# Modeling of P-N junction devices for photovoltaic applications

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Background

- A solar cell is typically a large area P-N junction device where electron-hole pairs are created by incident photons.

https://www.imagesco.com/articles/photovoltaic/photovoltaic-pg4.html
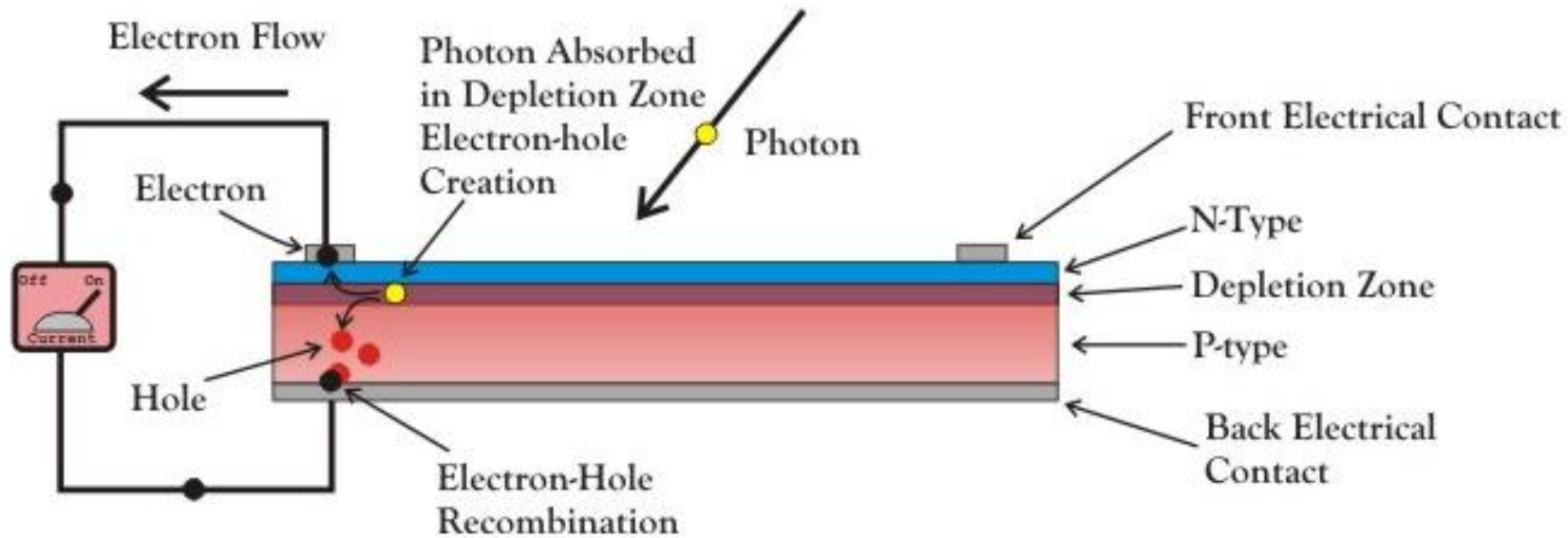
- Solar cells can be simulated using the tool ADEPT to obtain current-voltage (I-V) characteristics, band diagrams, External Quantum Efficiency (EQE) and parameters such as open-circuit voltage (V_{OC}) and short-circuit current (J_{SC}).

ADEPT

- The tool ADEPT (A Device Emulation Program and Tool) solves the semiconductor Poisson's equation, and the hole and electron continuity and transport equations (assuming drift-diffusion transport), subject to appropriate material parameters.

- ADEPT can be used to model single material solar cells (Si, GaAs), thin-film solar cells (CdTe, CIGS), and multijunction solar cells.

- There are three major aspects of the input file which are required to run ADEPT:
  - Material properties (bandgap, absorption profile, carrier mobilities and lifetimes, etc.)
  - Device parameters (no. of layers, boundary conditions, back surface reflection, etc.)
  - Operating Conditions (solar spectrum, temperature, etc.)

https://nanohub.org/resources/adeptnpt

Electronic and Optical Properties Calculation

- Density Functional Theory (DFT), a quantum mechanical modelling method, can be used to investigate the electronic structure of many-body systems, in particular atoms and molecules.

- DFT calculations can be carried out using the open-source code Quantum ESPRESSO.

- DFT is useful for calculating the band structure, bandgap, density of states, absorption coefficient, etc. of photovoltaic materials

https://nanohub.org/resources/dftqe

- Stanford Stratified Structure Solver (S4) can be used to simulate absorption properties of multi-layered structures (including patterned layers).

- S4 is a frequency domain code to solve layered periodic structures, using Rigorous Coupled Wave Analysis (RCWA) and the S-matrix algorithm.

https://nanohub.org/resources/s4sim