# Barrier properties of nanostructures GaP/PEDOT:PSS

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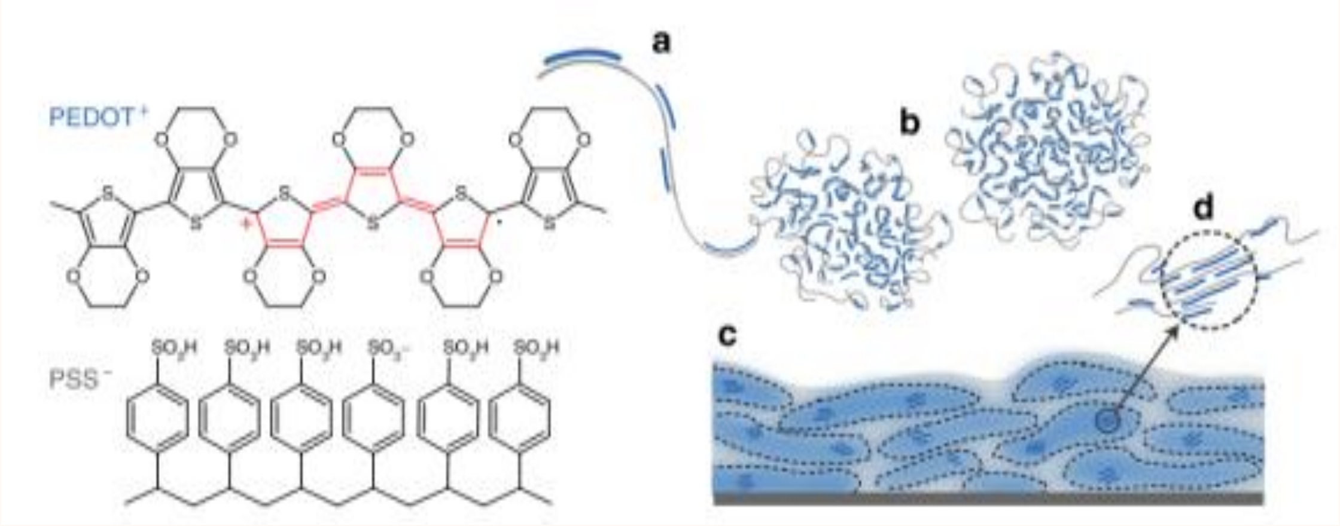
The most popular organic conductor today is the poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) composite. It is widely used in organic electronics, in particular to create photosensitive heterostructures such as organic/inorganic semiconductors, which are easy to manufacture due to the vacuum-free, low-temperature technology, and promising characteristics [1, 2]. PEDOT:PSS thin films reveals enough high conductivity with high transparency in visible range and considered now as alternative for ITO ones. In this work hybrid heterostructures based on n-type gallium phosphide single crystals and charge selective organic layer PEDOT:PSS. were fabricated to obtain barrier structures.

## Experimental details

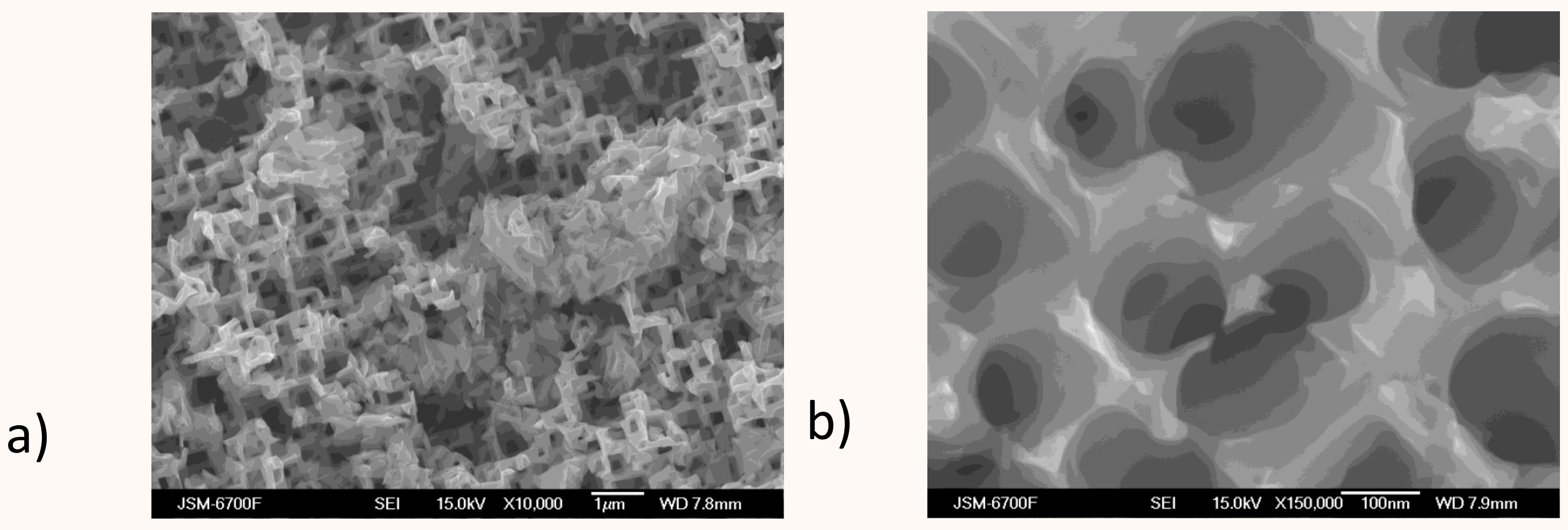


PEDOT:PSS structure and film morphology.

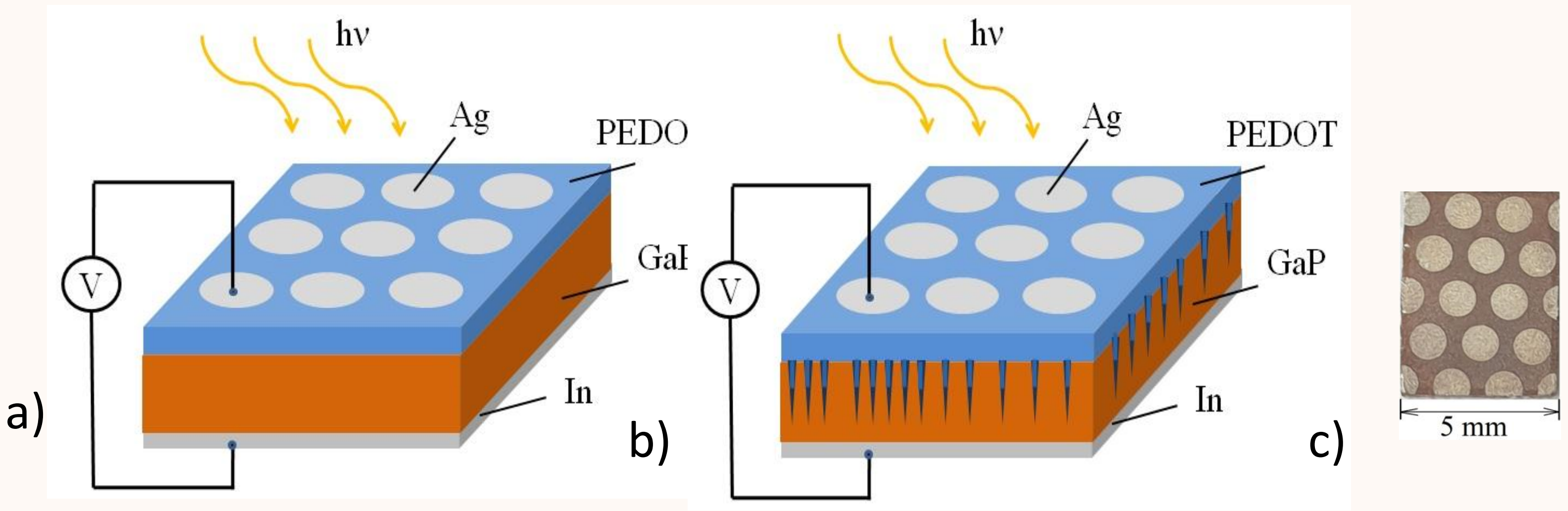
The chemical structure of PEDOT:PSS and commonly described microstructure of the conducting polymer system (a) synthesis onto PSS template, (b) formation of colloidal gel particles in dispersion and (c) resulting film with PEDOT:PSS-rich (blue) and PSS-rich (grey) phases. (d) Aggregates/crystallites support enhanced electronic transport [3].

Deposition of organic films was carried out by spin-coating followed by heating at T = 140-150ºC and washing of PEDOT:PSS films in ethanol. The thickness of the fabricated films determined by spectroscopic ellipsometry was in the range of 40-70 nm.

The back ohmic contacts were made by applying indium on the reverse side of the sample with prior removal of the oxide layer and sulfidation of the surface. The front contacts were created by physical vapor deposition of silver (35 nm) through the mask. Porous layers on GaP surface were fabricated by electrochemical etching in galvanostatic regim.



SEM images of porous GaP surfaces.



Schematic representation of the diodes design based on PEDOT:PSS on the flat (a) and porous (b) surface of GaP and image of the investigated structure (c).

## Optical properties of deposited PEDOT:PSS film

**SE-2000 SEMILAB**
(rotating compensator)
$\lambda$ = 250-2100 nm

Optical properties of PEDOT films were described by combining of the Cauchy and Drude models for dielectric constants *ε(E)*

$$\varepsilon(E) = \varepsilon_D(E) + \varepsilon_c(E)$$

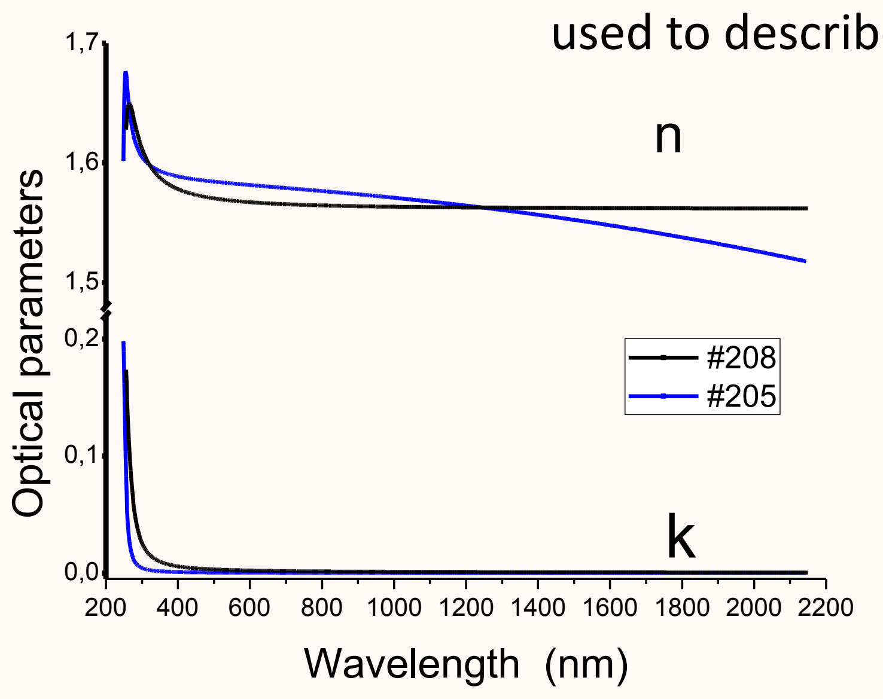
**Drude**

$$\varepsilon_D(E) = 1 - \frac{E_p^{\ 2}}{E^2 - iE \cdot E_\Gamma}$$

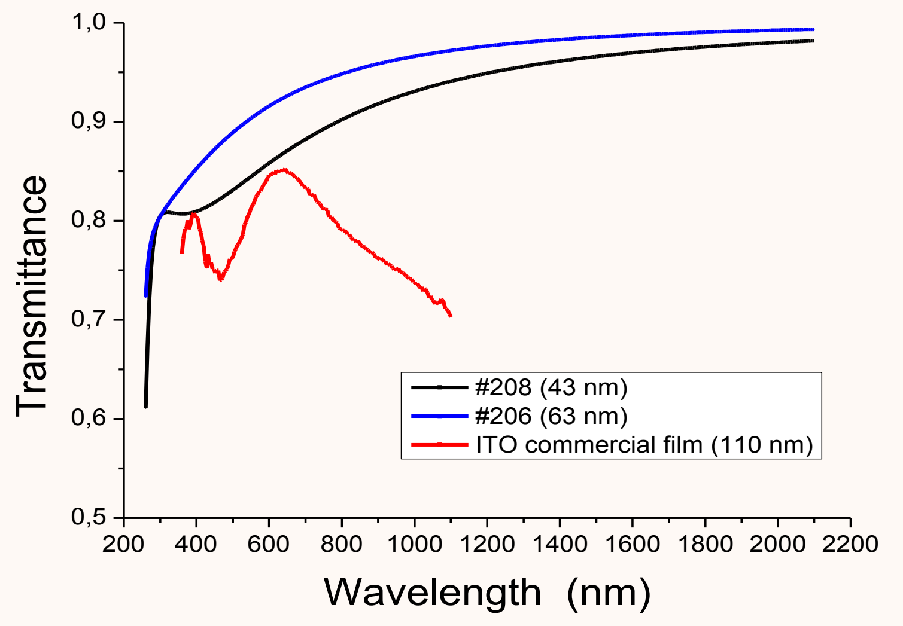
**Cauchy**

$$n(\lambda) = 1 + B/\lambda^2 + C/\lambda^4,$$

where $E_p$ is the plasmon energy, $E$ is the energy of incident quantum of light, and $E_\Gamma$ is the plasmon attenuation parameter; $B$ and $C$ are the empirical coefficients. Drude component $\varepsilon_D(E)$ describes the interaction of light with free carriers. Cauchy $\varepsilon_c(E) = n^2$ makes a major contribution to the refractive index of PEDOT:PSS in visible and often used to describe the optical properties of dielectrics.

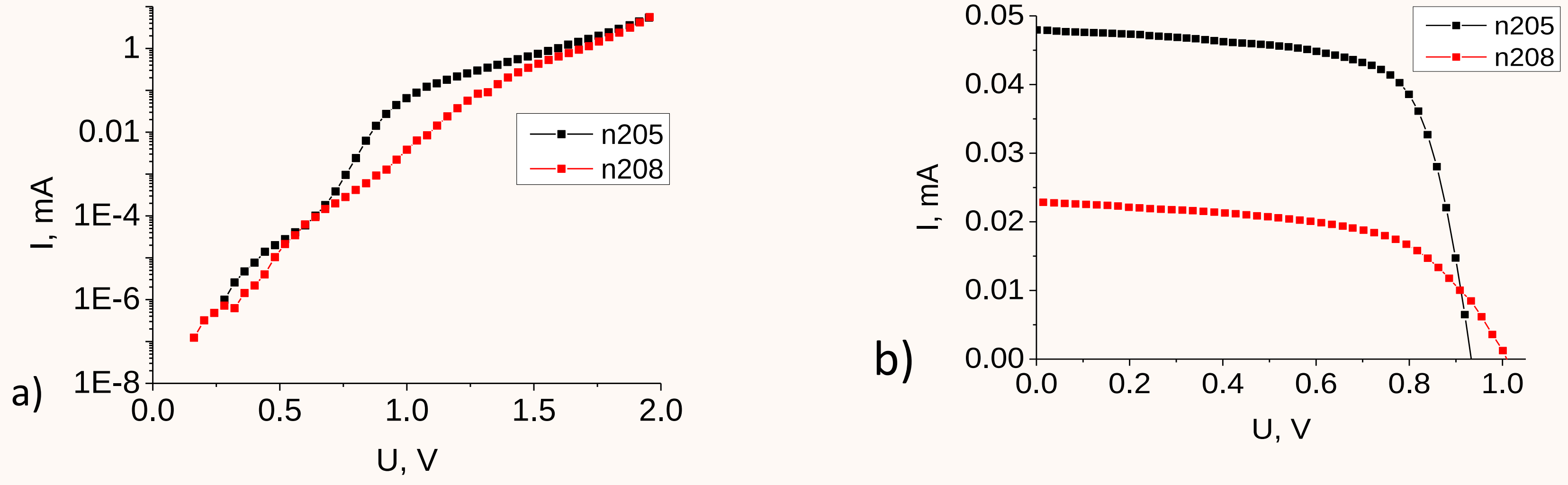


Spectral dependences of the refractive index n and extinction coefficient k of PEDOT:PSS films on GaP surfaces obtained from spectroscopic ellipsometry show film low extinction coefficient values



Transmittance spectra of PEDOT:PSS films #205 and #208 shows higher transparency in visible (photovoltaic) range than commercially available ITO film

## Current-voltage characteristics



Dark (a) and light (b) current-voltage characteristics of diodes (surface area 0.0133 cm²) based on GaP (measured under simulated illumination with a radiation power of P=136 mW/cm²).

| Sample | Open circuit Potential, V | Short circuit Current, mA/cm² | Fill factor, % | Max Efficiency, % |
|---|---|---|---|---|
| 201 | 0.7376 | 2.526 | 67.86 | 0.93 |
| 202 | 0.8948 | 2.756 | 44.20 | 0.80 |
| 203 | 0.7740 | 2.031 | 57.79 | 0.67 |
| 204 | 0.8213 | 1.620 | 65.71 | 0.64 |
| 205 | 0.9332 | 3.606 | 70.24 | 1.74 |
| 206 | 0.9867 | 8.937 | 35.24 | 2.29 |
| 208 | 1.0106 | 1.721 | 58.13 | 0.74 |

## CONCLUSIONS

The results for PEDOT:PSS/GaP heterostructures show that they have good barrier characteristics and further studies of these structures are promising. These may include, in particular, interface structuring, and the introduction of additional plasmon-active metal nanoparticles. Previous studies of similar heterostructures, based on nanoporous gallium phosphide and PEDOT: PSS charge-selective organic layer have shown that they are also barrier structures, but their characteristics depend significantly on the structure of the porous layer and further studies are needed to improve them.

[1] *P.Gao, Z. Yang, J. He, J. Yu, P. Liu, J. Zhu, Z. Ge, J. Ye*. Dopant free and carrier selective heterocontacts for silicon solar cells: recent advances and perspectives // Advanced Science.- 2018.-**5**. -1700547.
[2] *S.V. Mamykin, I.B. Mamontova, T.S. Lunko, O.S. Kondratenko, V.R. Romanyuk* . Fabrication and conductivityof thin PEDOT:PSS-CNT composite films // SPQEO. – 2021. – **24**, N2. – P. 148-153.
[3] *Jonathan Rivnay, Sahika Inal, Brian A. Collins, Michele Sessolo, Eleni Stavrinidou, Xenofon Strakosas, Christopher Tassone, Dean M. Delongchamp & George G. Malliaras.* Structural control of mixed ionic and electronic transport in conducting polymers. // *Nature Communications* .- 2016 .- **7**, Article number: 11287.