Photoluminescence of PCBM fullerene derivative confined in mesoporous glasses

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Introduction: Composites of fullerene derivatives with various polymers have been extensively used for more than two decades in in a wide range of applications in particular as electron acceptor in polymer-based organic solar cells and perovskite solar cells containing fullerenes.

In this report, we notify about the study of the influence of the surrounding environment - solvents, spatial limitation, temperature on the linear spectral properties of PCBM fullerene derivative.

Materials ant tools: It were prepared the next samples: PCBM solutions in acetonitrile and toluene.

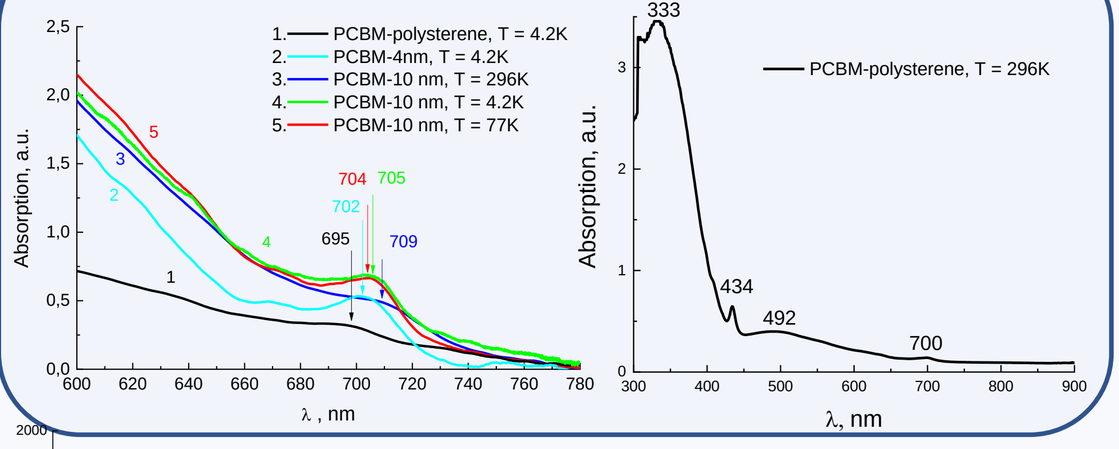
PCBM confined into PMMA and polystyrene matrices from toluene solution.

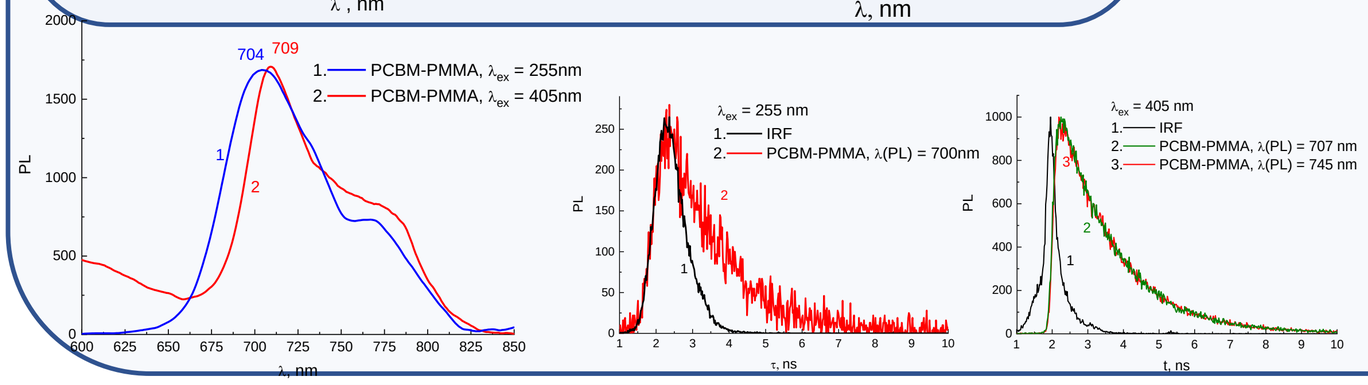
Also we used original sodium borosilicate glasses which leached in order to remove the sodium borate phase. The samples of PCBM in mesoporous glasses with pores diameters: 1, 3, 4, 10 and 44 nm were obtained by dipping the glasses into a saturated solution of PCBM in toluene and keeping in it for 24 h. After removal from the solution, the surface of the porous plates was wiped to remove PCBM residues on the surface, and then the plates were heated to remove toluene from the pores at 100 0C during 2 hours.

Concentration of PCBM in all toluene solution was C = 10^{-4} M.

The linear spectral properties of this molecule were investigated by optical absorption spectra, steady-state PL spectra, kinetic decay curves and PL lifetimes at λ_{ex} = 255, 325, 337.1, 405, and 532 nm; at room, liquid nitrogen and helium temperatures.

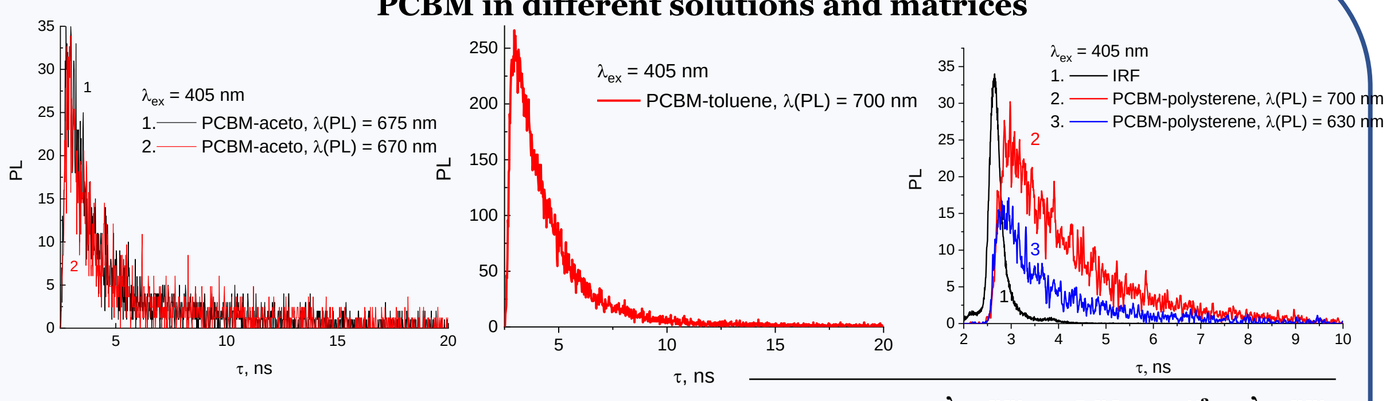
Optical absorption spectra of PCBM in different martices





	λ_{PL}, nm	τ, ns	χ^2	λ_{ex}, nm
PCBM-PMMA	700	1.4± 0.1	1.119	255
PCBM-PMMA	707	1.5± 0.1	1.102	405
PCBM-PMMA	745	1.55± 0.1	0.980	405

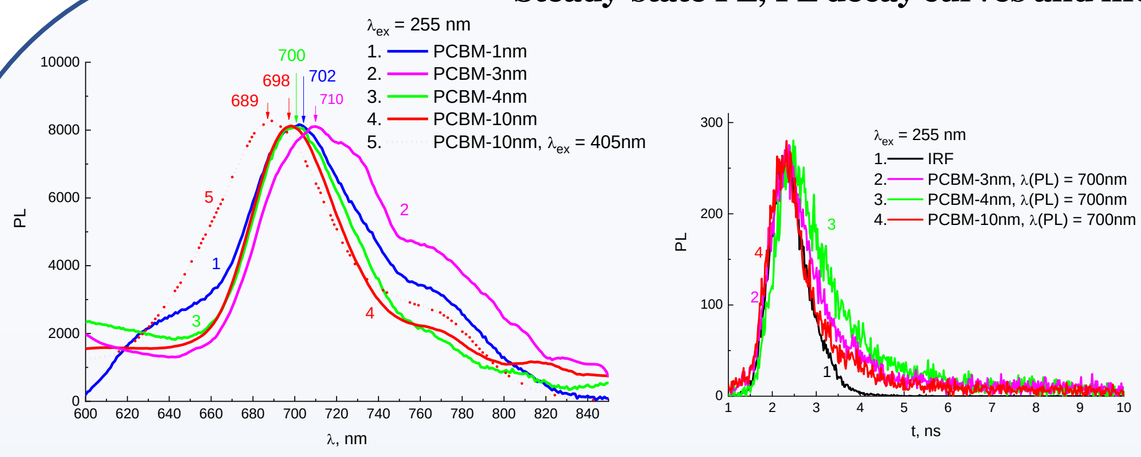
Steady-state PL, PL decay curves and lifetimes of PCBM in different solutions and matrices



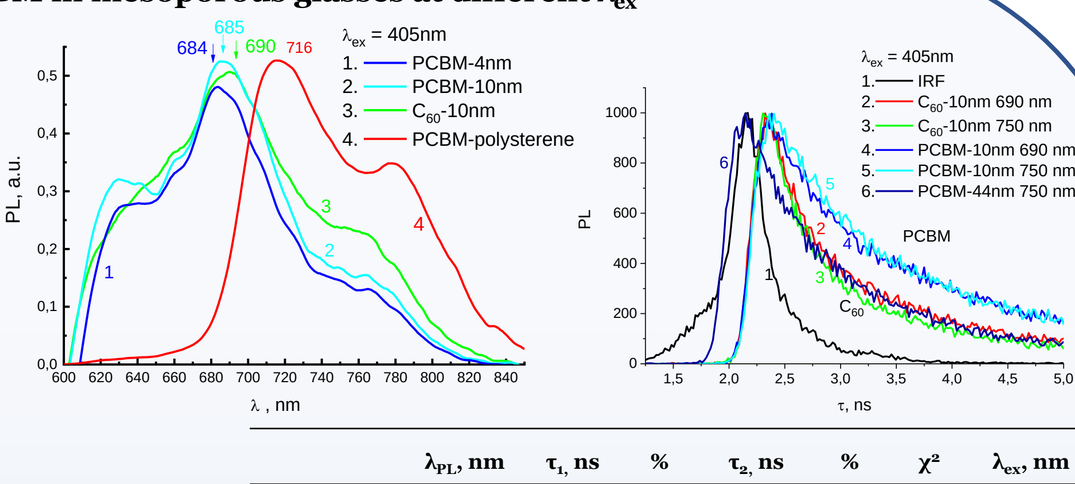
	λ_{PL}, nm	τ, ns	χ^2	λ_{ex}, nm
PCBM-aceto.	670	1.2 ± 0.1	1.185	405
PCBM-aceto.	675	0.9 ± 0.1	1.185	405
PCBM-toluene	700	1.6 ± 0.1	1.105	405

	λ_{PL}, nm	τ, ns	χ^2	λ_{ex}, nm
PCBM-polysterene	630	0.6± 0.1	1.031	405
PCBM-polysterene	700	1.2± 0.1	1.097	405

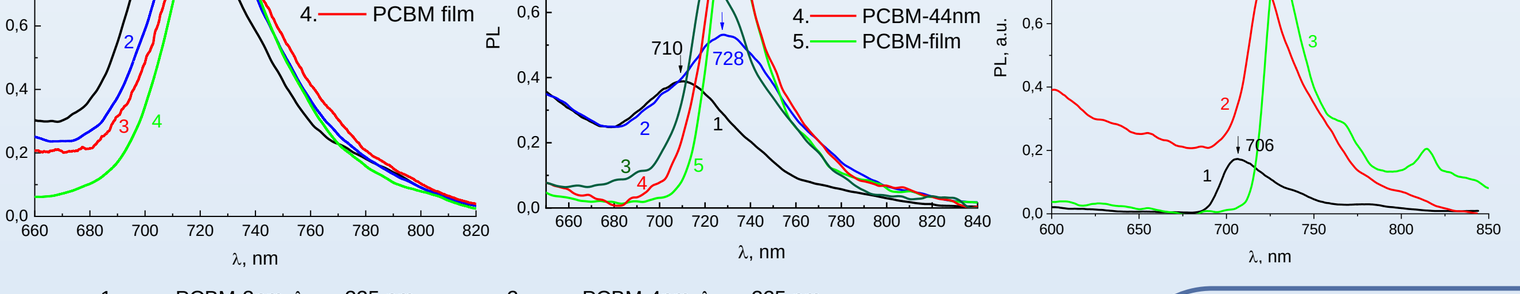
Steady-state PL, PL decay curves and lifetimes of PCBM in mesoporous glasses at different λ_{ex}



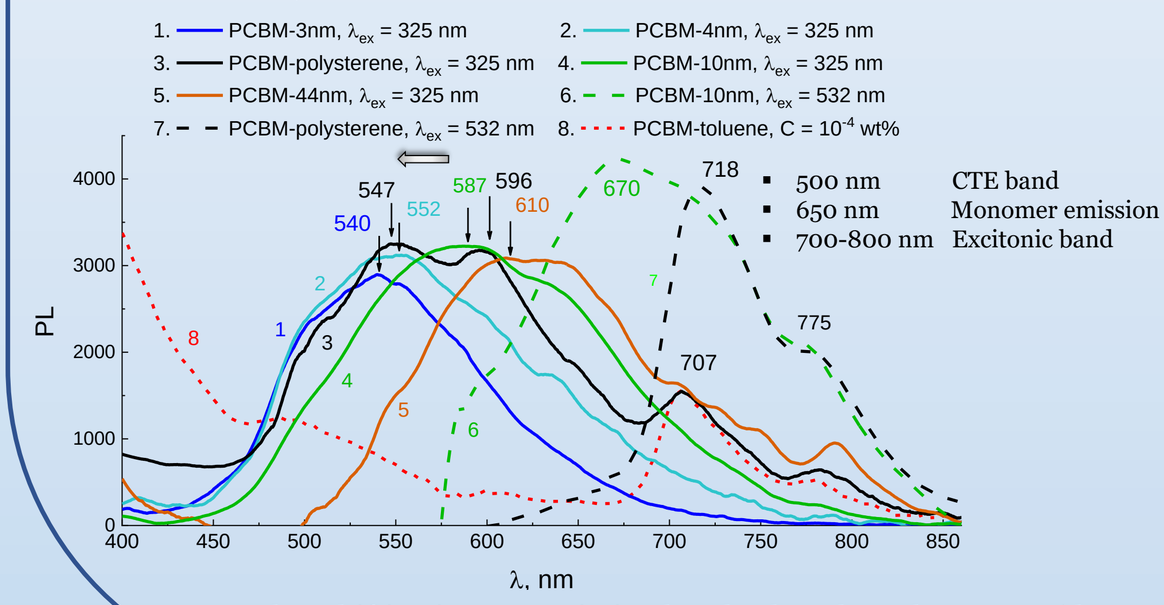
	λ_{PL}, nm	τ_1, ns	%	τ_2, ns	%	χ^2	λ_{ex}, nm
PCBM-4nm	700	0.3 ± 0.1	54	2.2 ± 0.1	46	1.169	255
PCBM-10nm	690	0.1 ± 0.1	75	1.4 ± 0.1	25	1.114	255
PCBM-10nm	700	0.2 ± 0.1	64	1.4 ± 0.1	36	1.121	255



	λ_{PL}, nm	τ_1, ns	%	τ_2, ns	%	χ^2	λ_{ex}, nm
C_{60}-10nm	690	0.5± 0.1	38	2.5± 0.1	62	1.207	405
C_{60}-10nm	750	0.4± 0.1	37	2± 0.1	63	1.297	405
PCBM-4nm	750	0.9± 0.1	41	3.1± 0.1	59	1.081	405
PCBM-10nm	690	0.9± 0.1	42	3.3± 0.1	58	1.109	405
PCBM-10nm	750	0.9± 0.1	40	2.9± 0.1	60	1.101	405
PCBM-44нм	750	0.7± 0.1	52	2.4± 0.1	48	1.175	405



Blue-shifting, when d_{pores} descreases, induced by the limitation of nanoaggregates sizes



Blue-shifting in CTE emission band, when d_{pores} descreases (d_{pores} <10 nm), induced by the **quantum size effect**

Conclusions:

- The linear spectral and time-domain decay properties of PCBM fullerene derivative in different media, in particular in mesoporous glasses at different excitation wavelengths were investigated.
- It was established the parameters of PL kinetic decay curves and lifetimes for PCBM in different media.
- The obtained bands in the PL spectra for PCBM were analyzed according to the model of the energy diagram of the electronic transitions in the molecule.
- Observed blue-shifting of the PL peaks maxima, which arises in the long-wave side of spectra with decreasing of pore diameters is induced by effect of spatial limitation the size of PCBM nanoaggregates.
- The blue-shifting of the PL peaks maxima, related with CTE emission band is induced by the quantum size effect. This effect leads to the spatial limitation of molecules forming the CT state with pore diameters less than 10 nm and as a consequence to observed blue-shifting.

*Kostetskyi, A. O., Piryatinski, Y. P., Verbitsky, A. B., Lutsyk, P. M., Rozhin, A. G. Photoluminescence of Melanin-Based Nanocomposites with Fullerene Derivative. *Semicond. Phys. Quantum Electron. Optoelectron.* **2022**, *25* (1), 49–57. https://doi.org/10.15407/spqeo25.01.049.