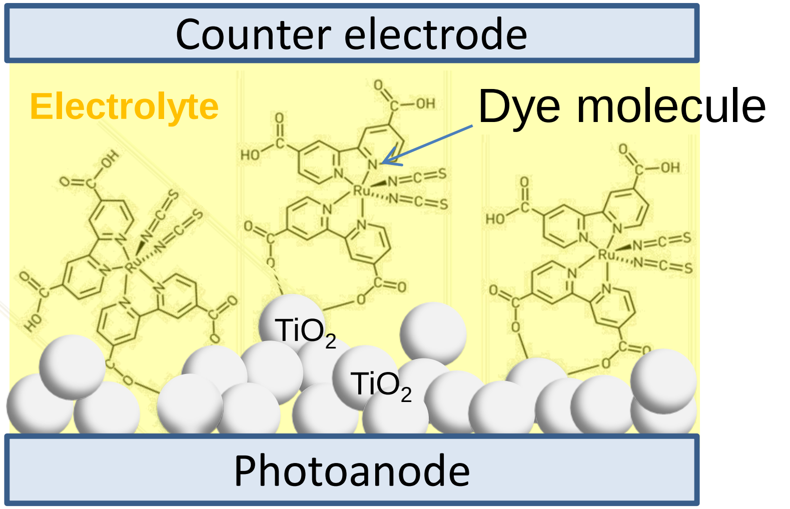
Dye Solar Cell

Dye sensitized Solar Cells (DSC): new generation solar devices. They are basically electrochemical cells and already reach an efficiency of 11% on small area

- Photoanode: semiconductor mesoporous medium (TiO_2), covered with dye molecules which make TiO_2 photoactive

- A region of liquid electrolyte in contact with a counter-electrode covered by a thin platinum layer



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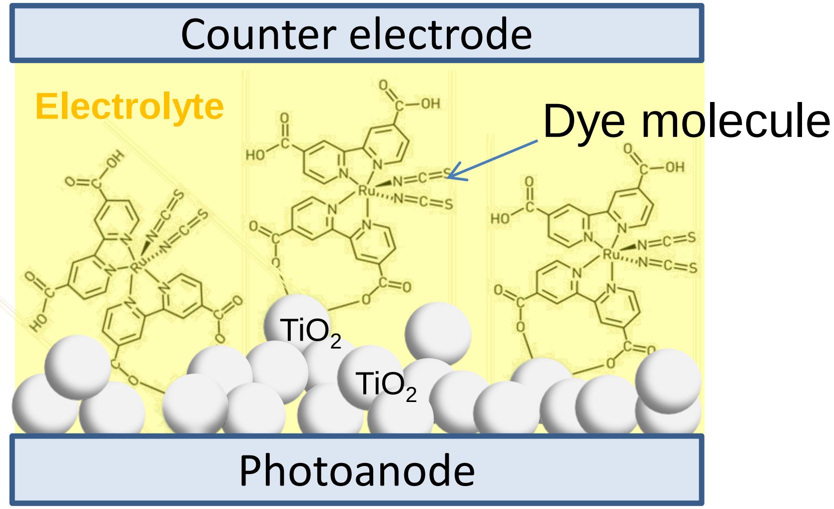

Photon is absorbed by a dye, it excites an electron in the porous material. Then, the electron percolates inside the porous material until it reaches the anode contact: a transparent conductive oxide (TCO).

The ionized dye is regenerated by the electrolyte by a redox process where iodide is oxidized and triiodide is formed.

$$3I^- + 2D^* \longrightarrow I_3^- + 2D,$$

Concentration gradient is formed that moves triiodide ions towards the counter-electrode and iodide ions towards the mesoporous material. Finally, the triiodide ions reach the platinum where they are reduced and transformed back in iodide ions, closing electric circuit.

$$I_3^- + 2e_{Pt} \longrightarrow 3I^- .$$

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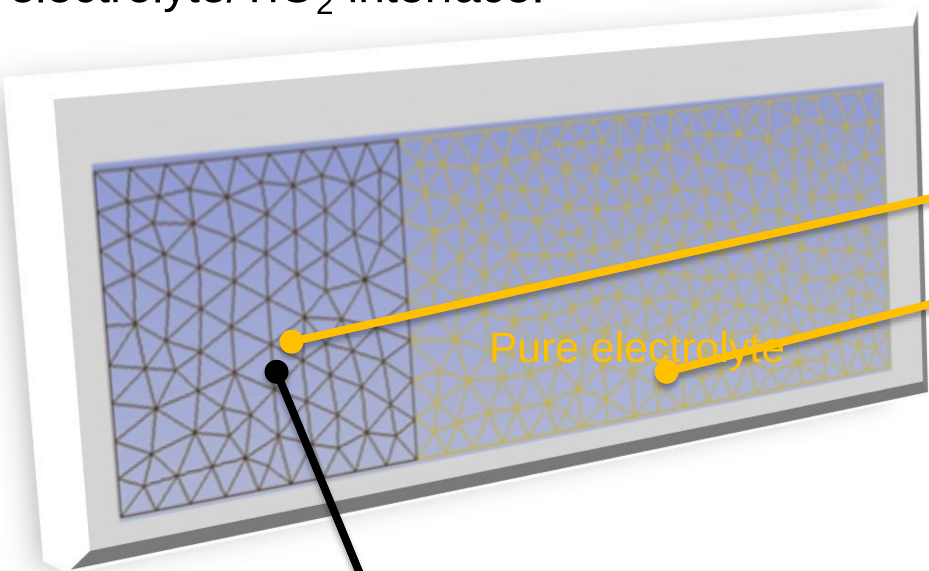
The model implemented is a steady state drift-diffusion set of equations for ionic charge carriers and electrons, coupled by the recombination term at the electrolyte/TiO_2 interface.



$$\nabla \cdot \left(\mu_{I_3^-} n_{I_3^-} \nabla \phi_{I_3^-} \right) = \frac{1}{2}(G - R)$$

$$\nabla \cdot \left(\mu_{I^-} n_{I^-} \nabla \phi_{I^-} \right) = -\frac{3}{2}(G - R)$$

$$\nabla \cdot \left(\mu_c n_c \nabla \phi_c \right) = 0$$

Drift-diffusion equations for the electrolyte (iodide/ triiodide pair + cation)

$$\nabla \cdot \left(\mu_e n_e \nabla \phi_e \right) = (G - R)$$

Effective mesoporous material TiO_2–electrolyte described by a porosity coeff. Generation and recombination term occur here.

Module
DSC

Module dssc{
  name = *somename*
  regions = *set_of_regions*

Physics
 { *somemodel* { } }

Contact *contact_name*
{}

Section
Physics

for simulation on a device under illumination

Poisson, Drift-Diffusion and Recombination parameters

Physics
{
generation = *dssc_generation*

parameters [porosity, k_dye, electron mobility, …]

}

Boundary cond.

Contact

Contact *anode*{
type = *ohmic*
[regions = (..)]
voltage = *$Vd*}

Contact *cathode*{
type = Pt
Ex_curr = *0.1*}

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Module
dssc_generation

Generation term for device under illumination

$$G = \int \alpha(\lambda)\Phi(\lambda)e^{-\alpha(\lambda)x}d\lambda,$$

$\alpha(\lambda)$ is the absorption coefficient (in μm^{-1}) of the chosen Dye, $\varphi(\lambda)$ the intensity of the light at wavelength λ of the light source

Module *dssc_generation* {

regions = *TiO2*
light_direction = *vector_light e.g. (1,0,0)*
light_intensity = *$x [units of Sun]*
dye = *dye_molecule_file_name*
illumination_spectrum = *source_spectrum (file name)*
}

Module ***sweep***

To perform the transition from dark condition to full short-circuit condition under illumination.

```
Module sweep
{
name = sweep_gen
solve = (dssc_generation, dssc)
variable = $x
values = (0, 1e-9, 1e-8, 1e-7, 1e-6,
1e-5, 1e-4, 1e-3, 1e-2, 0.1, 1)
plot_data = true
}
```

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Module
Sweep/2

The second sweep, (sweep_V), computes the I-V characteristic under illumination.

In case of dark simulation (application of an external bias without illumination) the first sweep is not needed.

```
Module sweep
{
name = sweep_V
solve = dssc
variable = $V
values = (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.62, 0.64,
0.66, 0.68, 0.7, 0.72, 0.74, 0.76, 0.78, 0.8)
plot_data = true
}
```