

### **3<sup>rd</sup> Symposium on Electrostatic Phenomena in Advanced Materials Science**

*Report prepared by:*

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On September 24 - 25, 2009, the 3<sup>rd</sup> Symposium on Electrostatic Phenomena in Advanced Materials Science was held at the Leibniz Institute of Polymer Research Dresden (IPF). The symposium aimed at reflecting the recent progress in both experimental and theoretical approaches to a quantitative understanding of interfacial charging. Invited and contributed lectures covered topics ranging from the electrokinetics and power conversion at aqueous interfaces over ion specific effects at bilayer lipid membranes to the electrohydrodynamics at soft surfaces. Some of the keynotes are briefly summarized below; the [complete program](#) and the [abstracts](#) for all oral and poster presentations can be accessed at the conference website of the IPF.

Johannes Lyklema of Wageningen University discussed overcharging effects and presented his strategy to solve the dilemma between physical and chemical interpretations of the effect. He pointed out that virtually all cases reported in literature can be interpreted in the “chemical way”, even those experiments that have been invoked as support for physical interpretations, such as the action of ion correlations. As he further explained, systems in which ion correlations occur, but masking of the phenomenon by chemical adsorption can be excluded, remain hard to find. In front of this background, Johannes Lyklema impressively demonstrated that the double layer on negatively charged mercury in the presence of  $\text{MgSO}_4$  solutions fulfills this condition, thus providing the first unambiguous proof for the operation of ion correlations in colloid science. A presentation given by Akihiko Tanioka from the Tokyo Institute of Technology concerned transport phenomena across nanomaterials. Nanomaterials, including nano-scaled and nano-structured materials, have attracted much attention due to their unique properties and potential applications in many fields of engineering, including separation technologies. Based on recent

results of his group, Akihiko Tanioka impressively demonstrated why surface electrochemical properties are important for the application of nanomaterials in those processes. He concluded with a preview on future research trends in this area.

Roland Netz from the Technical University of Munich gave a talk about the electrokinetics and power conversion at aqueous interfaces. Together with Douwe Bonthuis and Dominik Horinek, he studied the transformation of electric energy into mechanical energy at aqueous interfaces in micro-fluidic devices. It was shown how the proper choice of simulation conditions give zero pumping for fields constant in time, in agreement with continuum hydrodynamic theory, while imprudent use of cutoff schemes and cutoff lengths in simulations yields spurious pumping effects. Furthermore, he demonstrated that a rotating electric field induces an electro-osmotic flow, and thus a simple shear flow for large channels. Under these conditions, net fluid transport was obtained for asymmetric channels. He concluded by proposing different practical schemes for electro/mechanic power conversion on the nano-scale.

Werner Kunz from the University of Regensburg reviewed some striking examples of specific ion effects. Furthermore, he summarized some of the most promising attempts to model them and to understand the origin of these effects. Finally, he presented a simplified model for the prediction of the behavior of ions near biological surfaces and surfaces of typical association colloids (micelles, polymers, liquid crystals, etc.).

Pavel Jungwirth of the Academy of Sciences of the Czech Republic in Prague presented the results of molecular dynamics simulations on the interaction of alkali cations and halide anions with single and multicomponent lipid bilayer membranes. It was shown how the different ions adsorb at the lipids and compensate for the charge of the lipid head groups. The simulations represent a step forward in understanding ion-specific effects at biological membranes in physiological conditions.

Hiroyuki Ohshima of the Tokyo University of Science introduced a new theory on electrostatic interactions between soft particles. The presented analytical expressions covered various cases relevant for the application of soft particles in technical and biotechnological processes. With the

development of the new theory, he provided a base for the better understanding of electrostatic interactions in systems containing different types of hard and soft particles.

Lydéric Bocquet of the University of Lyon reviewed recent progress in the understanding of the fluidics in the Debye layer. Special emphasis was put on effects observed at superhydrophobic surfaces. These surfaces are characterized by very large slippage effects at their interface, with effective slip length in the micrometer range. It was shown that these nanotextured surfaces do not further enhance the electro-osmotic mobility, while a huge enhancement can be observed for other interfacial transport, such as diffusio-osmosis.

James Beattie from the University of Sydney explained his theory on the force that attracts hydroxide ions to hydrophobic interfaces. He demonstrated how the phenomenon can be related to the suppression of the collective dipole fluctuations of water molecules by the hydroxide ions. By combining a simple model for this fluctuation force with a modified Poisson-Boltzmann equation, he was able to reproduce the pH dependence of the zeta potential measured for various materials in aqueous electrolytes—including the low isoelectric points of about 4, typical for interfaces without ionizable surface groups. He concluded with the proposition of an explanation for the absence of a signal from the hydroxide ions in surface spectroscopic measurements and the failure of some molecular dynamics simulations to reproduce the experimental results.

Jérôme Duval, of Nancy-Université and CNRS UMR 7569, presented a generalization of previous electrokinetic models for the streaming current of charged gel layers by tackling the most general situation, where a diffuse-charged thin gel layer is supported by a charged rigid surface. He pointed out that the new theory does not suffer from any restrictions on the magnitude of the volume charge density of the gel, the electrokinetic potential of the supporting rigid surface or the thickness of the gel layer, and thus provides a versatile base for interpretation of streaming current data measured at soft surfaces.

It was generally felt that the presentations and the lively discussions during and after the symposium substantially helped to bridge the sometimes still-existing gap between theory and experiment. Likewise, the meeting stimulated future scientific collaboration between the

participating groups. While no final decision has been made yet, the next symposium of this series will probably be held in 2011. Please contact Dr. Ralf Zimmermann ([zimmermn@ipfdd.de](mailto:zimmermn@ipfdd.de)) if you wish to receive further information on this meeting.