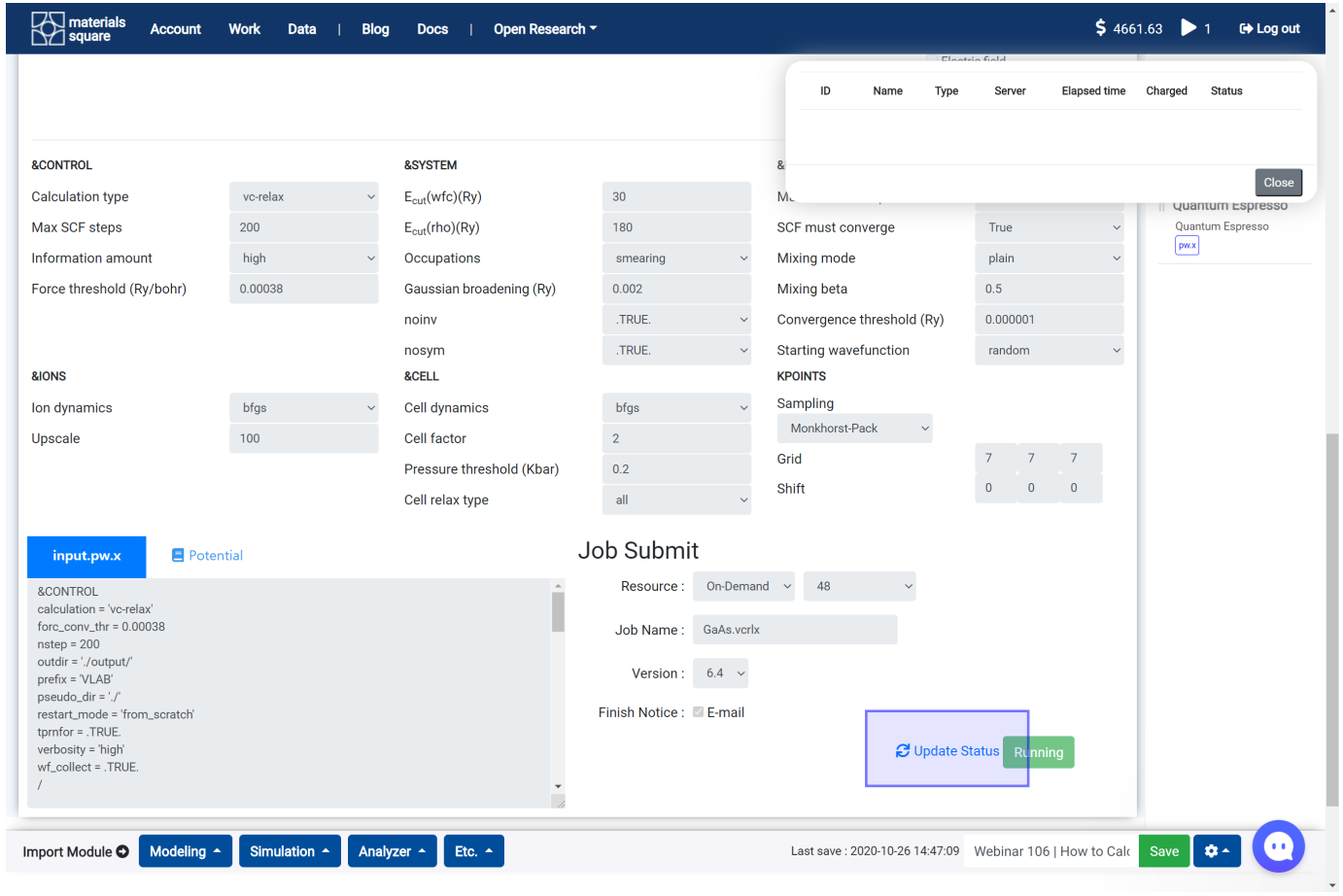


Step 2. Structural Relaxation

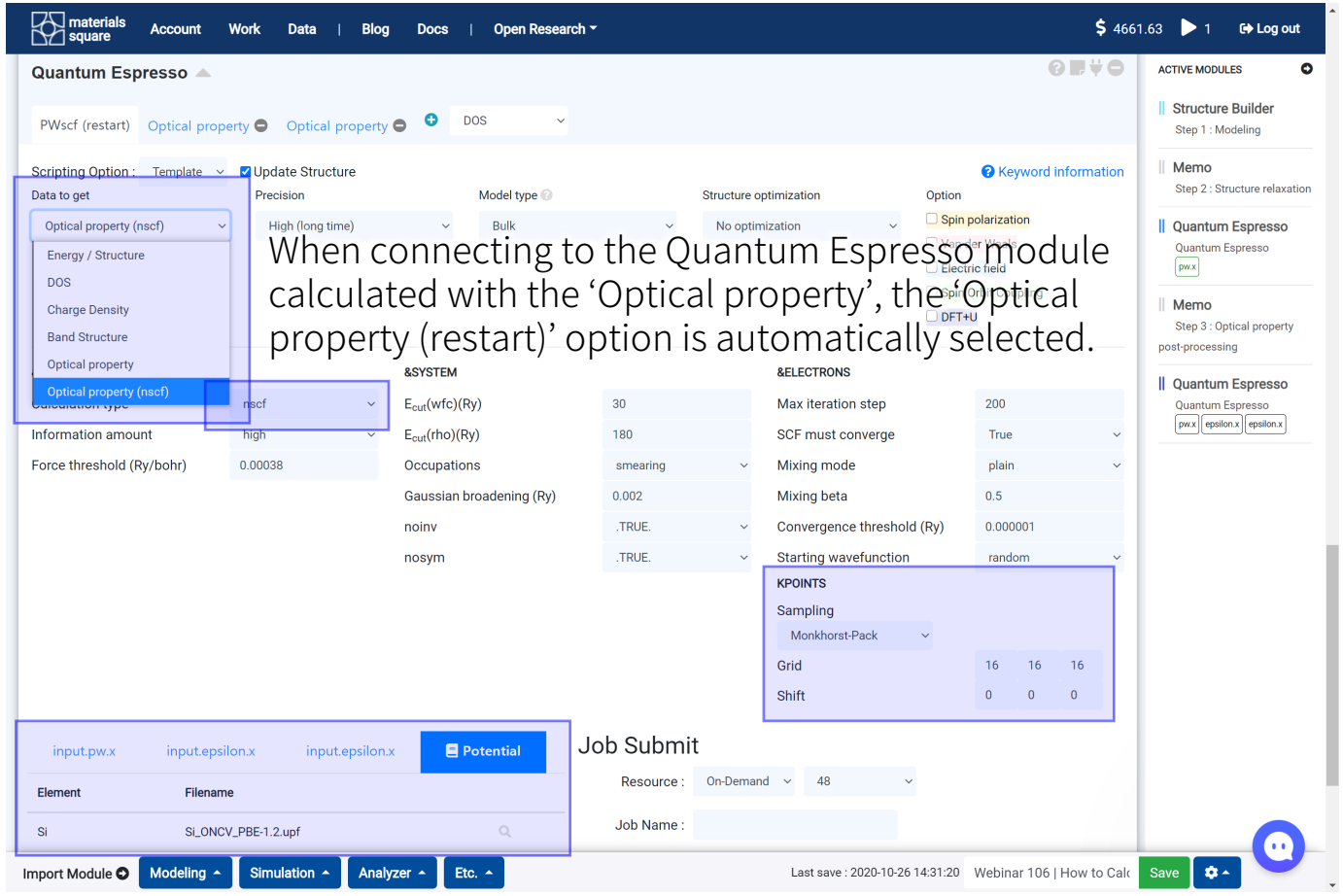
If you change the 'Data to get' option to 'Optical property', you can set the input more conveniently.



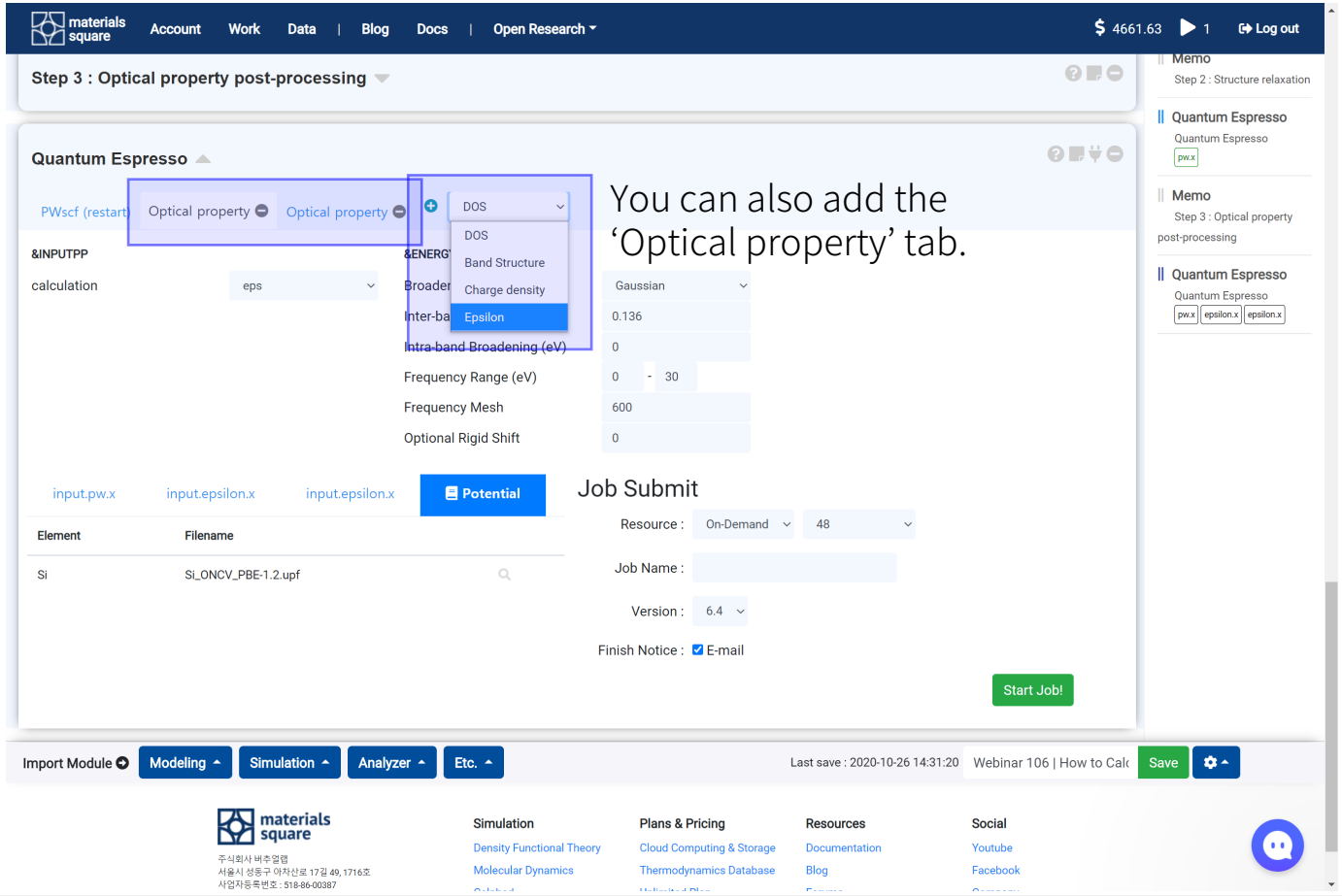
Step 3. When the calculation is finished, press ‘Update Status’ to update the status bar.



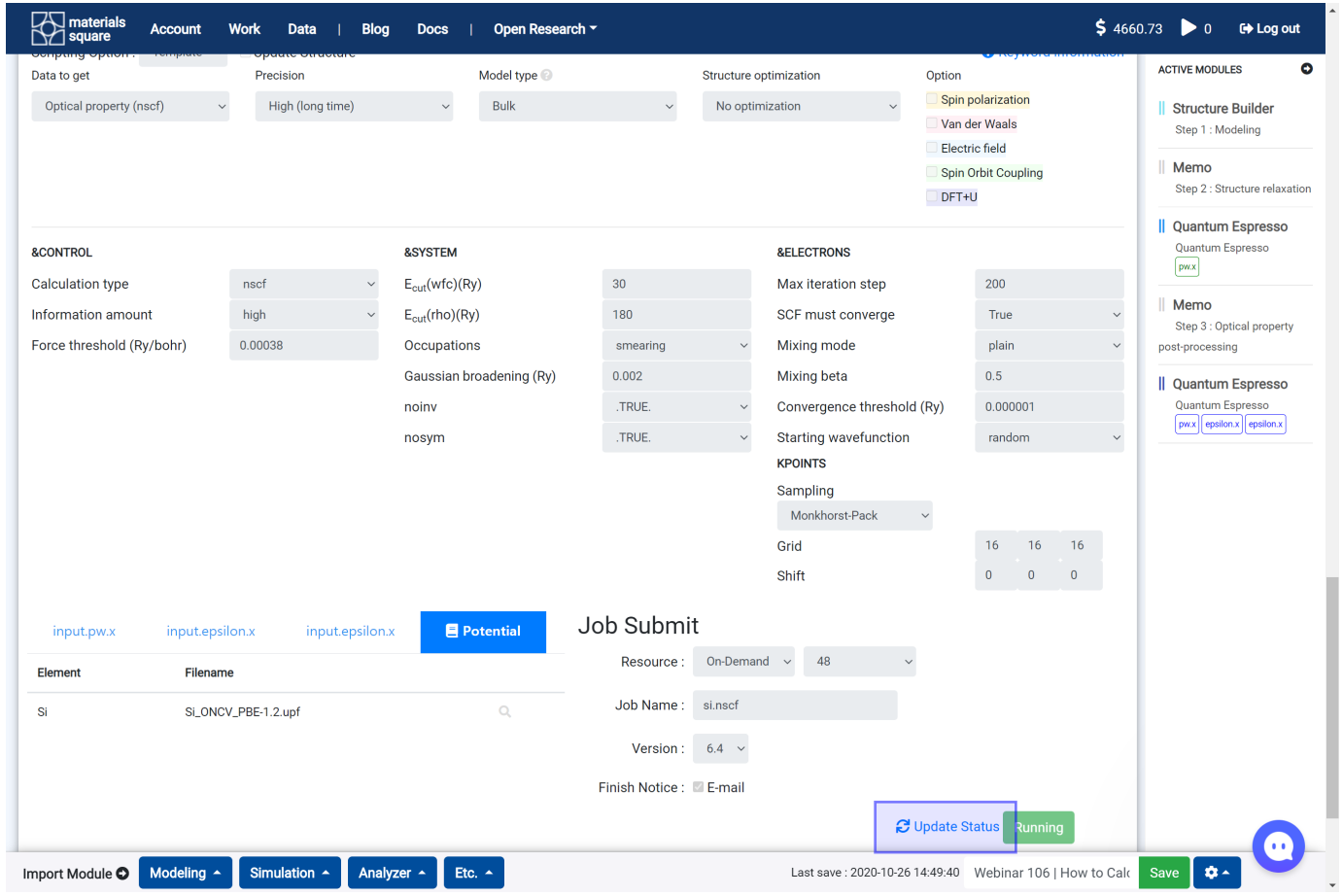
Step 4. NSCF Calculation



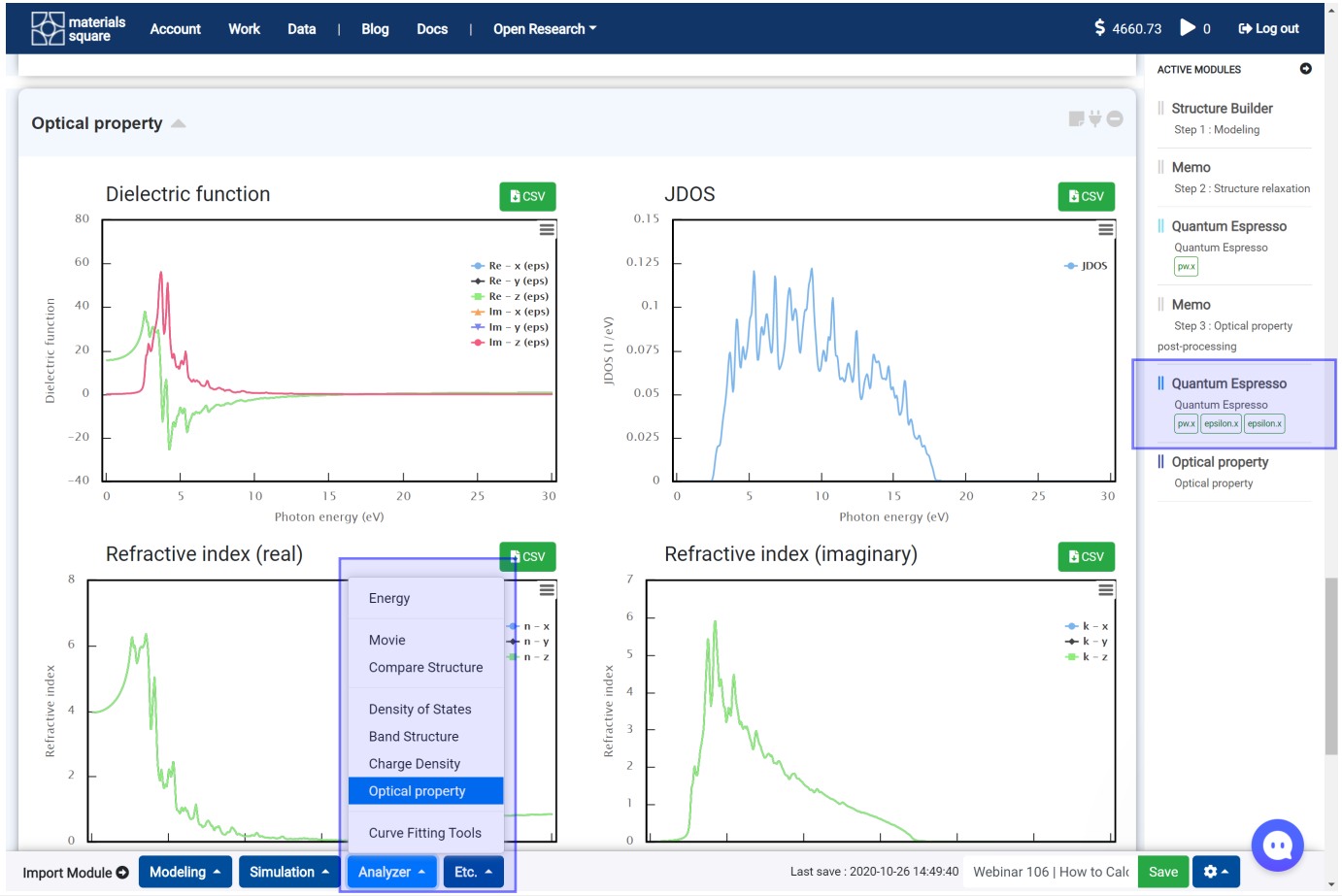
Step 5. Also, the ‘Optical property’ tab added.
In the ‘Optical property’ tab, you can set the input for epsilon.x calculation.



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



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



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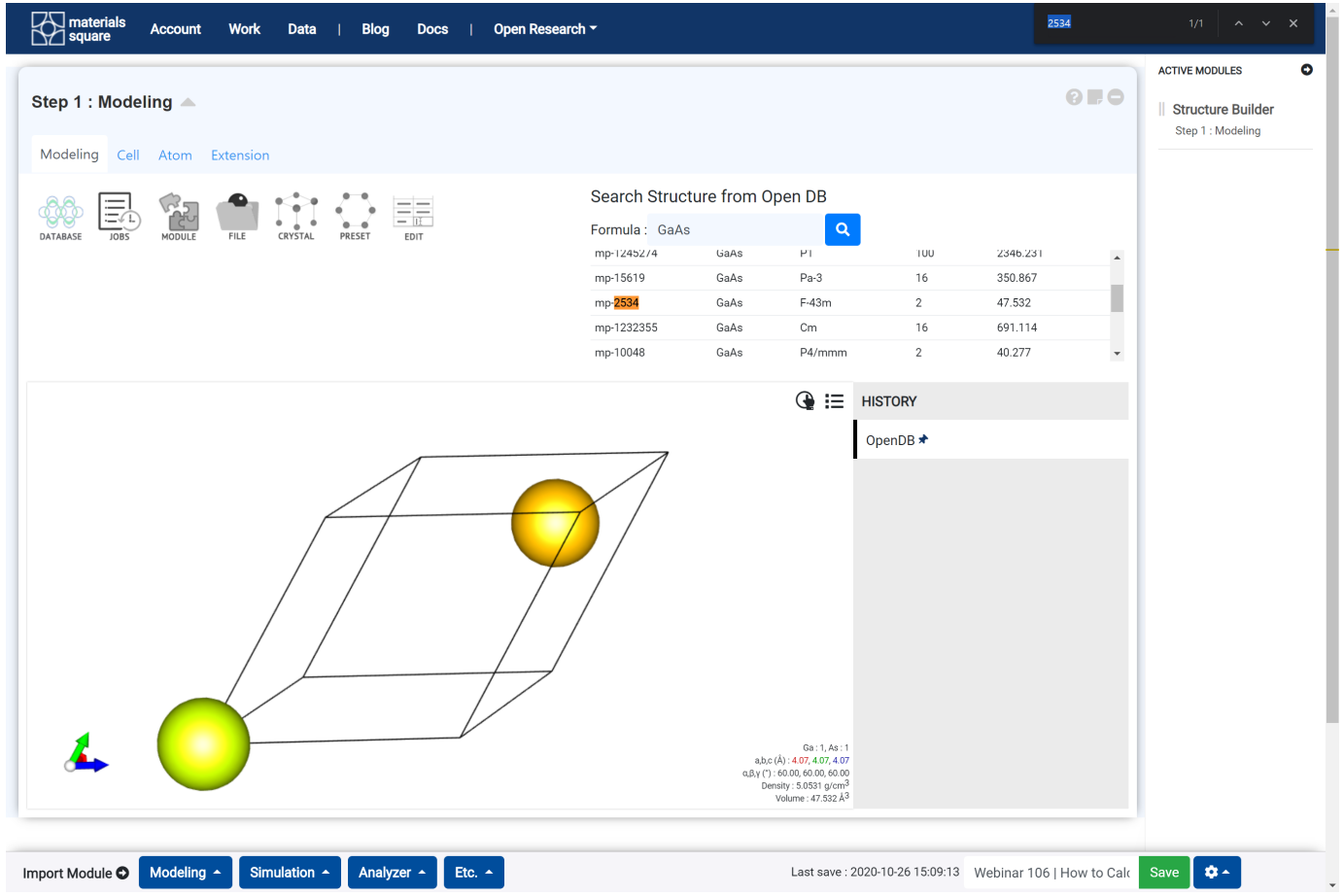

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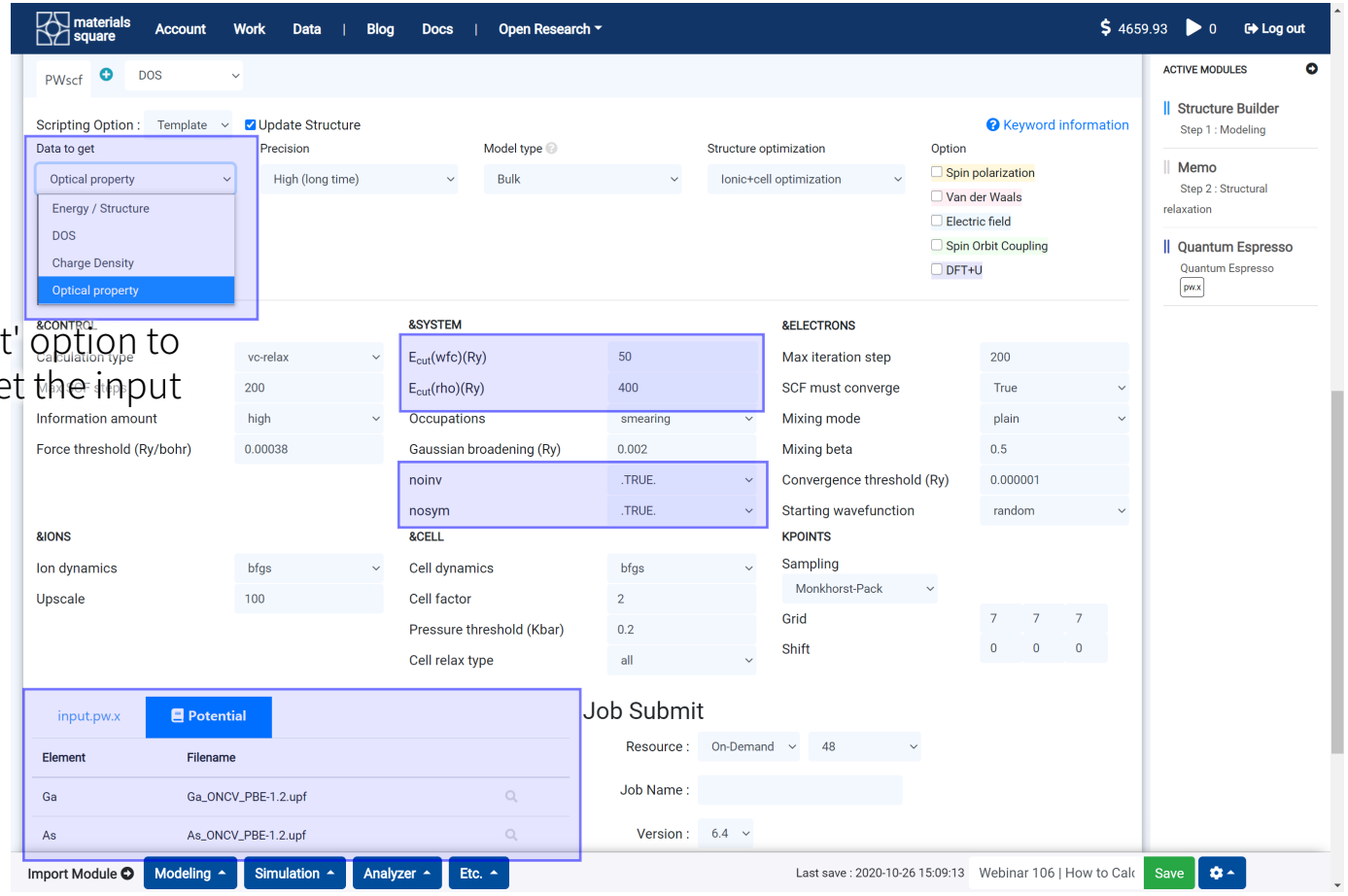

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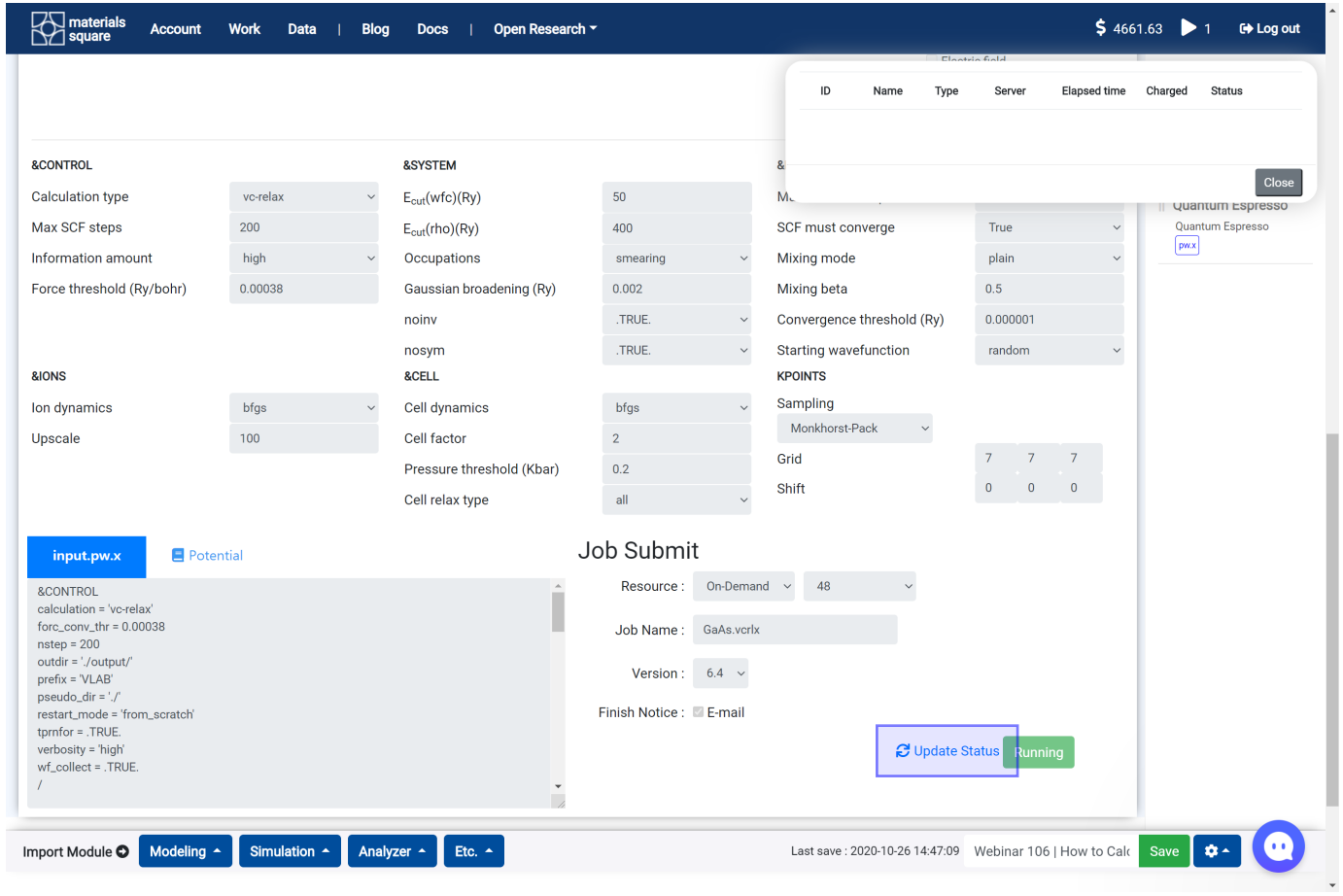

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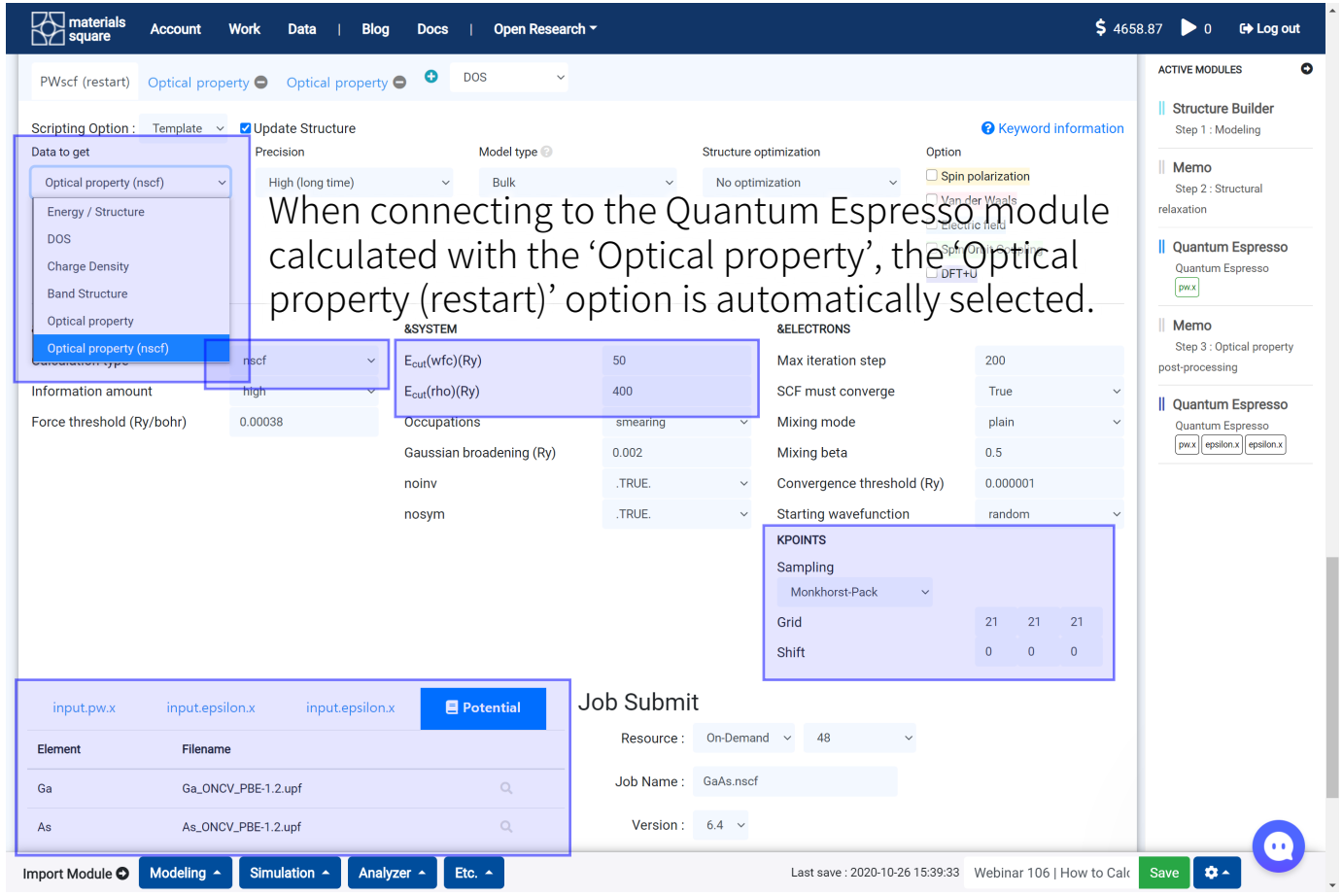

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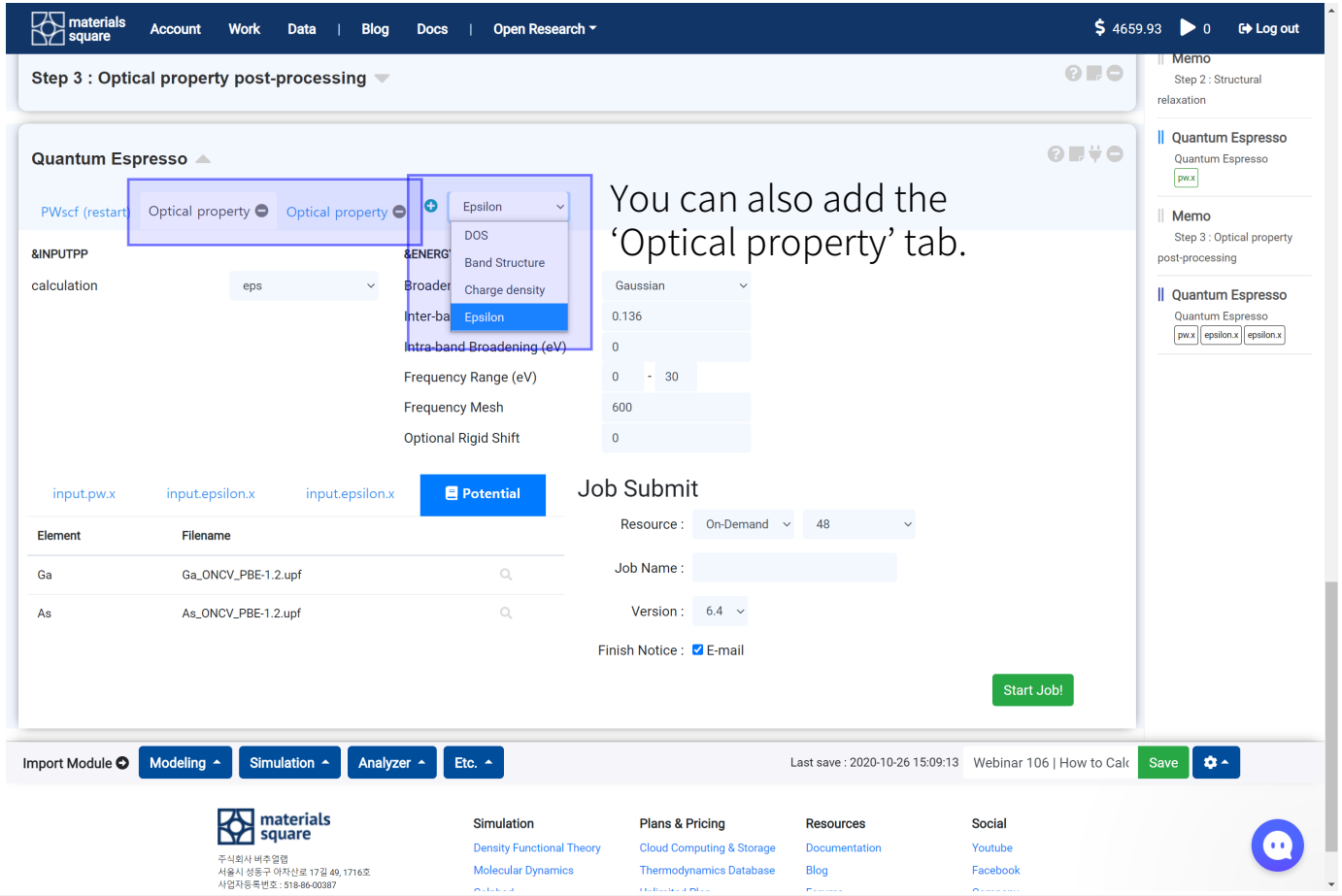

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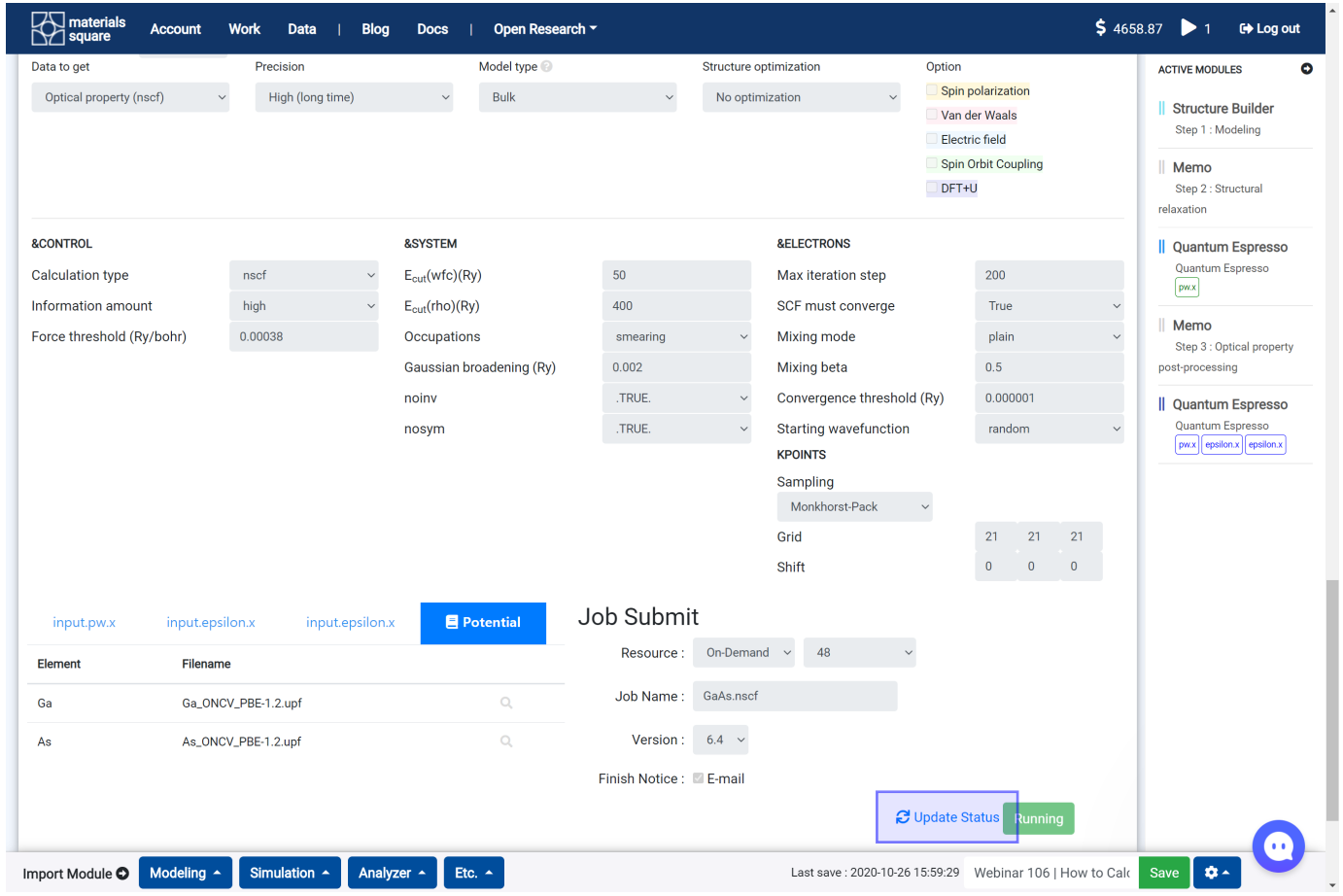
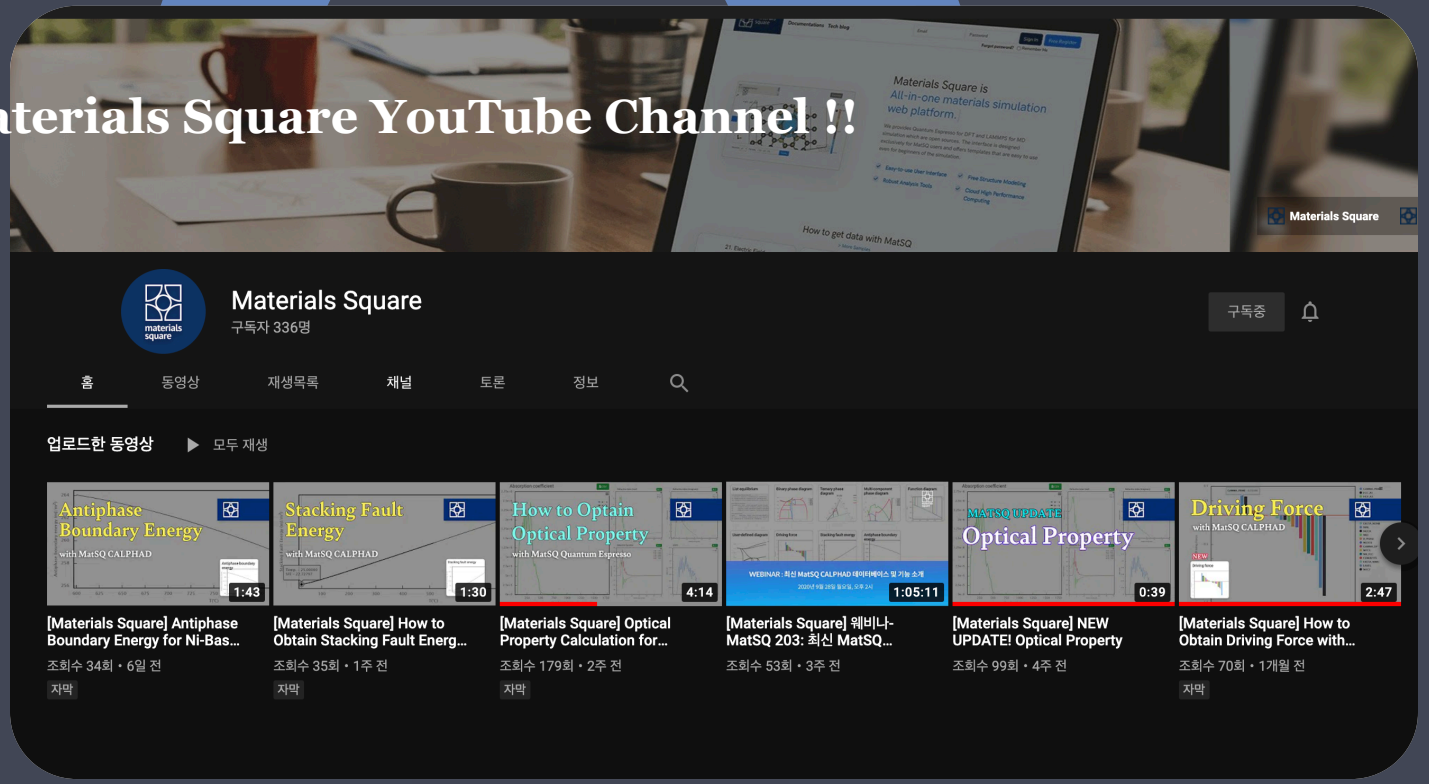


Step 7. Add the 'Optical Property' module, and connect that to the Quantum Espresso module with the 'Optical property' tab.

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



Any Questions

Thank You

Address

1716, Achasan-ro 17gil 49, Seongdong-gu, Seoul, Korea

Contact Number

02-3293-0204

Email Address

support@matsq.com