

01.12-31.12.2013

Department for the Modelling of Physico-Chemical Processes, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland

Worked on dissipative particle dynamics simulation of Poiseuille flows of oligomeric molecules in narrow slit-like channels with walls modified via stripes of polymer brush and on phase transitions in the lattice gas of Janus particles.

Discussions with P. Bryk and A. Patrykiewicz on:

- generalisation of simulation of Poiseuille flows for the case of the mixture of oligomeric solvents,
- an extension of viscosity coefficient evaluation for the case of wall bounded mixture of flowing fluid,
- a set of properties affected by molecular weight of the solvent.

Discussions with S. Sokolowski on:

- phase transitions in lattice gas of Janus particles,
- introducing of the set of order parameters related to the phase transitions from low-density to high density (lamellar) 2D phase in near-surface layers of Janus particles fluid.

Transfer of knowledge:

- learned on flow properties dependence on molecular weight and currently existing studies,
- shared algorithms for simulation of oligomeric solvent and for the analysis of their spatial distribution via gyration tensor and partial orientation order parameters,
- learned about the peculiarities of near surface phase transitions that are indicated by a stepwise behaviour of density vs chemical potential for the fluid of Janus particles,
- shared algorithmic knowledge on Hoshen-Copelman clusters identification approach and on analysis of cluster sizes and cluster metric distributions to identify the low-density to high-density phase transition.