Workshop Scientific Report (ESF)

Workshop: Perspectives and challenges of simulations of bio-materials interfaces

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I. Summary

The workshop “and challenges of simulations of bio-materials interfaces” was held at the University of Bremen, Germany from October 10th to October 14th 2011. In total, 65 participants from Bulgaria, Germany, USA, UK, Canada, Denmark, Japan, Poland, Sweden, Italy, Iran, France, China and Switzerland attended the workshop.

The programme consisted of 29 invited lectures, one poster session and different social events allowing for scientific discussions and exchange. The lectures were scheduled to last 40 min, including 10 min discussion time. In addition to this extended time for discussion, the chairpersons were instructed to introduce the subject of the session and to actively participate in the discussion. This “Gordon-conference-style” was essential to guarantee a vivid discussion. The organizers ensured that well-established scientists acted as invited speakers and chairpersons.

Concerning the poster session, we accepted only 22 posters to allow for an intense exchange of ideas at each single poster. Here, we encouraged in particular the young scientists to ask questions. The participation of young researchers were supported by partly covering local accommodation costs.

Due to the compact organization and accommodation in one hotel only all participants had to stay together for the whole time of the conference, which additionally enforced the scientific discussion which was mandatory since scientists from various separated fields, i.e. advanced quantum chemistry, quantum Monte-Carlo, many-body perturbation theory, time-dependent DFT, etc. were attending the meeting to merge ideas and formulate a common goal for future method developments.

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II. Scientific content and discussion

The physical/chemical behavior of hybrid bio-organic/inorganic interfaces in the focus of the workshop results from a delicate interplay between the electronic or mechanical properties of the inorganic phase and the surface bonding of biological molecules, which may undergo a drastic change of their structure and thus of their functionality upon interaction with the solid. Chemical reactions at the phase boundaries and other processes involving the transfer of electrons or the exchange of ions across the interface characterize uniquely the behavior of the composite material. Since such effects are not trivial to be analyzed with high resolution experiments or predicted a priori, computer modeling offers a viable way to investigate them on the basis of fundamental physical principles, thus complementing and expanding the information obtained by means of experimental techniques.

The investigation of phenomena at hybrid biomaterials interfaces poses so far unresolved challenges to accurate, atomistic computational methods, since it involves dealing with mutually interacting phenomena spanning multiple time and length scales and requiring different levels of precision. In the biological community, deciphering the physics of complex units from motor proteins to ribosomes, from membrane channels to DNA packaging in the cell nucleus or DNA-sequencing has become possible by the advent of many new technologies to analyze and manipulate molecular systems at highest precision. Combining high-resolution structural analysis with high-performance computing enabled furthermore to simulate how the intrinsic structural movements of biological nano-scale systems combined with their optical, electrical or mechanical properties control or regulate their functions. Also aided by high-performance computing, new functional hybrid-materials were designed, some of which were inspired by biological systems. Understanding life from its molecular foundation on a qualitative level, learning from it for technical applications and elucidating how the interactions between living structures interact and the technical world may stimulate novel routes for materials design has become a very attractive field of research these days.

To accomplish this goal successfully computational research request different methods from quantum and classical atomistic simulations through coarse grained techniques and further bottom upscale to finite element methods (FEM), and this is done traditionally in quite separate research communities.

Since the subject of the workshop is so interdisciplinary, also the background and scientific communities of the lecturers and participants were quite diverse. It was therefore the aim of the workshop to familiarize the participants with different subjects, to encourage interdisciplinary interactions, and to share experience of different research fields with one another. In this way, we managed to foster the exchange of ideas and methods, to highlight the most recent advances in experiments and computational method developments and applications, and hopefully stimulated new and fruitful collaborations and future projects across subject boundaries.

III. Assessment of the results and impact on future direction of the field

It became apparent from the presentations and the corresponding discussions that the modelling in each component of bio-materials interfaces is indeed very challenging. In some areas of the research field the methods and approaches have still not matured, so that intrinsic technical and conceptual problems persist.

In the workshop the following key objectives have been achieve:

The main advantages and disadvantages of currently available modeling techniques for the specific case of simulations of biological/inorganic interfaces have been discussed and specified. The techniques considered comprise (but not are limited to): (i) QM: essentially DFT-based techniques for ground states configurational sampling, including Order-N techniques; (ii) MM: atomistic force fields and many-body potentials; (iii) QM/MM: hybrid quantum/classical with static QM zones; (iv) D-QM/MM: hybrid quantum classical with dynamically moving and evolving QM zones; (v) CG: coarse-grained; (vi) HCG hybrid coarse-grained coupling different levels of precision.

The workshop impressively demonstrated the already existing intense collaboration between experiment and theory being the basis for improving our understanding of fundamental interactions and the functional interplay at bio-materials interfaces. To foster this process even further invited overview talks by highly recognized experimentalists have been presented.

In the workshop future directions for method developments and improvements of existing techniques to address physical and chemical phenomena at bio-organic/inorganic interfaces have been discussed. This has set the basis for scientific collaborations between the participants in order to foster methodological advances with respect to the state of the art.

October 19th 2011

The Organizers