POLISH NATIONAL AGENCY FOR ACADEMIC EXCHANGE

STER PROGRAMME

name of the unit:

DIVISION OF MOLECULAR MODELING

Department of Molecular Physics, Lodz University of Technology

symbol:

K-31

http://www.kfm.p.lodz.pl

head of the unit:	potential promoters:	contact person:
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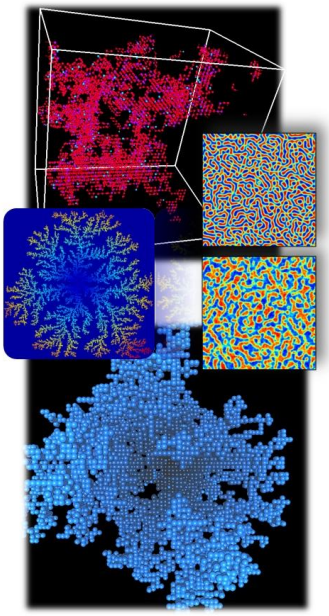
scope of activities:

The mainstream of research includes computer simulations of complex polymer systems using Monte Carlo methods. In the simulations of simple and complex fluids we mainly use the Dynamic Lattice Liquid (DLL) model. DLL is a simple model of fluid dynamics that assumes cooperative particle motion in the form of closed loops. The model does not require empty spaces, which allows to simulate dense systems, while the timescale is naturally included as loops are parallelly generated in whole the system. This model has been successfully applied in many fields of research: dynamics of chains, brushes, stars, polymer networks and the solvent, phase separation process, molecular aggregation, polymer diffusion problems, modelling of chemical reactions, including controlled polymerization, molecular transport in constrained geometry systems. Additionally, we perform molecular dynamics (MD) simulations of polymer mixtures and solutions as well as quantum calculations for organic compounds for use in organic and biologically active electronics. Another field of interest is the use of dedicated computing machines in molecular simulations, such as the FPGA-based Analyzer of Real Complex Systems (ARUZ) built in the Bionanopark in Łódź. We are also working on the implementation of new computer models, also with the use of parallel computing techniques. We work closely with experimenters in the field of chemistry, polymer physics and electronics.

graphic material



present activities:

- Computer simulations of the dynamics of polymer and solvent brushes.
- Study of the relationship between structure and dynamics in polymer systems with different geometries.
- Modelling of a controlled polymerization of macromolecules.
- Simulations of molecular transport in constrained geometry systems.
- Application of dedicated machines (ARUZ) in molecular simulations.
- Quantum computing for organic compounds for organic and biologically active electronics (adenosine derivatives, metallocarboranes).
- Simulations of molecular dynamics of polymer mixtures, eg PMMA, PLA and derivatives as well as water systems.
- Correlation of experimental and simulation results obtained with the use of models with different levels of generality.

Future activities:

Development of computer models for simulating complex systems, development of methods for dedicated computing machines

Keywords:

computer simulations, cooperative dynamics, molecular dynamics, complex polymer systems

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".

List of internship proposal in this research team:

- Simulations of molecular dynamics and macroscopic properties of polymer mixtures.
- Implementation of new numerical models for Monte Carlo simulations.

List of attachments:

- K. Hałagan, M. Banaszak, J. Jung, P. Polanowski, A. Sikorski, "Polymerization and Structure of Opposing Polymer Brushes Studied by Computer Simulations"; Polymers 13(24), 4294 (2021). DOI: 10.3390/polym13244294
- P. Filipczak, K. Hałagan, J. Ulanski, M. Kozanecki, "Surface-Enhanced Raman Scattering of Water in Aqueous Dispersions of Silver Nanoparticles"; Beilstein J. Nanotechnol. 12, 497-506 (2021). DOI: 10.3762/bjnano.12.40
- P. Polanowski, A. Sikorski; "The structure of polymer brushes: The transition from dilute to dense systems: A computer simulation study"; Soft Matter 17(46), 10516–10526 (2021). DOI: 10.1039/d1sm01306h
- R. Kiełbik, K. Hałagan, W. Zatorski, J. Jung, J. Ulański, A. Napieralski, K. Rudnicki, P. Amrozik, G. Jabłoński, D. Stożek, P. Polanowski, Z. Mudza, J. Kupis, P. Panek; „ARUZ - Large-scale, Massively Parallel FPGA-based Analyzer of Real Complex Systems"; Computer Physics Communications 232, 22 – 34 (2018). DOI: 10.1016/j.cpc.2018.06.010