



1st Winter School on “Modeling Chemical and Biological (Re)Activity”

January 2 to 22, 2014

**Center for Computational Natural Sciences and Bioinformatics
International Institute of Information Technology, Hyderabad**

Conveners: Prof. U. Deva Priyakumar, Prof. G. Narahari Sastry

Modeling Chemical and Biological (Re) activity (MCBR) is a series of Indo-German workshops/symposia. The concept of MCBR symposia (Indo-German meetings on “Modeling of Chemical and Biological (Re)Activity”) was developed by Prof. G. N. Sastry (IICT), and Prof. Hendrick Zipse (LMU) and the first meeting (MCBR-I) was held in IICT, Hyderabad (2007), followed by MCBR-II in Wildbad Kreuth (2009) and MCBR-III in Chandigarh (2013). In January 2014, Prof. G.Narahari Sastry and Prof. U. Deva Priyakumar, as an extension to the scientific meetings organized the first Winter School on MCBR. The next symposium (MCBR-IV) and the second winter school will be held in Heidelberg (Germany) next year which will be organized by Prof. P. Comba.

After the immense success of this series of scientific conferences in the field of Computational Chemistry and Biology, MCBR team planned to get a step ahead this time. Thus after lot of planning and efforts, DST-SERB supported “First 21-day Winter School on Modeling Chemical and Biological (Re)Activity” was organized by the Center for Computational Natural Sciences and Bioinformatics at the International Institute of Information Technology, Hyderabad from January 2 to 22, 2014. Prof. Comba, Heidelberg University was one of the key players in this initiative. Being the first ever winter school of its kind held in India, the workshop consisted of an intensive training program of three weeks, very well scheduled, covering almost all the topics in the field of computational natural science starting from the very basics up to cutting edge research level. Out of over 200 applications received, top 40 research students from all the leading institutes in different corners of India were selected for participation here. Along with them, 10 people from industry also participated making a total count of 50 participants across the country. This talented pool of students got a golden opportunity to interact with the renowned scientists of their field of research from different parts of India as well as abroad, who were invited to teach in this winter school.

The key objective of this winter school was to provide appropriate theoretical background and to train with methodologies of computational Chemistry and Biology. In accordance with it, along with the lectures, hands-on practical sessions and post-dinner discussion sessions were an integral part of the program. The well-thought schedule allowed students to first learn the basic concepts through lectures and thereafter practically applying the concepts learnt by actually solving exercises with the use of computational software packages under the supervision of experts. All this was followed by post-dinner question session, where all the participants were allowed to share any kind of technical or conceptual problem they faced and these questions were addressed by experts as well as fellow participants leading to superb exchange of experiences.

Another unique feature of this winter school was teaching the advanced topics from the very basics. It touched upon four broad classes of the subject namely Molecular Mechanics, Quantum Chemistry, Hybrid QM/MM and Computer Aided Drug Design. Topics included were basic



quantum mechanics, approximation methods, Born-oppenheimer approximation, Hartree-Fock and post Hartree-Fock methods, Density Functional theory, electron correlation, basis sets, potential energy surface, reaction mechanism, force field parametrization, biomolecular simulations, and various aspects of drug designing using computational techniques. All of these topics were beautifully covered, starting from the basics and then finally up to the level of case studies of real life applications of these in the research problems. The practical sessions led to even deeper understanding. It is important to mention that each topic was covered several times, each time by a new expert, adding a new perspective to it and leading to a wider understanding of it.

Most of them spent more than a week each in this winter school and made themselves available for interaction/discussion with interested students from morning 08:30 up to the post-dinner session everyday, which went up to 11 PM. Their vicinity benefitted the participants academically, but also inspired them to do simple things the right way. They could see how great scientists work and approach a problem, by listening and talking to them about their research career experiences. The informal discussion of students with them during lunch and dinner was equally productive as formal interactions during pre-defined sessions.

Another element of uniqueness of this winter school was the flexible dynamic schedule which kept on evolving as per the immediate needs of the participants and speakers. This led to better fitting in of the program as per the requirements of the students, as observed by the organizers. The schedule was really intensive with participants left with no time for any other activity. Thus, organizers also periodically conducted fun events during the winter school, with a dual objective of recreation and more importantly allowing close interaction among the members of MCBR family. Sundays were used for outing to nearby places.

A general survey of participants, after the completion of these intense three weeks, clearly reflects the increased level of confidence amongst them about their field of interest. All of them were already experts of one or the other part of the broad spectrum of computational science, but after attending this winter school they all gained an insight of the overall picture of the whole spectrum. The most important thing was that they could succeed in learning the areas which they were afraid of and always feared to encounter. They were able to connect the little pieces of knowledge they had and put them at the right place in the realm of computational Chemistry and Biology. Both organizers as well as participants seem to be very much excited with the success of this unique winter school organized in the country. This first of its kind attempt generated immense output they believe and has set an example and laid the foundation for more such events in future with higher level of rigor involved and higher opportunity of participation for students as well as teachers.

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