Interpolation & Its Application to Solar Cells

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Introduction…

- An important part in a scientist's life is the interpretation of measured data or theoretical calculations.

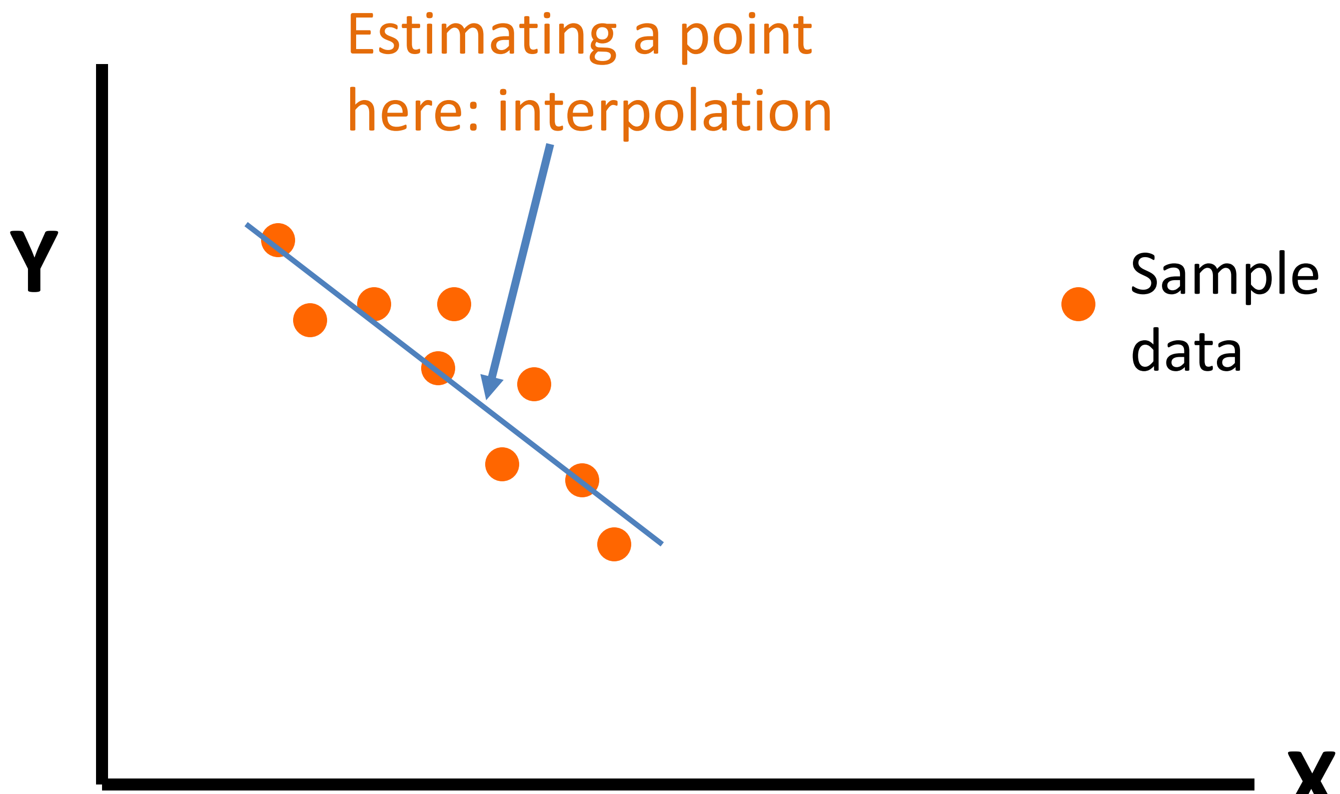
- Usually when you do a measurement you will have a ***<u>discrete</u>*** set of points representing your experiment.

- Assume that the data is represented by pairs of values:
  - an independent variable ***"x,"*** which you vary
  - quantity ***"y,"*** which is the measured value at the point *x*.

x_0	x_1	x_2	x_3
y_0	y_1	y_2	y_3

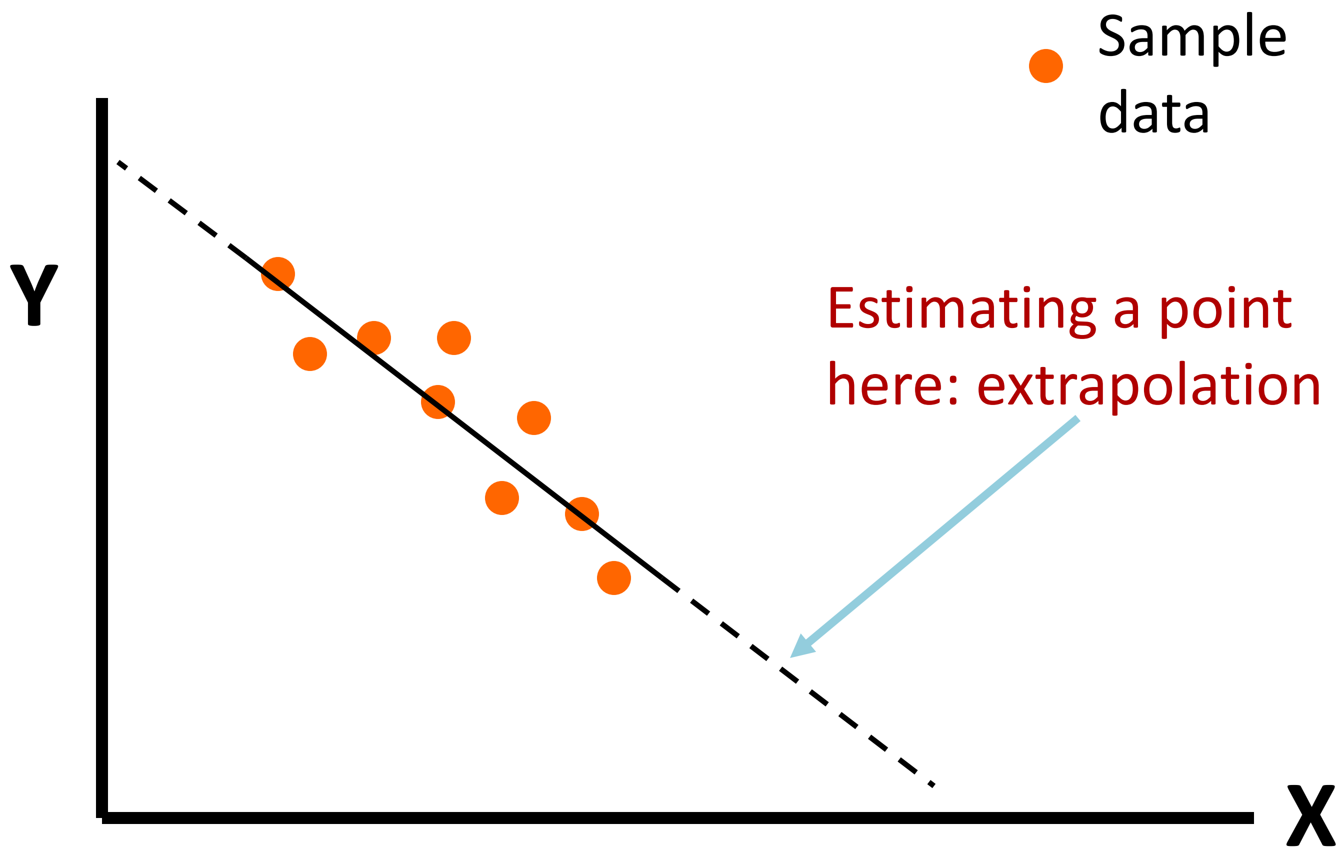
Definition: Interpolation

✓ Estimating the attribute values of locations that are <u>**within**</u> the range of available data using known data values.



Definition: Extrapolation

✓ Estimating the attribute values of locations **outside** the range of available data using known data values.



Interpolation

Interpolation is carried out using approximating functions such as:

1. **Polynomials**
2. Trigonometric functions
3. Exponential functions
4. Fourier methods

Interpolating Polynomials

Following interpolating methods are most popular:

1. Lagrange Interpolation (unevenly spaced data)
2. Newton's Divided Difference (evenly spaced data)
3. Central difference method

Lagrange's Interpolation

i	x	y
0	x_0	$f(x_0)$
1	x_1	$f(x_1)$
2	x_2	$f(x_2)$
3	x_3	$f(x_3)$

The interpolation polynomial is

$$P(x)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}f(x_0)+\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}f(x_1)$$

$$+\frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}f(x_2)+\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}f(x_3)$$

Newton's Method:

1. Forward difference interpolation formula
2. Backward difference interpolation formula
3. Central difference interpolation formula

Newton's Interpolation Method

- The nth degree polynomial may be written in the special form:

$$p(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1) + \cdots + a_n(x-x_0)(x-x_1)\cdots(x-x_{n-1}).$$

- If we take a_i such that $P_n(x) = f(x)$ at n+1 known points so that $P_n(x_i) = f(x_i)$, $i=0,1,\ldots,n$, then $P_n(x)$ is an interpolating polynomial.

Newton's Forward Difference Method

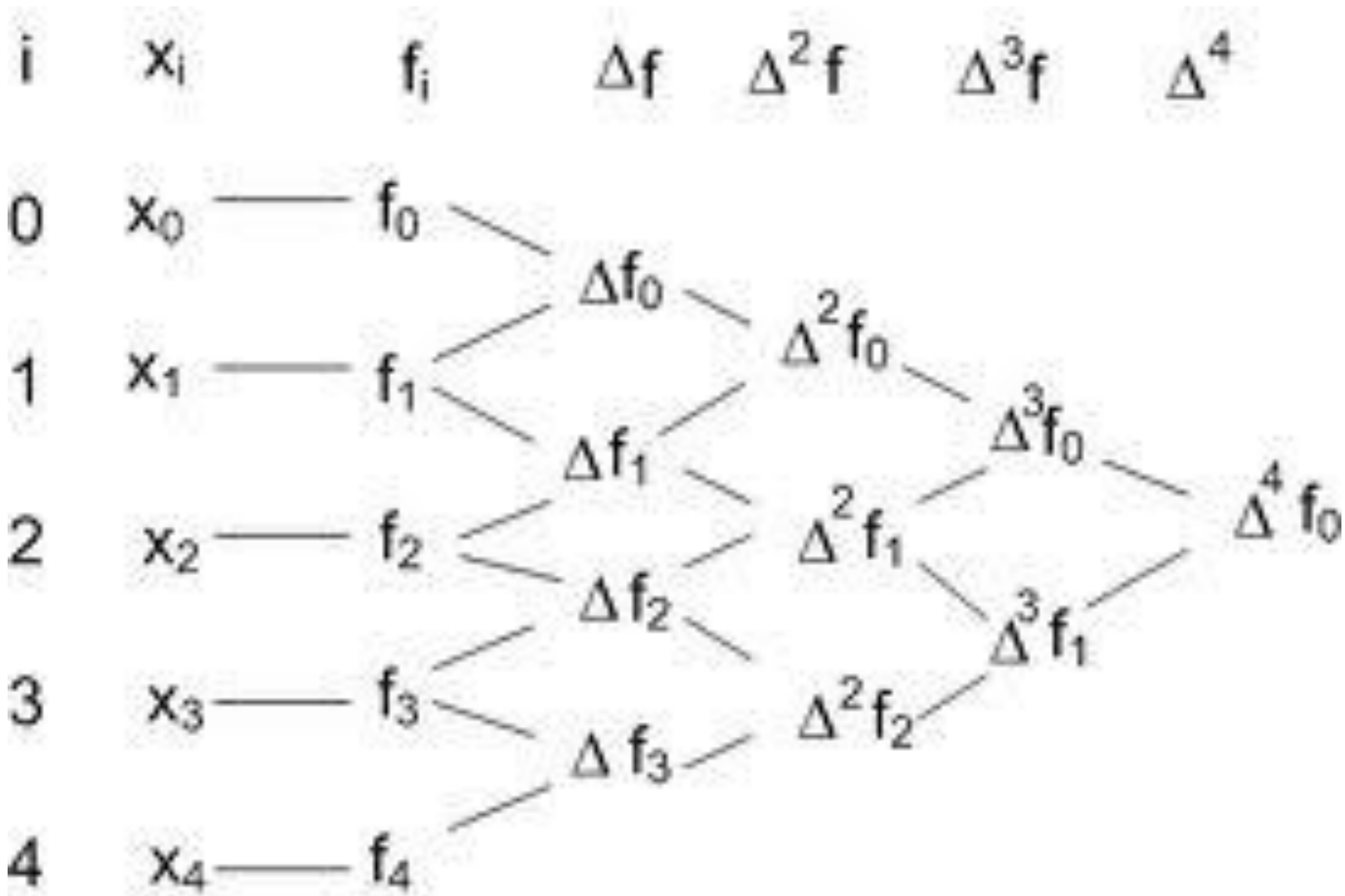
Let $(X_{0,}, Y_0)$, $(X_{1,}, Y_1)$, …, $(X_{n,}, Y_n)$ be the given points with

$X_{i+1} = X_i + h$, $i = 0,1,2,\ldots,(n-1)$.

Finite Difference Operators

- Forward difference operator
  $\Delta f(x_i) = f(x_i + h) - f(x_i)$

Forward Difference Table



NEWTON GREGORY FORWARD INTERPOLATION

For convenience we put $p = \frac{x - x_0}{h}$ and $f_0 = y_0$. Then we have

$$P(x_0 + ph) = y_o + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots + \frac{p(p-1)(p-2)\,L\,(p-n+1)}{n!}\Delta^n y_0$$

Backward Difference Table

i	x_i	f_i	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$
0	0	1					
1	1	2	1				
2	2	4	2	1			
3	3	8	4	2	1		
4	4	16	8	4	2	1	
5	5	32	16	8	4	2	1

NEWTON GREGORY BACKWARD INTERPOLATION

Taking $p = \frac{x - x_n}{h}$, we get the interpolation formula as:

$$P(x_n+ph) = y_0 + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \cdots + \frac{p(p+1)(p+2)\ldots(p+n-1)}{n!}\nabla^n y_n$$

Extrapolation Methods

Linear extrapolation

Polynomial extrapolation

Conic extrapolation

Linear Extrapolation

- Linear Extrapolation means creating a tangent line at the end of the known data and extending it beyond that limit.
- Linear extrapolation will provide good results only when used to extend the graph of an approximately linear function or not too far beyond the known data.
- If the two data points nearest to the point x_* to be extrapolated are (x_k, y_k) and (x_{k-1}, y_{k-1}), linear extrapolation gives the function

$$y(x_*) = y_{k-1} + \frac{x_* - x_{k-1}}{x_k - x_{k-1}}(y_k - y_{k-1}).$$

Polynomial Extrapolation

A polynomial curve can be created through the entire known data or just near the end. The resulting curve can then be extended beyond the end of the known data. Polynomial extrapolation is typically done by means of Lagrange interpolation or using Newton's method of finite differences to create a Newton series that fits the data. The resulting polynomial may be used to extrapolate the data.

Program for Lagrange's Interpolation

```
#include<iostream.h>
#include<conio.h>
int main()
{
    int n,i,j;
    float mult,sum=0,x[10],f[10],a;
    clrscr();
    cout<<"Enter no of sample points ? ";
    cin>>n;
    cout<<"Enter all values of x and corresponding funtional value: "<<endl;
    for(i=0;i<n;i++)
        cin>>x[i]>>f[i];

    cout<<"\nEnter your x for calculation : ";
    cin>>a;

    for(i=0;i<=n-1;i++)
    {
    mult=1;
        for(j=0;j<=n-1;j++)
        {
            if(j!=i)
            mult*=(a-x[j])/(x[i]-x[j]);
        }
        sum+=mult*f[i];
    }
    cout<<"\nThe estimated value of f(x) = "<<sum;
    getch();
    return 0;
}
```

Results: Lagrange's Interpolation

f(x) = xlogx

At x=5, the actual value is **3.4948**

C:\TCWIN451\BIN\NONAME00.EXE

```
Enter no of sample points ? 4
Enter all values of x and corresponding funtional value:
3
1.4313
7
5.9156
9
8.5881
12
12.9501

Enter your x for calculation : 5

The estimated value of f(x) = 3.50811
```

For 4 sample points, answer = **3.50811**

For 7 points answer = **4.49477**

C:\TCWIN451\BIN\LGRNFINA.EXE

```
Enter no of sample points ? 7
Enter all values of x and corresponding funtional value:
3
1.4313
4
2.4082
6
4.6689
7
5.9156
9
8.5881
12
12.9501
14
16.0458

Enter your x for calculation : 5

The estimated value of f(x) = 3.49477
```

Results: Lagrange Inverse Interpolation

Lagrange interpolation formula can also be used for finding the value of x for given value of y.

```
C:\TCWIN451\BIN\LGRNFINA.EXE
Enter no of sample points ? 4
Enter all values of x and corresponding funtional value:
1.4313
3
5.9156
7
8.5881
9
12.9501
12

Enter your x for calculation : 3.50811

The estimated value of f(x) = 4.97812
```

```
C:\TCWIN451\BIN\LGRNFINA.EXE
Enter no of sample points ? 4
Enter all values of x and corresponding funtional value:
1.4313
3
5.9156
7
8.5881
9
12.9501
12

Enter your x for calculation : 3.4948

The estimated value of f(x) = 4.9662
```

$$f(x) = 8x^2 - 6x + 1$$

At x=5, value obtained: **171**

Exact Value: **171**

C:\TCWIN451\BIN\LGRNFINA.EXE

```
Enter no of sample points ? 4
Enter all values of x and corresponding funtional value:
0
1
3
55
6
253
9
595

Enter your x for calculation : 5

The estimated value of f(x) = 171_
```

Results: Lagrange Extrapolation

Exact value = 17.6413

C:\TCWIN451\BIN\LGRNFINA.EXE

```
Enter no of sample points ? 7
Enter all values of x and corresponding funtional value:
1
0
3
1.4313
6
4.6689
7
5.91568
10
10
12
12.9501
13
14.4812

Enter your x for calculation : 15

The estimated value of f(x) = 17.6738_
```

C:\TCWIN451\BIN\LGRNFINA.EXE

```
Enter no of sample points ?
4
Enter all values of x and corresponding funtional value:
0
1
1
3
3
55
5
171

Enter your x for calculation : 9

The estimated value of f(x) = 595_
```

Results: Newton- Gregory Forward Interpolation

f(x) = xlogx

C:\TCWIN451\BIN\FWDINTP.EXE

```
enter the eqally spaced values of x::>
4
6
8
10

enter the corresponding values of y::>
2.4082
4.6689
7.2247
10


          FORWARD DIFFRENCE TABLE IS:::>

         4    2.408         2.3         0.3     -0.076
         6    4.669         2.6        0.22
         8    7.225         2.8
        10       10

enter the value of x for which y(x) needs to be calculated
5


          when x=5         y[5]==3.5191
```

C:\TCWIN451\BIN\FWDINTP.EXE

```
enter the corresponding values of y::>
2.9394
4.072
5.2839
6.5629
7.9
9.2883
10.7225


        FORWARD DIFFRENCE TABLE IS:::>

     4.5    2.939        1.1      0.079    -0.012     0.0032    -0.0011     0.0006
     5.5    4.072        1.2      0.067    -0.009     0.0021    -0.0005
     6.5    5.284        1.3      0.058   -0.0069     0.0016
     7.5    6.563        1.3      0.051   -0.0053
     8.5      7.9        1.4      0.046
     9.5    9.288        1.4
    10.5   10.722

enter the value of x for which y(x) needs to be calculated
5


        when x=5        y[5]==3.5006
```

7 input values, answer = 3.50

4 input values, answer = 3.52

Results: Newton's Extrapolation

```
C:\TCWIN451\BIN\FWDINTP.EXE
enter the eqally spaced values of x::>
5.5
6.5
7.5
8.5

enter the corresponding values of y::>
4.07199
5.2839
6.5629
7.9


        FORWARD DIFFRENCE TABLE IS:::>

     5.5   4.072        1.2      0.067     -0.009
     6.5   5.284        1.3      0.058
     7.5   6.563        1.3
     8.5     7.9

enter the value of x for which y(x) needs to be calculated
5


        when x=5        y[5]==3.4792
```

Results: Newton- Gregory Backward Interpolation

$f(x) = x\log x$

C:\TCWIN451\BIN\BWDINTP.EXE

```
enter the corresponding values of y::>
-0.0775
0.3266
0.9125
1.6165
2.4082
3.2699
4.1898


       BACKWARD DIFFRENCE TABLE IS:::>

    0.8 -0.0775
    1.6  0.3266       0.4
    2.4  0.9125      0.59      0.18
    3.2   1.617       0.7      0.12    -0.064
      4   2.408      0.79     0.088     -0.03     0.033
    4.8    3.27      0.86      0.07    -0.018     0.013    -0.021
    5.6    4.19      0.92     0.058    -0.012    0.0059   -0.0068     0.014

enter the value of x for which y(x) needs to be calculated: 5


       when x=5        y[5]==3.521
```

C:\TCWIN451\BIN\BWDINTP.EXE

```
enter the eqally spaced values of x::>
2.5
3.5
4.5
5.5

enter the corresponding values of y::>
0.9948
1.9042
2.9394
4.0719


       BACKWARD DIFFRENCE TABLE IS:::>

    2.5  0.9948
    3.5   1.904      0.91
    4.5   2.939         1      0.13
    5.5   4.072       1.1     0.097    -0.029

enter the value of x for which y(x) needs to be calculated: 5


       when x=5        y[5]==3.526
```

For 4 points with smaller value of h (interval)

C:\TCWIN451\BIN\BWDINTP.EXE

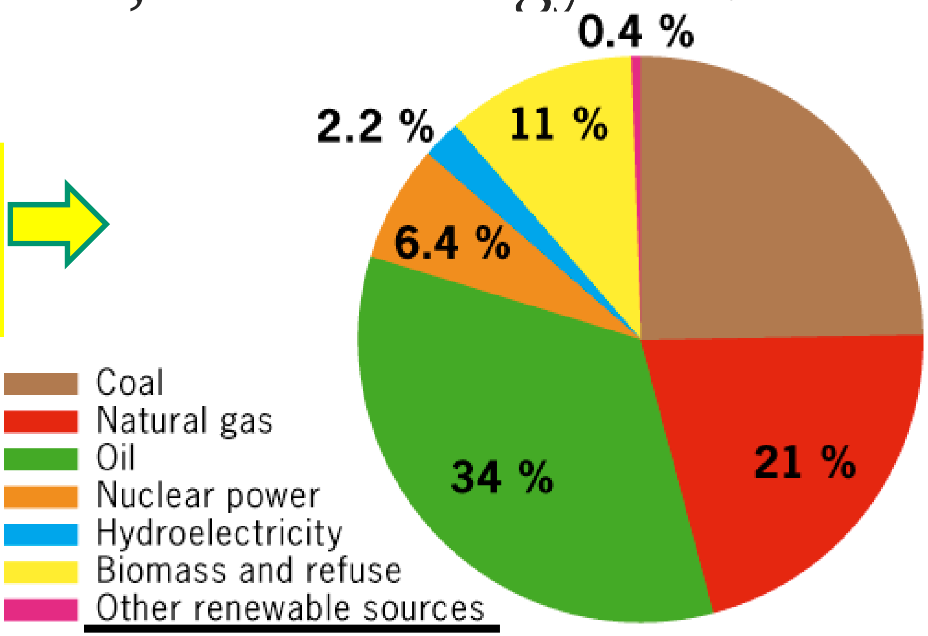
```
enter the eqally spaced values of x::>
4
4.4
4.8
5.2

enter the corresponding values of y::>
2.4082
2.8312
3.2699
3.7232


        BACKWARD DIFFRENCE TABLE IS:::>

         4   2.408
       4.4   2.831       0.42
       4.8    3.27       0.44      0.016
       5.2   3.723       0.45      0.015   -0.0011

enter the value of x for which y(x) needs to be calculated: 5


        when x=5        y[5]==3.499
```

Solar Cells

ENERGY!!

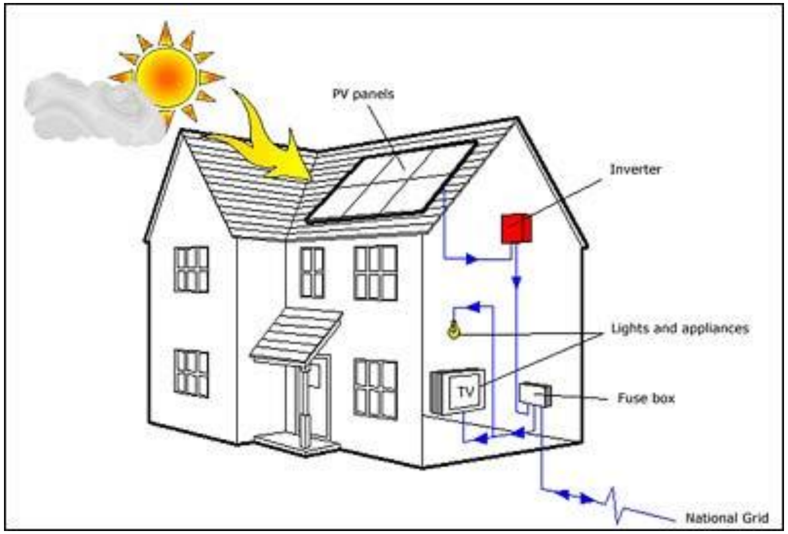
- Main concern in present time
- Conventional sources are limited and polluting
- In search for renewable and cleaner energy resources
- Wind, hydroelectric, solar energy etc. are being developed

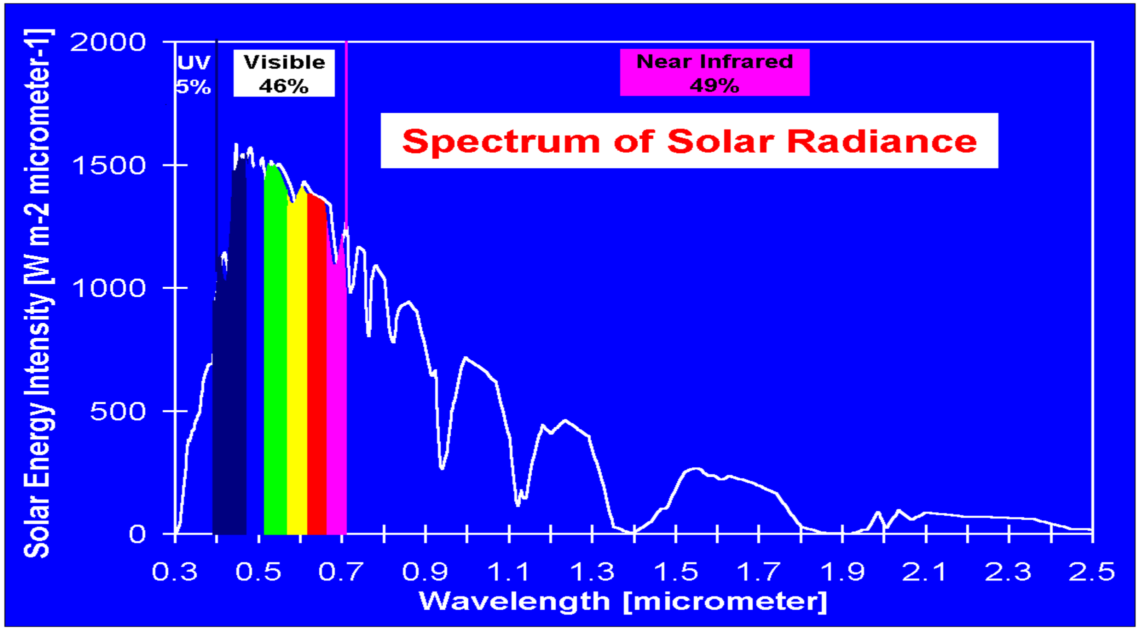
Percentage distribution of energy consumption from different resources.



Solar Energy

- **Solar energy is one of the solutions to this problem**

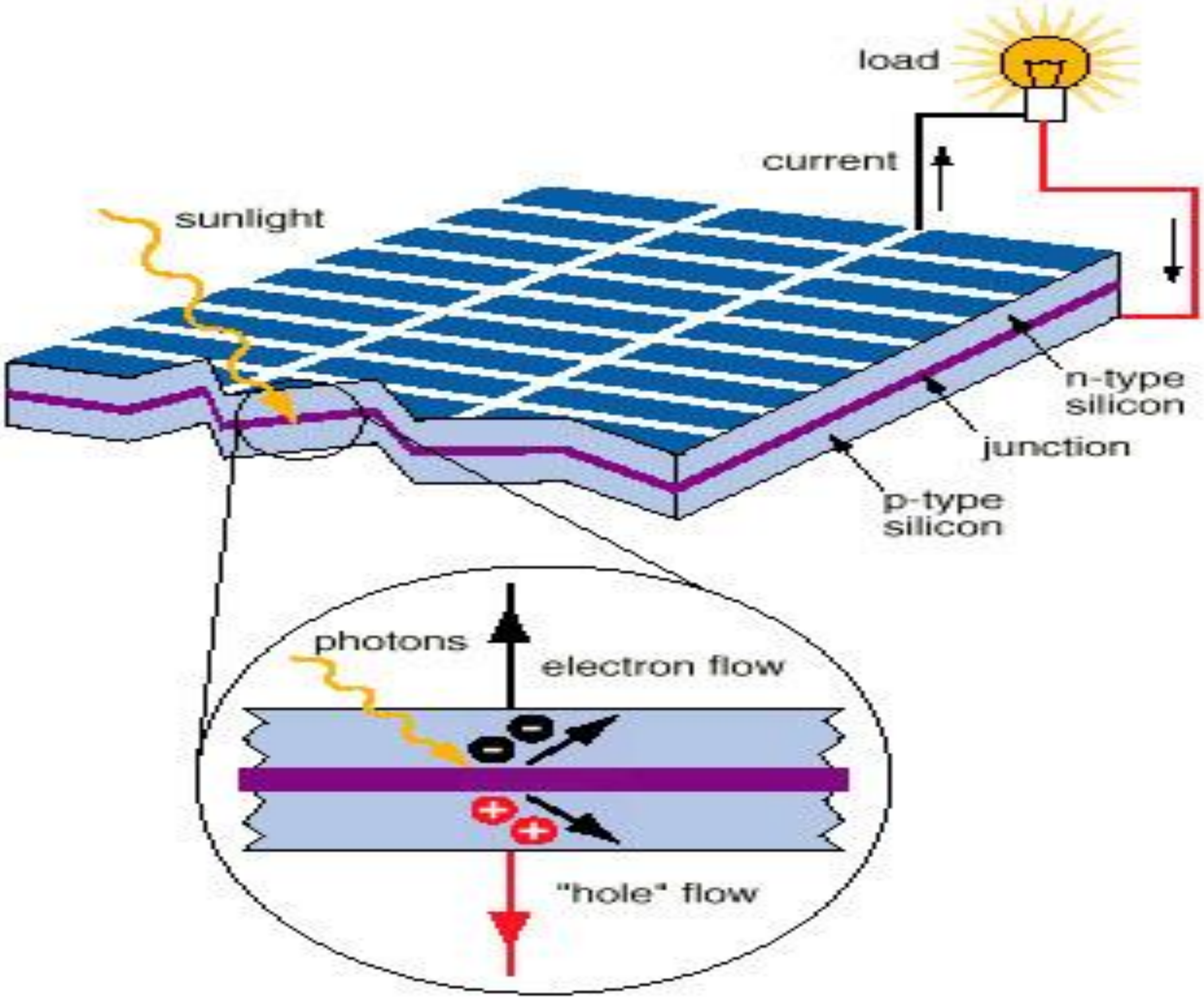




- **Power reaching earth is 1.37 KW/m^2**

Solar Cells

Solar cells are devices that take light energy as input and convert it into electrical energy.



Uses of Solar Cells

Photovoltaics can be used in a variety of applications including:

- consumer products such as watches, toys and calculators
- emergency power systems
- vaccine and blood storage refrigerators for remote areas
- aeration systems for ponds
- power supplies for satellites and space vehicles
- portable power supplies for camping and fishing

Types of Solar Cells

Inorganic Solar Cells

- Mono-crystalline Solar Cells
- Poly-crystalline Solar Cells
- Amorphous Solar Cells

Organic Solar Cells

- Polymer Solar Cells
- Small Molecules Solar Cells
- Dye-sensitized Solar cells

Hybrid Solar Cells

Brings together the advantages of both inorganic and organic solar cells. Inorganic particles (Ag, ZnO, FeS_2, TiO_2, etc.) are incorporated in organic materials. This may improve the efficiency and lifetime of solar cells.

Importance of Organic Solar Cells

Inorganic solar cells have dominated the market so far. The efficiency of inorganic SC might have reached high value but some drawbacks of inorganic solar cells are:

- cumbersome processing
- inflexibility
- difficult to make in large area
- high cost of materials

Research interest has inclined towards organic materials due to:

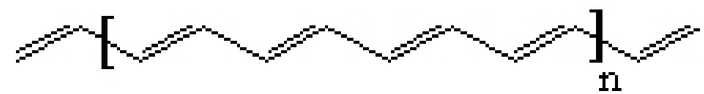
- Their ease of processing
- Mechanical flexibility
- Potential for low cost fabrication of large areas
- Chemical flexibility for modifications of the active layer

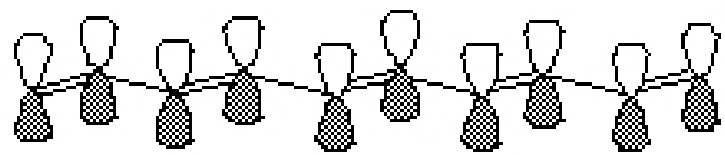
Drawbacks of organic solar cells over inorganic devices:

- Very low efficiency
- Fast degradation/less stable
- Small life-time
- Small absorption spectrum

Polymer materials

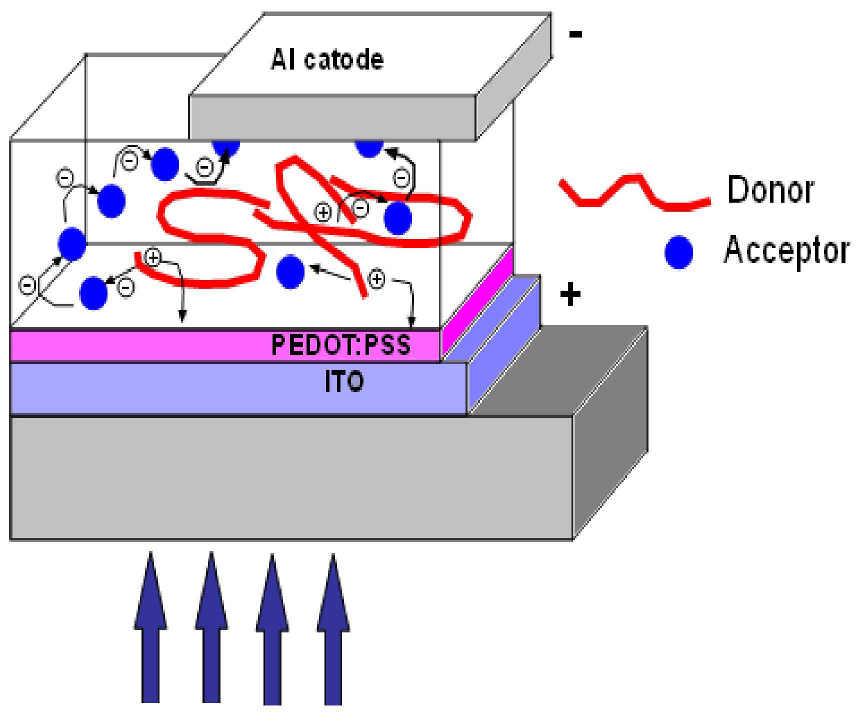
- Polymers are generally insulating
- Alternating single and double bonds (conjugated)
- π electrons able to delocalise into clouds above and below the chain
- Bandgap suitable for absorption of sunlight

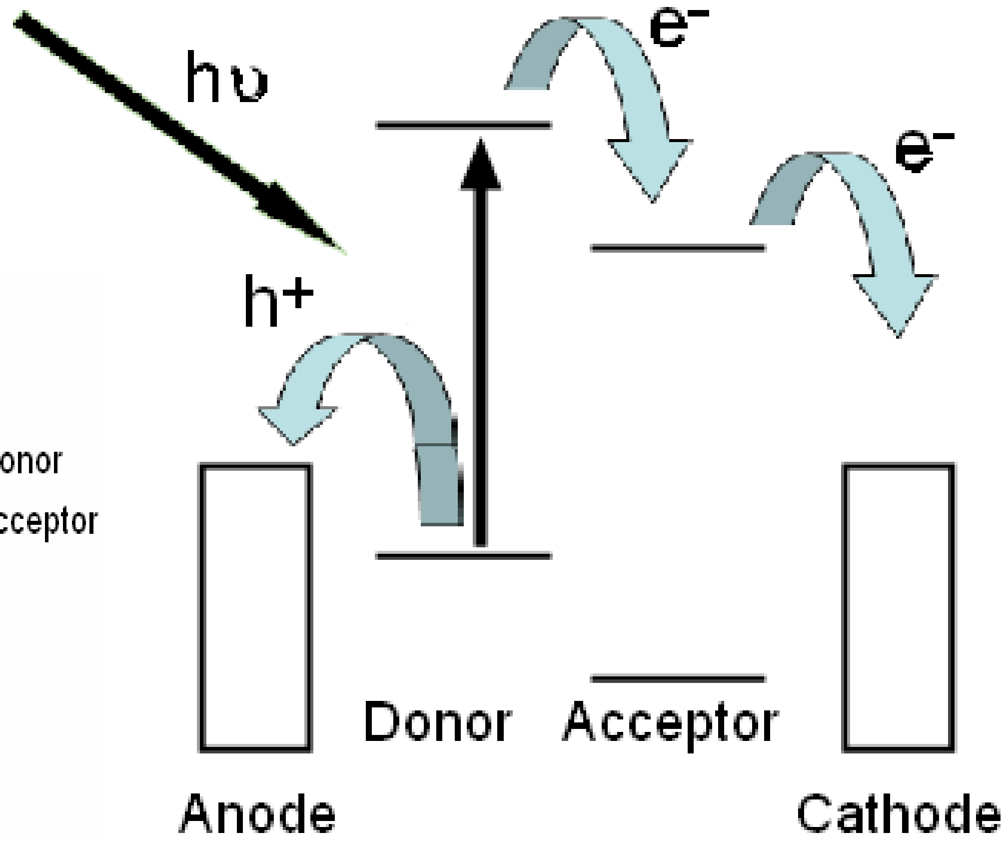




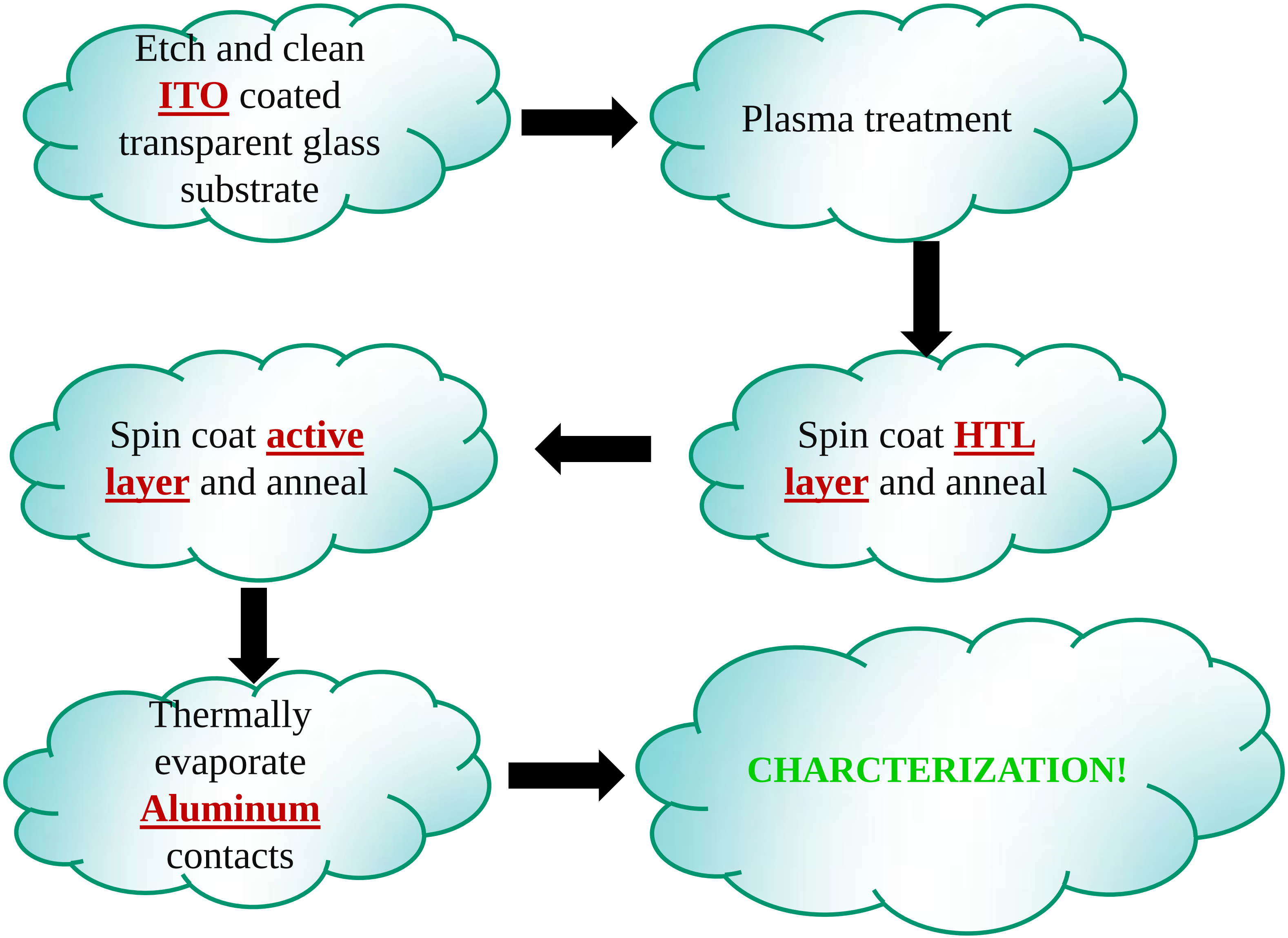
Working Principle

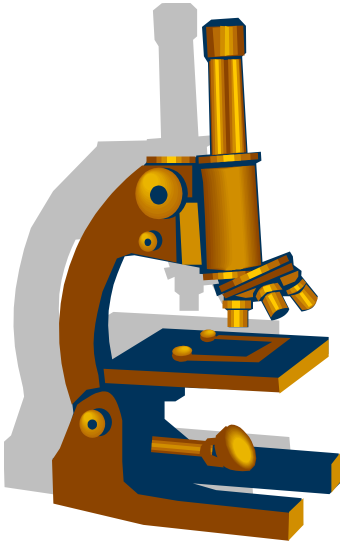
General Structure of the fabricated solar cell.

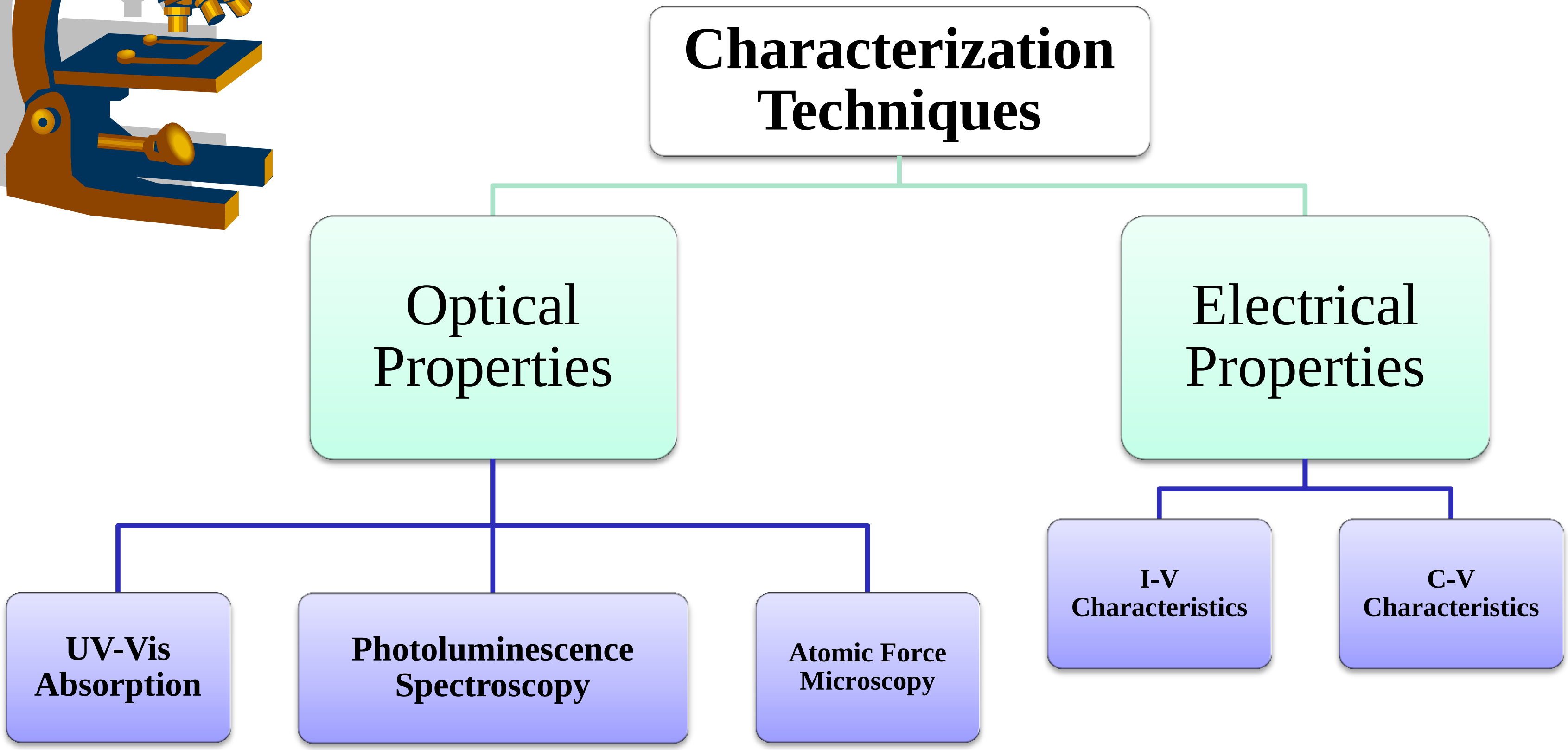




Fabrication Process



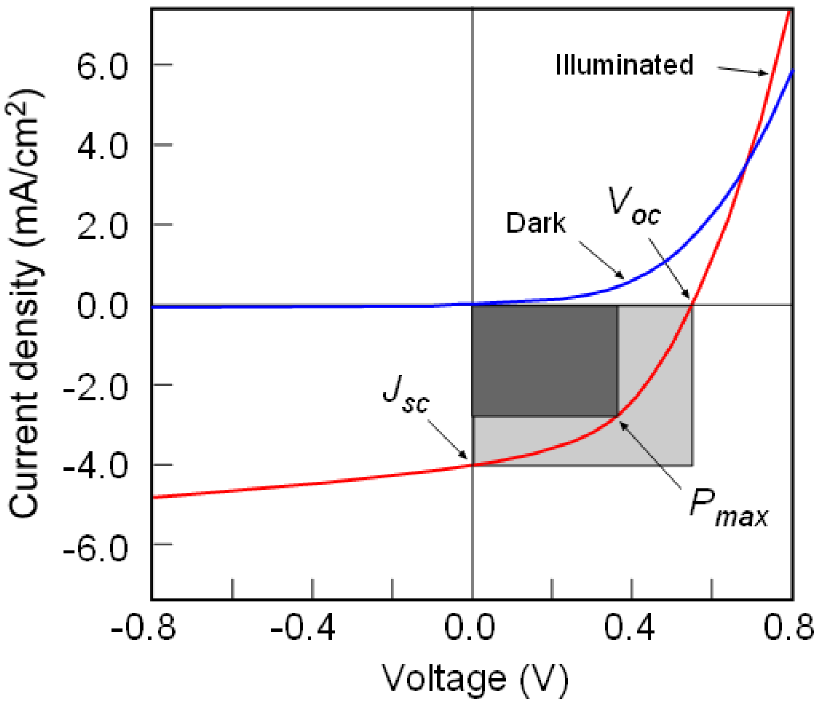



Characterization Techniques
Optical Properties
Electrical Properties
UV-Vis Absorption
Photoluminescence Spectroscopy
Atomic Force Microscopy
I-V Characteristics
C-V Characteristics

Electrical Properties

The performance of an organic solar cell is determined by measuring its current-voltage (*I*-*V*) characteristics in dark and under sun light illumination. The *I*-*V* characteristic of a solar cell under illumination gives several photovoltaic parameters such as

- short circuit current (J_{sc})
- open circuit voltage (V_{oc})
- fill factor (*FF*)
- power conversion efficiency (η) at an instance.



The typical *J*-*V* characteristics of an organic solar cell in dark and under light illumination

Photovoltaic Parameters

Short circuit current (J_{sc})

J_{sc} is the current driven from the illuminated solar cell under short circuit condition.

Open circuit voltage (V_{oc})

V_{oc} is the voltage developed across the electrodes of an illuminated solar cell when no current is driven from the cell.

Fill Factor (*FF*)

FF of a solar cell is the measure of the power that can be extracted from the cell.

$$FF = \frac{J_{\max} V_{\max}}{J_{sc} V_{oc}}$$

Power conversion efficiency (η)

The power conversion efficiency is simply the ultimate measure of the efficiency of the device to convert the light photons into electricity.

$$\eta = \frac{I_{sc} V_{oc} FF}{P_{light}}$$

Optical Properties

UV-visible absorption spectrophotometer

Spectrophotometer is an instrument which measures and compares the incident, reflected and transmitted light of a sample. The ratio of the two light intensities, transmitted light (I) over the incident light (I_0) is known as the transmittance of the sample. Absorbance is calculated by

$$A = -\log\left(\frac{I}{I_0}\right)$$

It is useful to study the wavelength range in which the active layer absorbs.

Spectrometer

A spectrometer is an optical instrument which is used to study the properties of light emitted by a material, over the specific portion of the electromagnetic radiation. Spectrometer is used to get the spectrum of the light intensity as a function of wavelength.

It is useful to study the emission spectra of thin films which should be less for better performance of the device.

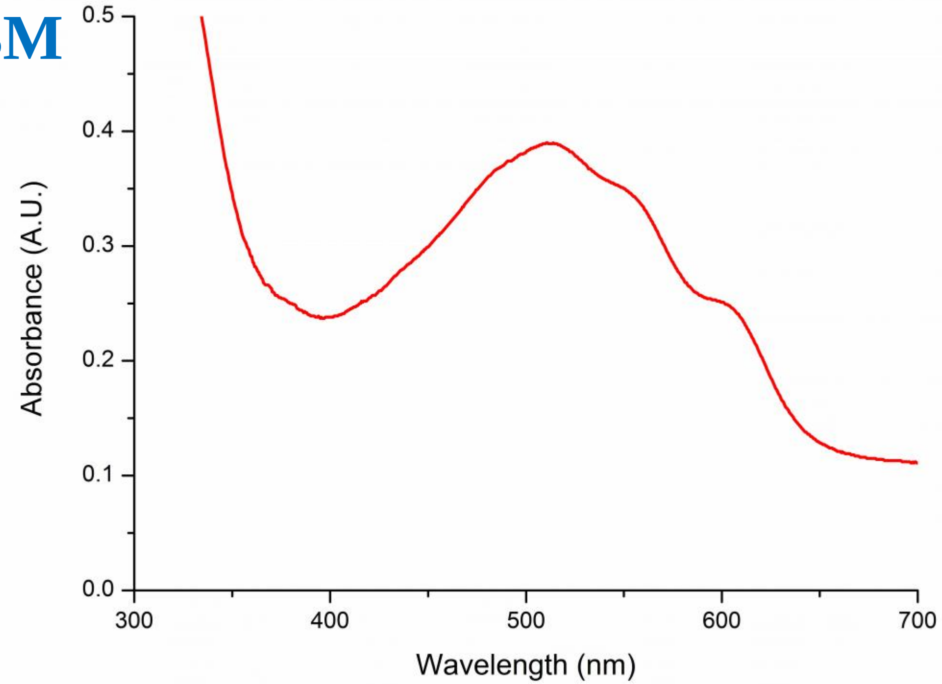
Atomic Force Microscope

AFM is based on the interactive forces called the van der waal's force between the sample and the tip.

It is useful to study the morphology and surface roughness.

UV-Visible Spectrum

- **Samples were prepared on thoroughly cleaned glass substrates.**
- **Mixture of donor and acceptor material in 1:1 ratio were spin coated on the substrates.**
- **Donor material: P3HT**
- **Acceptor material: PCBM**



Energy Band Gap Calculation

- **Calculated using absorption spectrum.**
- **Absorption coefficient, α, can be extracted from absorbance:**

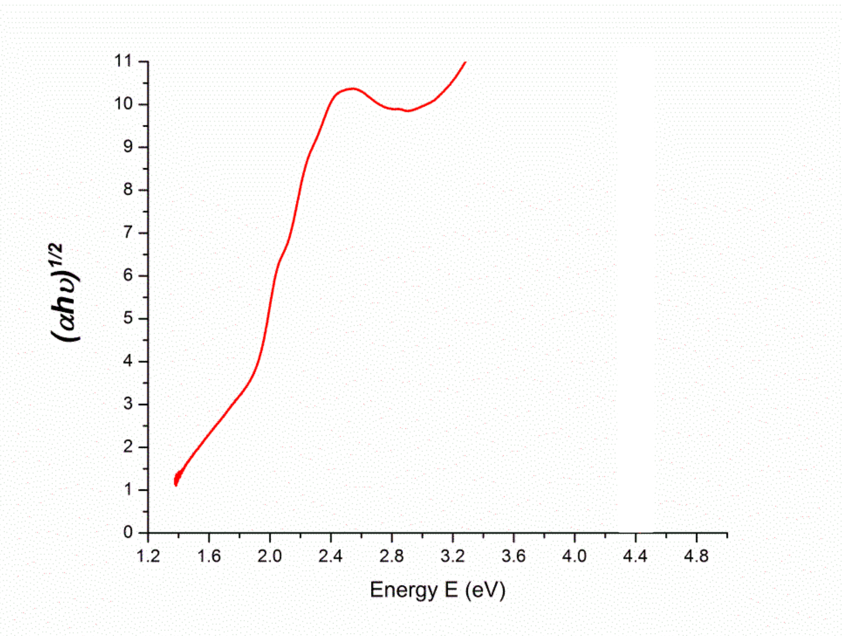
$$\alpha = A/t$$

Where t = thickness

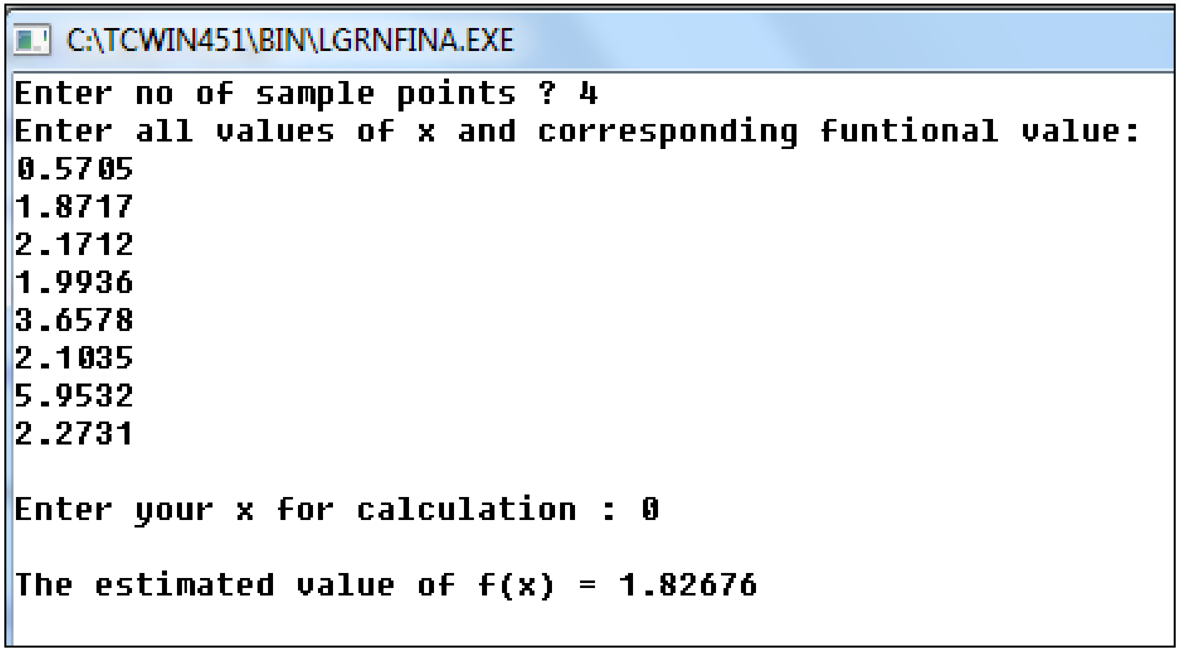
- **A graph between $(\alpha hv)^{1/2}$ and Energy E can be used to find the energy band gap.**

$$E = 1240/\lambda$$

- **E_g can be calculated by extrapolating the linear region**



Results: Energy Band Gap Calculation by Lagrange Extrapolation



```
C:\TCWIN451\BIN\LGRNFINA.EXE
Enter no of sample points ? 4
Enter all values of x and corresponding funtional value:
0.5705
1.8717
2.1712
1.9936
3.6578
2.1035
5.9532
2.2731

Enter your x for calculation : 0

The estimated value of f(x) = 1.82676
```

- **Reported band gap of P3HT:PCBM les between 1.85 - 2 eV.**
- **Band gap has been observed to vary with the concentration ratio of the materials used.**

Turbo C++ - [c:\tcwin451\bin\coupled.cpp]

File Edit Search View Project Debug Tool Options Window Help

```cpp
#include <iostream.h>
#include <fstream.h>
#include <iomanip.h>
#include <conio.h>
#include <math.h>

int main()
{
int i;
float x[100], y[100], z[100],  min, num, jsc, FF, PCE, A;
float c1[100];
ifstream ins; // input stream
ifstream ins1; // input stream
ofstream outs; // output stream
ins.open("volt.txt");
ins1.open("crnt.txt");
//outs.open("power.txt");
cout<<"\n Enter the pixel of cell\n";
cin>>A;
for (i=0; i<100; i++)
{
ins >> x[i];
ins1 >> y[i];
//power = x[i]*y[i];
z[i] = x[i]*y[i];
c1[i] = y[i];
//outs << "" << setprecision(10) << power << endl;
//outs1 << "" << setprecision(6) << absorb << endl;
}
ins.close();
//outs.close();
ins1.close();
min=0;
for (i=50; i<80; i++)
{
if (z[i]<min)
min = z[i];
else
num = min;
}
```

```cpp
num = min;
}
cout<<"\nThe maximum power is "<< setprecision(10)<<num;
jsc = c1[50];
cout<<"\n\nThe short circuit current density is\n ";
cout<<setw(8)<< setprecision(10)<<jsc;
FF = num/(jsc*0.54)*100;
cout<<"\n\nThe fill factor is\n ";
cout<<setw(8)<< setprecision(10)<<FF;
PCE = -jsc*A*0.54*FF;
cout<<"\n\nThe power conversion efficiency is\n ";
cout<< setw(8)<< setprecision(10)<<PCE;
return 0;
}
```

Program for calculation of various Solar Cell Parameters

Steps

1. **Read in data files containing current and voltage values.**
2. **Get value of short circuit current (ie value at V=0)**
3. **Multiply current – voltage to get power.**
4. **Sort data to get maximum power value in fourth quadrant .**
5. **Calculate fill factor using formula:**

$$FF= P_{max}/J_{SC}*V_{OC}$$

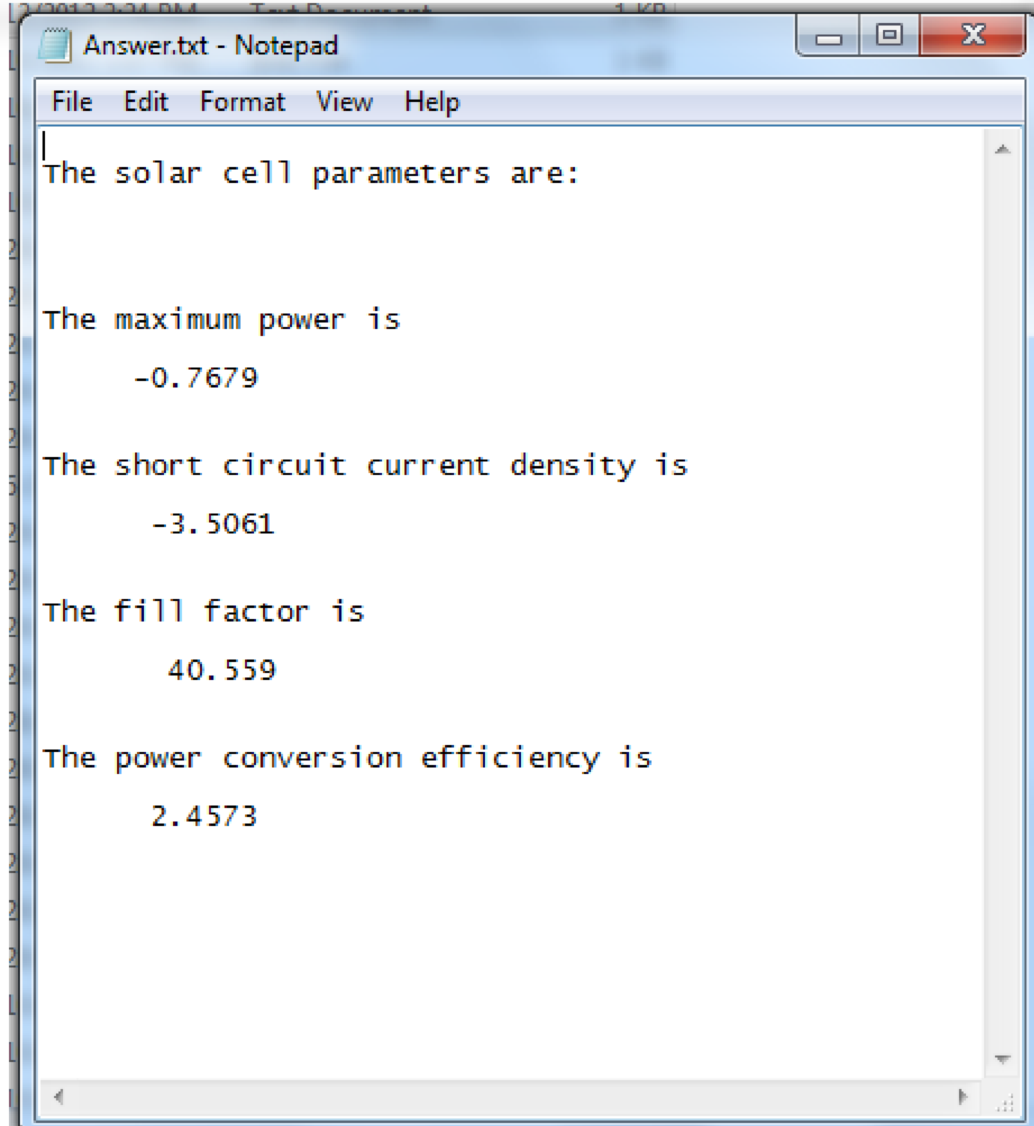
6. **Calculated efficiency using:**

$$PCE = J_{SC}*V_{OC}*FF/P_{in}$$

where P_{in} = incident power

Results

1. **Input values needed:**
   Pixel size of the sample



Thank You