Stefan Sokołowski, visit to Departamento de Fisicoquímica, Instituto de Química de la UNAM, Mexico City, November 6 – December 3, 2013.

1. Scientific developments.

Together with O. Pizio we developed a new computer code for the description of structure, thermodynamic and electric properties of a fluid involving Janus (or amphiphilic molecules) and a solution of an electrolyte in contact with a solid surface. The program was based on a density functional theory. The amphiphilic molecules were modeled as spheres composed of "attractive'" and "repulsive'" parts. The electrolyte solution was treated employing the restricted primitive model. The density functional approach combined the fundamental measure theory for hard sphere mixtures, weighted density approach for inhomogeneous charged hard spheres and a mean-field approximation for describing the anisotropic interactions. We have extensively tested the program by comparing the obtained results with some existing literature data and, after tests, we have started the production runs. Our aim was to publish a paper, entitled "The structure and properties of a mixture of amphiphilic Janus molecules and ions at a solid surface" Therefore, an appropriate schedule of the calculations was proposed. We plan to finalize the manuscript of that work druring (private) visit of O. Pizio to UMCS at the beginning of March 2014.

2. Meetings and TOK.

I had three meetings with undergraduate and graduate students of O. Pizio, during which the problems connected with modelling and computer simulations of confined complex fluids were discussed. I also discussed several scientific, as well as technical problems connected with different applications of Molecular Dynamics with dr. Hector Dominguez.