Ministry of Higher Education
and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- The seventh lecture -

Stage 4

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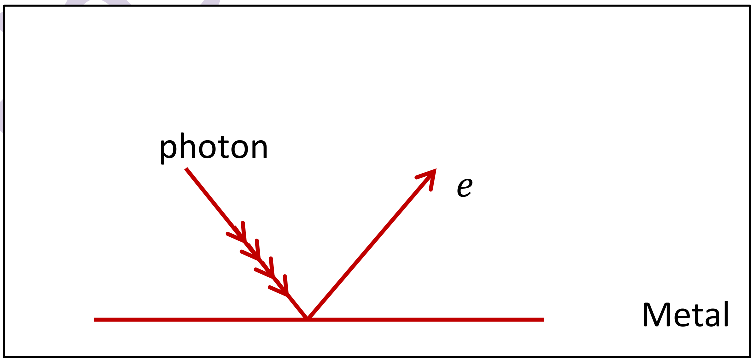
Photo electric effect

One of the first applications of quantum chemistry hypotheses is the interpretation of the photoelectric effect by the einstein world (1905). Photoelectric effect

(The emission of electrons from the surface of some elements by light and this effect is the basic rule in the work of the photovoltaic cell that is sensitive in detecting and measuring electromagnetic radiation)

So it's a way to convert light into electric power like in the shape.

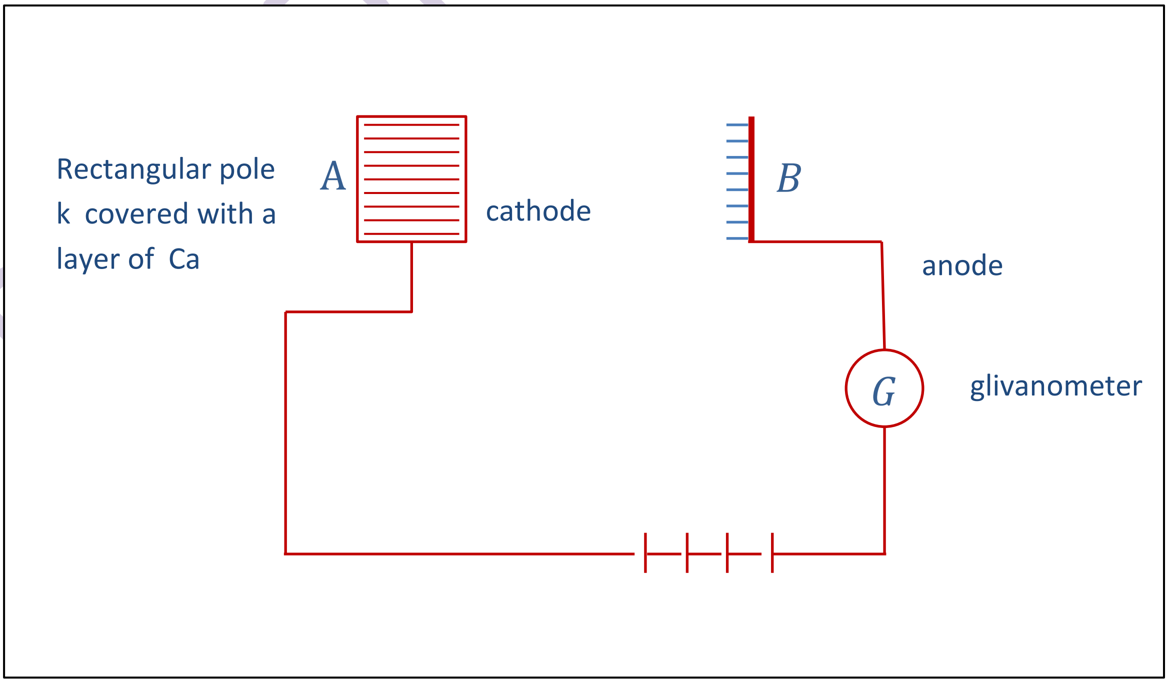


Hertz 1887 illustrated the phenomenon of photoelectric effect in his experiment. The device consists of a treadmill of air (why)?

It contains two electrode, one positive (B) and the other negative (A)

The electrode (A) is covered with an active metal or compound for active metal or alloy for that active metal with elements such as bluntness and tin. Caesium was selected in the manufacture of photovoltaic cells. Then he shed pv radiation (UVrays) on the surface of the metal, the electrons move from A→B, i.e. when the future electrode is exposed to light at a certain frequency, the electrons will be emitted from the cathode electrode to the anode and the circle will be completed. The current passing through the kelvanometer is directly proportional to the number of electrons emitted per second.

Thus, the number of protons that collide with the pole surface is proportional, as in the following form, which shows the PV cell and the electrical circuit.



We conclude:

1 Use different frequencies and tensions:

When you take a certain frequency there is no emission but another frequency occurs a emission so there must be a certain frequency called the threshold frequency (ther shold frequency)

It is the lowest frequency of light required to emit electrons, so if the frequency is lower than the limit frequency, there is no emission.

2 The value of the photoelectric current (number of electrons emitted) is proportional to the energy of the fallen radiation

3 The kinetic energy of the electrons emitted is proportional to the frequency of radiation dropped expelled and does not depend on the intensity of the fallen light

Interpretation of the phenomenon of photovoltaic effect

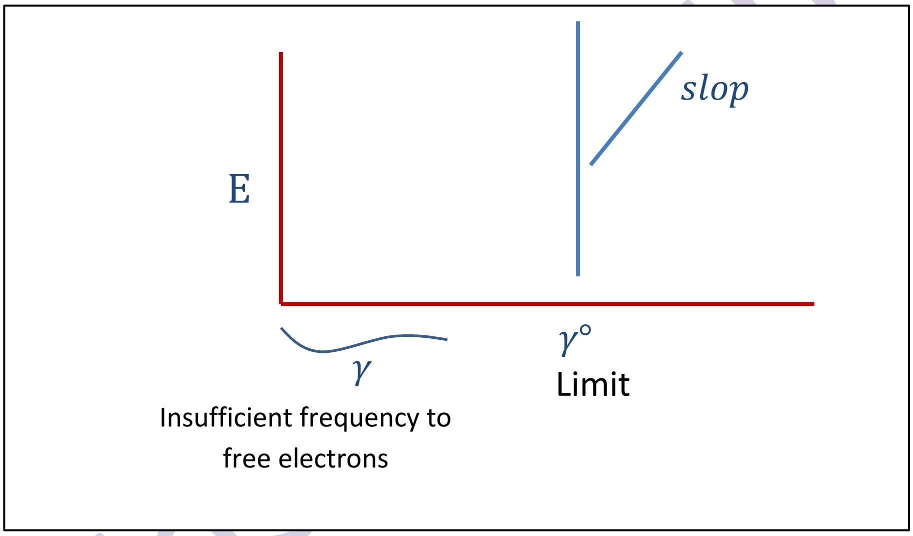
When photons collide with electrons on the surface of the metal, their energy is transferred to the electron, where part of the energy is consumed to overcome the gravitational force of the surface, and the rest appears as an electron's kinetic energy and increases with increased frequency.

That is, when metals absorb light, the total energy of photon hy is given to one electron of metal.

If this energy is enough, the electron can penetrate the potential barrier of the metal surface.

This can be explained by the following form.

Represents the relationship between energy as a function of radiation frequency and as follows



The relationship between photon energy and electron kinetic energy

$$E_{Kin} = hy \quad \dots \dots \dots (1$$

$$= h(y - y_o) \quad \dots \dots (2)$$

Critical frequency y_o critical frequency: frequency needed to free the electron only without giving it kinetic energy

$$\because E = \frac{1}{2}mv^2$$

$$\frac{1}{2}mv^2 = h(y - y_o)\_\_\_\_\_(3)$$

$$\frac{1}{2}mv^2 = hy - hy_o \_\_\_\_\_(4)$$

So the amount of energy needed to extract the electron is hy_o, a constant called work function (w_o)

So the relationship becomes:

$$\frac{1}{2}mv^2 = hy - w_o \_\_\_(5)$$

therefore:

a. If $w_o = hy$ it's zero, the power is zero.
b. If the critical frequency is greater than the fallen rays, there is no electron emission.

So we deduce from the equation (5)

The energy in which the electron is emitted is less than the fallen photon energy by hy_o and is called the metal's work allowance.

where $E_{max} = T_{max} = \frac{1}{2}mv^2$

(If the limit frequency and wavelength are required, Tmax = 0)

So we conclude. $hy = w_o \; \ldots \; \ldots \; \ldots (6$

Thus, the total number of photons can be found from the relationship as:

$$No\ of\ photon = \frac{E_{totoal}}{E_{photon}}$$

$$= \frac{watt * \frac{J.sec}{watt} * t}{hy}$$

$$1pm = 10^{-12}m$$

$$1A^{\circ} = 10^{-10}m$$

$$1nm = 10^{-9}m$$

$$1\mu = 10^{-6}m$$

$$1ev = 1.6 * 10^{-19}J = 1.6 * 10^{-12}\ erg$$

Important conversions

Application for photo electric effect

1- Einstein principle (dualting light)

2- Compton effect

3- debroglie principle (dualting matter)

4- Hisen brag uncertainty principle

First: Einstein principle (dualting light)

Einstein Principle (Principle of Duality)

Duality of light: wave-particle wave and minute wave

In traditional physics, some phenomena explain the wave properties and the minute properties where the minute properties or semi-minute properties of electromagnetic radiation were discovered through the electromagnetic effect as well as the Kosptin effect, so Einstein developed and based on the plank hypothesis the following:

$$1\text{-}E = h\,y \quad plank\ theory \_\_\_\_\_(1$$

$$2\text{-}E = mc^2 \quad Eimstien\ theory \_\_\_\_\_(2$$

$$hy = mc^2$$

$$hy = mc\,c$$

$$hy = p\,c$$

$$p = \frac{hy}{c} \qquad \because \frac{y}{c} = \frac{1}{\lambda}$$

$$p = \frac{h}{\lambda} \; or \; \lambda = \frac{h}{p} \_\_\_\_\_(3$$

The first equation was based on frequency, which is a characteristic of the wave and the second equation depended on body mass, which is a minute trait (physical), so the frequency and particle were linked by the Einstein and De Broly equation.

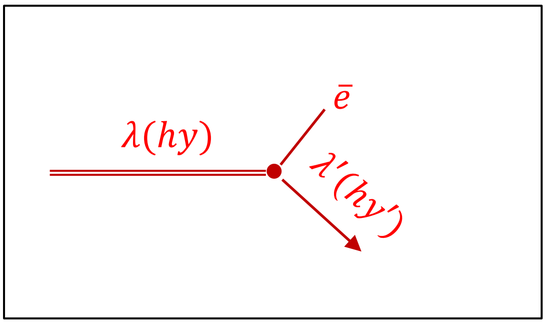
Q/ What is the difference between Einstein's idea and Max Planck's idea of estimating the phenomenon of electromagnetic radiation

II: Kombtn Effect Compton Effect

When a single-wavelength X-ray was shed on carbon, it was noted that the broken rays included the longest wave longer than the controlled rays.

This phenomenon was interpreted on the basis of diffraction refraction.

Due to the collision between x-ray photons and the single electron in the target as in the following chart



Thus, through the Compton phenomenon, a discovery has been developed (an equation linking the change between the wavelength of light and the$\Delta\lambda\emptyset$ scattoing angle dispersion angle) that illustrates the next relationship.

$$\Delta\lambda = \frac{2h}{m\,c}\,sin^2\emptyset$$

This relationship illustrates the relationship of the refractive angle with the energy of the fallen light.

Third: Duplicity de Broglie debroglie principle

(Each object in a state of movement accompanied by a wave that is inversely proportional to the momentum)

De Bruley assumed that Einstein's waveform and minute behavior also applies to matter when the material is for atomic dimensions.

$$\lambda = \frac{h}{p}$$

Represents the characteristic of the wave λ:

It's a particle. p:

Thus, the electron, neutron and other particles show this characteristic and the wavelengths associated with them are within the boundaries of the inter-atom distances of solids, so the relationship becomes

$$\lambda = \frac{h}{mv}$$

We conclude that whenever the momentum is small, the wavelength is large and vice versa, so the de Yeroli hypothesis was achieved through the refractive relationship of a bundle of electrons by a crystalline material where the vegetation occurs when wavelengths match the dimensions between the crystalline levels and thus conclude

$$E = \frac{1}{2} mv^2 = \frac{p^2}{2m}$$

Fourth: The principle of indymination of **Hisenberg uncertainty principle**

Hayescoineda principle that states that

(Any pair of specific variables cannot be determined simultaneously with high accuracy))   According to quantum mechanics:

1- possition and momentum

2- energy and time

Simply put, the location and momentum of the electron cannot be set at the same time with high accuracy. There is a limit on the duration of accuracy if the location is determined (displacement)

The inaccuracy in the value of momentum increases, and if time is set for the molecular or atomic state with accuracy, the inaccuracy in the determination of the state's energy increases.

So the mathematical expression of the principle of indeceration of Heisnberk can be derived on the basis of de Broley's relationship and Einstein's relationship.

1) $p = \frac{h}{\lambda}$ ______(1)

2) $E = hy$ ______(2)

For the wave movement, it is given according to the wave equation, which is

$$\psi_{(x,t)} \cdot A\, sin2\pi \left(\frac{x}{\lambda} - yt\right) \_\_\_\_(3$$

$\psi_{(x,t)}$ Represents the wave function

A wave capacity

X Removal (coordinateor location)

Y frequency

t- Time

And you can write an abbreviation where hard $k = \frac{1}{\lambda}$

So it's the relationship.

$$\psi_{(x,t)} = A\, sin2\pi\, (kx - yt) \_\_\_\_(4$$

And by integrating Forer with the order and abbreviation we get the wave movement instead of the cases that follow

1) $\Delta x \cdot \Delta k = \Delta x \cdot \frac{1}{\lambda} \geq \frac{1}{4\pi} \quad \_\_\_\_(5)$

2) $\Delta t \cdot \Delta y \geq \frac{1}{4\pi}$ ______(6)

ΔK ← represents inverted wavelength

ΔY ← frequency change

Δt ← time needed for wave passage

Δx ← the extent of the wave pocket in space (displacement)

So you can find a relationship with Heisnberk as follows:

أ) Heisnberk's relationship with location and momentum

$$\lambda = \frac{h}{p} \quad \_\_\_\_\_\_(1)$$

$$\frac{1}{\lambda} = \frac{p}{h} \quad \_\_\_\_\_\_(2)$$

Inthe relationship above, we conclude.

$$\Delta x \cdot \Delta p / h \geq \frac{1}{4\pi}$$

$$\because \hbar = \frac{h}{2\pi}$$

And when compensated for the relationship above

Conclude

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2\pi}$$

Any inaccuracy in momentum * Inaccuracy in the site equals or greater than if $\frac{\hbar}{2\pi}$ the accuracy in measuring the site increases in accuracy with momentum

With heisenberk's energy relationship with time.

Through the relationships that have been made

$$E = hy \quad \_\_\_\_\_\_\_(1)$$

So change with energy. $\Delta E = h\ \Delta y$ _____(2)

By compensation in the frequency-to-time relationship, we conclude.

$$\Delta t \cdot \Delta E/h \geq \frac{1}{4\pi}$$

$$\because \hbar = \frac{h}{2\pi}$$

$$\therefore \Delta t \cdot \Delta E \geq \frac{\hbar}{2\pi}$$

This means that the longer the time frame of the situation raised is short, the more inaccuracy in the energy level increases, so when the atomand the molecule in theground state are stable, i.e.

Its time life is long, so the inaccuracies at the level are low, i.e. the energy level is more specific.

Heisnberk equations are not experimental errors based on instruments, but something inherited in quantum mechanics, and because of the inaccuracy of these results, quantum mechanics calculations are expressed in a probability.

Q:- what is un certainty for momentum if you know the un certainty for position is 100 pm