name of the unit:

LABORATORY OF COMPUTATIONAL PHYSICS AND CHEMISTRY

Institute of Applied Radiation Chemistry, Faculty of Chemistry,
Lodz University of Technology

symbol:

I-34

http://mitr.p.lodz.pl

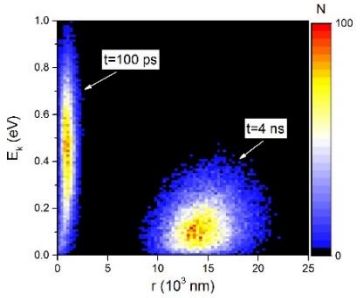
head of the unit:	potential promoters:	contact person:
Prof. Mariusz Wójcik, PhD, DSc	Prof. Mariusz Wójcik, PhD, DSc	Prof. Mariusz Wójcik phone: 42-631-3194 mariusz.wojcik@p.lodz.pl

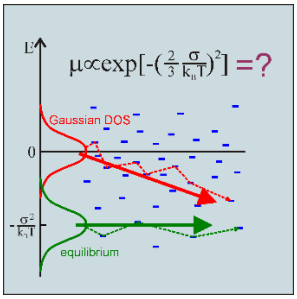
scope of activities:

The main research fields in our laboratory are:

- computer modelling of radiation-induced and photochemical processes
- electron-ion recombination in ionized systems
- charge-carrier transport and recombination in organic solids, modelling the operation of organic photovoltaic cells
- electron transport in dielectric liquids, including liquefied rare gases
- modelling the electronic processes in elementary particles detectors, especially the liquid-argon based detectors
- theoretical studies of diffusion and diffusion-controlled reactions
- development of computer simulation methods

graphic material





present activities:

We develop computer simulation methods and other computational tools which are useful in the modelling of particle transport processes in disordered media. We apply these methods to study various systems where a transport and reactions of excess charged particles are observed, such as organic photovoltaic cells, or elementary particle detectors.

To give an example, we study how the electron-hole separation probability, which determines the efficiency of organic solar cells, is affected by the type and magnitude of disorder in a particular medium. We also take into account the device construction details. We have recently found that the well-established previous theory of electron-hole recombination has serious flaws and proposed new solutions of practical importance.

We also work in quite a different field related to elementary particle physics. Our simulation model of electron transport in liquid argon was found to be useful in describing the operation of elementary particle detectors. We were invited to participate in a large international project, called DarkSide, which aims to explain the nature of dark matter by detecting its hypothetical particles using many tonnes-scale liquid argon detectors.

future activities:

We plan to continue our activities, both in the field of organic photovoltaics and in connection with detector physics. We want to provide useful hints for construction of efficient solar cells. We also want to assist the particle physicists in explaining the secrets of dark matter.

The portfolio of research groups was created as part of the Programme "STER" – Internationalisation of doctoral schools" as part of the realization of the project "Curriculum for advanced doctoral education & taining – CADET Academy of Lodz University of Technology".

publications/patents, awards, projects:

- M. Wojcik, I. Zawieja, K. Seki, "Charge transport in disordered organic solids: Refining the Bässler equation with high-precision simulation results", J. Phys. Chem. C 124, 17879 (2020)
- E. Collado-Fregoso, S. N. Pugliese, M. Wojcik, ... , "Energy-gap law for photocurrent generation in fullerene-based organic solar cells: The case of low-donor-content blends", J. Am. Chem. Soc. 141, 2329 (2019)
- P. Agnes, I. F. M. Albuquerque, ... , M. Wojcik, ... , "Low-mass dark matter search with the DarkSide-50 experiment", Phys. Rev. Lett. 121, 081307 (2018)
- M. Wojcik, A. Nowak, K. Seki, "Geminate electron-hole recombination in organic photovoltaic cells. A semi-empirical theory", J. Chem. Phys. 146, 054101 (2017)

keywords:

computer simulation, recombination, electron, hole, organic photovoltaics, elementary-particle detectors

list of internship proposals in this research team:

We offer a possibility of internship in the field of computer modelling of physicochemical processes.