Concluding the School: School aspects

P.Varilly

To investigate the structural and dynamical properties of confined water all the available methods: RX, NS, RAMAN, IR, fluorescence, dielectric spectroscopy, NMR, have been used. We are interested to get results from other techniques: optical KERR, digital microscopy. Where to go from here? Simulations, modeling can provide what can get out from experiments.

Come up with a model that can describe the whole data.

Among results, surprising results:

- Protein wrapped with polymers (M. Weik)
- New phenomena: use of strong electric field (A. Luzar). How to explore experimentally such new phenomena?

Time resolved experiments must be considered.

Define model systems, but in biology there are no model systems.

T. Yamaguchi

The School provides with a lot of inspiration for the future work.

There was a chance to chat in the evening. The School was a very important opportunity for young people who will become 10 years later professor in their university.

X-ray free electron laser in Japan, femtosecond spectroscopy; there is a hint what science can be done with these new techniques.

Computer simulations by Tarek offer a good opportunity to progress in science. Water is important for life and new progresses have to be made in the future.

M. Vogel

View over different fields and different methods.

It is important to bring together different methods plus simulations. There is some progress. We need more for the future.

Interesting questions: How much specificity of surfaces matter for the water? For one water monolayer dynamics is more driven by the surface. What do water-water interactions? What about the 2^{nd} and the 3^{rd} layer of water? Compare NS plus dielectric, from MD calculate the observables and understand the differences between the different methods. Bring together all these methods and compare with the MD results.

MCM41 are not always similar. There is a problem into the definition of model or perfect system. Sample matters a lot. From the School one must find a way to exchange and compare samples. We are working too much individually.

V. Kempter

Thanks to organize Ionic liquids (IL's) session. Difficult to follow session on biology. VK feels that IL's may serve as realistic model for biology.

Close to polymers coated myoglobin (M. Weik).

IL's lead to segregation phenomena, pattern formation, similar confined phenomena in biology.

From Ouchi talk, working with confined IL's is easier than with water. You can prepare surfaces under ultra high vacuum. You can prepare deposit, starting from sub-monolayer deposits up to multilayers, study by photoelectron plus optical spectroscopies. See similar chemically active groups in IL and biological systems.

Theory on IL's is one step in front of the treatment of biological systems. One can use ab initio methods, check the force fields.

What are the outstanding questions in IL's area that you trigger interest for simulations?

-Interaction of IL's with the surfaces?

-What is the origin of the bonding within/between IL's? (H-bonding?) No agreement on that.

T. Elsaesser

The School was a mix of many topics. The connection of tools is quite important. How do we link structure and dynamics? Structure is measured with different time scale: X-ray and NMR. We need to have links with MD from which we can extract the different structures. We need to perform non-linear spectroscopy to go to lower frequencies in time resolved spectroscopy (ps). There are new possibilities with time resolved X-ray diffraction (free electron laser?) to locate oxygen atoms transiently.
-limitation for NS
-limitation for IR
One should think to another conference.
Concerning Tarek lecture: advantage to use a group of techniques to study one object.

S. Meech
S. Meech learnt new and different aspects of water. Novel featues like simulations (electroevaporation) look to be an important and exciting growth area. Some new techniques like ultrafast spectroscopy, Brillouin scattering bring new information and challenges for theory. The methods that are not represented here and may make important contributions in the future are single molecule fluorescence plus modeling, time resolved electron diffraction (problem of penetration?), femtosecond X-ray absorption. There are problems as always to pick up well defined systems.

B. Bouvier
There were not too many repetitions. The School was good.
B. Bouvier mentioned his collaborations with many experimentalists concerning the thermodynamics. He works at room temperature (force fields). What is the behavior at temperatures different from room temperature? Water mediates the nonspecific interactions. It is important to understand this effect of water. His community is more interested by dynamics, time resolved experiments. From the biological point of view, it is interesting to simulate large systems (coarse graining technique). But there is a problem for water, no model of coarse graining.