Lab 2. Fabrication and characterization of hybrid perovskite solar cell devices

Organic Materials for Energy and Optoelectronics

Equipment and applicated solutions:

- Spin coater SM-150 (Sawatec);
- Spin coater NEWBY;
- Evaporator (vacuum chamber) MBraun
- I-V simulator AM 1.5G + Advantest R6240A;
- Glass substrates with covered transparent conductive layer (indium-tin oxide, ITO);
- 10% wt. solution of SnO_2 particles in water;
- 1.4M solution of methylammonium lead(II) iodide (MAPI) in DMF;
- 6 mg/mL solution of Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine (PTAA) in chlorobenzene;
- V_2O_5 powder and Al pieces.

During this Lab work, students can get hands-on experience with some methods used to make laboratory-scaled solar cells. Here, the photovoltaic devices based on hybrid organic-inorganic perovskite material ($CH_3NH_3PbI_3$) are proposed for fabrication. Its schematic composition is shown in Figure 1.

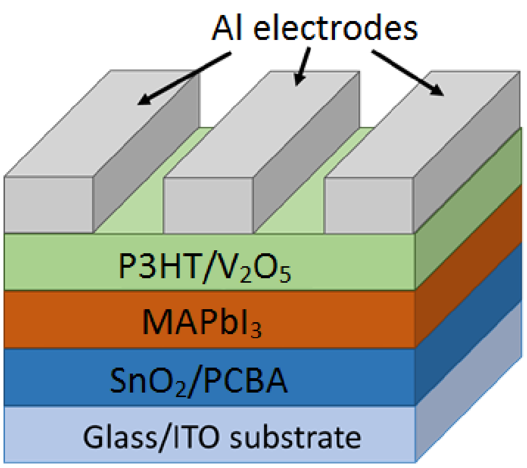

Figure 1. The architecture of MAPI-based solar cell

Progress of Lab work

Step 0. Glass substrate preparation + SnO_2 layer deposition (will be completed and provided to students)

Step 1. PCBA layer preparation

- Heat the ITO/SnO_2-covered substrates in glove box at 160 °C during 5 min;
- Turn on the spin coater and set the following parameters of rotation mode: 3000 rpm, 30 s;
- Draw up 50 µL of PCBA solution into the pipette and put them on the substrate surface without rotation;
- After 3-5 s, turn on the rotation.

Each deposited layer then must be heated (100 °C, 10 min).

Step 2. MAPI layer preparation

- Set the following parameters of rotation mode: 4000 rpm, 60 s;
- Filtrate the MAPI solution through the PTFE filter;
- Turn on the rotation and drop 65 µL of MAPI solution sharply, then (on the 13^{th} second) drop 160 µL of toluene (which was prepared beforehand);
- Leave the resulted substrate for 10-12 min without heating;
- Heat the plate to 50°C and put the substrates on it; then increase the temperature to 80°C and leave them for 5 min.

Step 3. PTAA layer preparation

- Set the following parameters of rotation mode: 4000 rpm, 30 s;
- Turn on the rotation and drop 30 µL of PTAA solution sharply.

Step 4. V_2O_5 and Al electrode deposition

- Transfer the substrates to the glove box with MBraun evaporator;
- Fill the vacuum chamber with inert atmosphere and open it;
- Scratch the substrates in the middle with thin spatula to release ITO layer;
- Put the substrates in special mask (deposited layers down!) and place the mask into the vacuum chamber;
- Prepare the materials for evaporation by placing them on the tungsten boats
  - V_2O_5 must be placed on source #1 (closer to operator);
  - Al must be placed on source #2 (farther to operator);
- Close the chamber and evacuate atmosphere inside it;

- Make sure that rotary holder and shutter are turned off (white buttons);
- Turn on the deposition controller (Inficon SQC-310C);
- Wait for the pressure reducing ($2 \cdot 10^{-5}$ mbar or less);
- Choose the preset program for V_2O_5 evaporation;
- Press “Start layer”;
- Increase the power to xxx%;
- After 20 s continue to slightly increase the power to yyy%
- After evaporation process beginning, regulate the power to keep the evaporation rate in range of 0.20-0.50 Å s^{-1};
- Wait the creation of 3-5 nm thickness layer, after:
    - Turn on the rotary holder (green button);
    - Simultaneously press “Zero” button on deposition controller and turn on the shutter (green button);
- Proceed the evaporation process and stop it when the layer thickness reaches 30 nm by turning off the rotary holder and shutter;
- Turn off the source #1 and choose the program for Al evaporation from source #2;
- Repeat the sequence highlighted with grey color for the Al layer deposition using:
    - Average power of 30-32%;
    - Average deposition rate of 1.0-2.0 Å s^{-1};
    - Aimed thickness of 170-200 nm;
- Turn off the source #2 and fill the chamber with atmosphere.

Step 5. Current-voltage measurements of devices

- Turn on the solar simulator lamp and wait about 10-15 min before using it;
- Place a metal mask with rectangular cutout on the simulator surface;
- Turn on the program LabView and use the preset program for measurements;
- Place the device on it (deposited layer up!) and put the wired negative electrode on ITO/V2O5/Al layer;
- Put the wired positive electrode on the ITO/…P3HT/V_2O_5/Al layer;
- Write down the device “name” in program;
- Start the measurements;
- Provide one measurement of the device in a dark mode (at switched off simulator).

Take into account that the measurements save automatically but still need to be transformed into .txt files.

- After the measurements, use the script to transform initial files for the tabular format.

Tasks for the Lab analysis

1. Taking the measured I-V data, plot the J-V curves (where J is a current density, *mA* cm^{-2}; V is a voltage, *V*). Find the V_{max} and J_{max} from these data. Confirm the automatically calculated FF and PCE using the formula (1):

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{max}J_{max}}{P_{in}} = \frac{V_{oc}J_{sc}FF}{P_{in}} \quad (1)$$

2. Match the plots of one device measured both in a dark and light modes. Explain the distinguishes of the processes in device when the non-zero voltage is applied.

Questions for the Lab analysis

1. What is the function of each specific layer in fabricated solar cell device?

2. What are the restrictions of proposed methods for layers fabrication: spin coating and thermal evaporation?

3.What is the Schockley-Queisser limit? Estimate the maximum PCE value for MAPI semiconductor.

4. What are the parameters of V_{oc} and J_{sc}? What factors may they depend on?