

M. Borówko and S. Sokółowski, UMCS Lublin, visits to UNAM, Mexico

In Mexico (UNAM, Institute of Chemistry) S. Sokółowski continued, with O. Pizio, the work on the manuscript „Restricted primitive model for electrolyte solutions in slit-like pores with grafted chains: Microscopic structure, thermodynamics of adsorption, and electric properties from a density functional approach.” (described in the report of O. Pizio), This task consisted of running several computer jobs, discussion of the obtained results and discussions of future calculations, necessary to get a deep knowledge of the observed phenomena. We collected numerous results and started to write the manuscript. The paper was submitted for publication in April, 2013 and was published in Journal of Chemical Physics in May 2013. Moreover, we began preparation of a review paper, entitled „Description of liquid - tethered polymer brushes interfaces: advances in density functional theories and off-lattice computer simulations”, in which our previous achievements in the fields connected with the description of fluids in contact with surfaces modified by tethered chains are reviewed. This work has been done together with J. Ilnytskyi (ICMP, Lviv). Of course, we did not finish that paper, but the work on it was continued during next months. Finally, the Manuscript was submitted for publication in May 2013.

Borówko worked on the preparation of the manuscript, entitled „ Terminally grafted chain layers in oligomer-monomer solutions: predictions from a density functional theory”. She carried out numerous discussions with the people from Institute of Chemistry, UNAM and with O. Pizio in particular. This paper was submitted for publication in Journal of Physical Chemistry B by the end of April 2013.

Both M. Borówko and S. Sokółowski attended the international Conference „4th Meeting on Molecular Simulations”, that was organized by Universidad Autonoma Metropolitana, Mexico City, Dec. 5-7 and took part in conference discussions on possibilities of simulations of complex systems. They also discussed several problems that can be encountered performing computer simulations of complex systems with G. Chapela, J. Alejandre (UAM, Mexico City) and W. Smith (University of Ontario Institute of Technology, Canada), who also attended that conference.