Report on a European Training School on Advanced EPR

held at

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Summary

During the past decade EPR spectroscopy has undergone a change from being focused on mainly continuous-wave techniques, frequencies below 40 GHz and native paramagnetic centers to widespread use of pulsed techniques, frequencies of 94 GHz and higher, and application of site-directed spin labeling of biomacromolecules. The European Training School under the auspices of the European Federation of EPR groups addressed the educational needs of Ph.D. students and young postdoctoral co-workers arising from this development by a series of educational lectures, tutorials, and lab courses, as well as by two research lectures by renowned experts, Prof. Dr. Jack Freed (Northwestern University) and Prof. Dr. Brian Hoffman (Cornell University), and two lectures on important aspects of application of EPR spectroscopy in the life sciences.

The 14 lectures (format 45 minutes + 15 minutes discussion) on basic aspects of EPR theory, instrumentation, and experimental techniques provided a complete, if rather condensed overview of the foundations of the field. In addition, 4 advanced lectures were given on quantum chemical computation of EPR parameters, dynamic nuclear polarization, advance high-field EPR instrumentation, and spin correlated radical pairs, all by top experts in the respective fields. The important application fields of metalloproteins, site-directed spin labeling, EPR imaging, optically excited systems, and solid-state materials were covered in depth by altogether 7 lectures.

Students could deepen their knowledge and abilities by choosing from 27 tutorials on 12 distinct topics (75 minutes each, up to about 10 participants) and 15 lab courses on 5 distinct topics (150 minutes each, up to 4 participants). A general question session and a feedback session were organized.

Students evaluated the summer school with good to very good grades. On a scale from 1 to 5 (best grade 5), overview was graded 4.29 (standard deviation 0.74), course materials 4.45 (0.71), tutorials 4.44 (0.88), and lab courses 4.5 (0.67).

Scientific Content and Discussion at the Event

Except for the first research lecture, which was given as an opening lecture by Jack Freed, the sequence of lectures was based on the idea that as few as possible previous knowledge of students should be supposed. This principle was deemed necessary because of the expected heterogeneity of the students, with experience varying from master level to PostDoc and the main field being almost evenly distributed between physics (35.3%), chemistry (38.2%), and biology (26.5%). We think that the principle was successful, also due to the cooperation of virtually all teachers in emphasizing didactics. Our assessment is based on the evaluation of the students, which graded difficulty of the lectures as 3.30 (standard deviation 0.72) on a scale where 1 was to easy and 5 too difficult (ideal result would have been 3.00).

Almost 50% of all lectures, altogether corresponding to a one term course with one lecture hour per week, were devoted to topics that would feature in an introductory lecture course on EPR spectroscopy. The level and depth of theses lectures was higher than would be expected in an undergraduate course. We made a strong and successful effort to ensure a lively discussion of each lecture (including the more advanced and specialized lectures) by the students. For that purpose, questions by other lecturers were strictly forbidden and moderators of the discussion insisted until the first student came forward with a question. After this procedure had been established on day 1 and the ice was broken, students did not need further encouragement to ask. The moderator just needed to make sure that they found sufficient time to think about questions.

Tutorials were given with typical group sizes of 10-12 people, although limitations were not strictly enforced. The format differed between demonstrations on the black board, work of students on exercises, and 4 different computer-based tutorials (altogether 11 sessions) with explanation and hands-on experience. Student activity in the tutorials was good to very good. The concept caught on so much that two lecturers spontaneously offered extra tutorials on advanced topics (Stefan Stoll and Brian Hoffman). Distribution of tutorials materials was on discretion of lecturers, although we did offer help with printing/copying. A majority of tutorials had printed materials, most notably the tutorial on the quantum chemistry software package ORCA came with the complete manual of the package (plenty of copies were provided and all were taken). Most tutorials were running overtime.

The typical size of a lab course group was three students and one teacher, in exceptional cases four students. For spectrometer capacity reasons not all students (>70%) could be assigned to lab courses, places had been distributed on “first come first served” basis. Lack of spectrometer capacity was also the reason for offering additional lab course spots for advanced students on Sunday, September 5th at ETH Zurich. This offer was indeed taken by 8 students.

Lab courses were discussed in detail in the feedback session, prompted by one lab tutor who asked the question whether such short lab courses make any sense. Several students vigorously defended the concept. As organizers, we were surprised by the demand for the “Basic pulse EPR” lab course, to which we had to assign 7 of the 15 available slots. Feedback from the tutors and students indicates that these basic courses were very valuable and should be a part of any future school, spectrometer capacity permitting.

Most students did have the opportunity to take part in one lab course (150 minutes) and up to seven tutorials (75 minutes), in addition to the 30 lectures (45 minutes + 15 minutes discussion) and the poster session on Tuesday evening. This made for a fairly condensed program, and most students took some time off on tutorial afternoons for informal discussions, often in front of their posters. The relatively short time assigned to poster discussion (one evening) made for the worst average grade given by students in the evaluation (“Time for poster discussion was sufficient”, grade 3.43, std. dev. 1.41, 12.5% assigned the worst grade 1). We could observe poster discussions even in the morning before lectures and during lunch breaks. This may explain why another 30% of the students awarded the best grade 5 in this question. In fact, the statement “Time for informal contacts between students was sufficient” received a grading of 4.03 (std. dev. 1.1).

We made an effort to have lecturers present for the whole week or at least for a significant time after their lectures. Most lecturers did cooperate, the ones who did not usually had very good reasons. Students got a good impression regarding this point. The statement “Lecturers were sufficiently accessible beyond lecture times” got a grading of 4.23 (std. dev. 0.89).

The whole school had a focus on EPR basics and methodology (14 basic lectures + 4 advance lectures + all bit one tutorial + all practical). Our reasoning was that an interest in basics and methodology was the only unifying feature of all students. The evaluation question about the main interest of the students revealed that about 1/3 mentioned methods as main interest, while 41.7% mentioned biological applications and 20.8% materials science applications. This distribution was also apparent in the large interest in tutorials on techniques that are of main interest in work on biological systems. While the scientific program catered well to this large group, we feel that the students with a main interest in materials science (a larger fraction than we expected) should have been offered one or two tutorials geared to their interests.

The lectures on topics beyond EPR spectroscopy (Protein Crystallography and Current Trends in Molecular Biology) were given by local experts, Prof. Kay Diederichs and Prof. Elke Deuerling, thus taking advantage of the strength of University of Konstanz in the fields of Biology and Chemical Biology. As gauged by the lively discussion after these lectures, both topics were of great interest for the students (and the EPR lecturers).

Assessment of Results and Impact on the Future Direction of the Field

The EPR Summer School in Konstanz was distinguished by a good and friendly spirit among students and lecturers over the whole week. This is also certified by the response of students to the evaluation statement "Lecturers were engaged and engaging" (average 4.13, std. dev. 0.91). The 11 statements of the evaluation sheet, most of which were already discussed above, received an average grade of 4.12. With respect to content the most negative evaluations were for the statements "Connections between different topics became clear" (avg. 3.71, std. dev. 0.93) and "Topics were covered in sufficient depth" (avg. 3.85, std. dev. 1.03). For a training school with such a broad scope we still consider these responses as good. Probably an overview of connections in the Curriculum would be a good addition to course materials, as some of these connections appear to be much less obvious to students than to teachers. Altogether we consider the Training School as a great success, made possible by the tradition of such schools since 1999 and continuous feedback from students, teachers, and organizers of previous schools.

We identify two main results with respect to the students. First, the scope of the whole school has made many students aware of aspects of EPR spectroscopy that are relevant for their work, but were never encountered by them in their previous education. Such a lack of depth of the students is a typical feature of a relatively small scientific field such as EPR spectroscopy, which does not feature prominently and in some places does not feature at all in undergraduate curricula. With respect to this we see a clear competitive advantage of European science compared to the USA, where such a training school for EPR spectroscopy does not exist. In Europe such schools have been held every three or two years since 1999, so that in principle all Ph.D. students had an opportunity to take part. Significantly, the students in Konstanz awarded the title of "Best Lecturer" to Stefan Stoll, who is a graduate of the 1st European EPR Summer School 1999 in Caorle, Italy and had organized the student feedback session in this school.

The second main result with respect to students came mainly from tutorials and lab courses. This is a spread of good practices in EPR experimentation, data analysis, and interpretation. In fact, we consider this as even more important than the widening of scope of the students. Advanced EPR spectrometers and advanced experimental techniques are currently spreading fast to groups who had no previous experience. In some cases groups have made the transfer without a principal investigator or even experienced PostDoc who had in-depth knowledge of these techniques. Some of the students who perform the work are biologists, with few general education in quantum mechanics, basics of magnetic resonance, and complex measurements. In this situation, a dedicated Training School is the only way to keep up high scientific standards in the field. We do think that many of the graduates of the Konstanz EPR Summer School will become teachers themselves in their

groups at home. They have also established a network with their peers and with tutors at the school that will help them to get advice.

Last but not least the school has also strengthened contacts among the teachers and, in many cases, the knowledge of principal investigators. This should not come as a surprise. Didactical lectures by top experts are rarely encountered at scientific conferences. Then, how can a principal investigator extend his knowledge of the foundations of his field? With the fast current development in EPR, textbooks are lagging the advances. In fact, experienced PostDocs of one of our groups suggested that there should be an advanced training school at an even higher level that addresses mainly experienced PostDocs and principal investigators. Whether something like this could be financed may be a matter of debate. Short of such a school, the Konstanz EPR school addressed at graduate students and young PostDocs has contributed to fill this gap.

As the main impact of the school on the field we consider the spread of good practice and high scientific standards. Informal networking of European EPR groups at Ph.D. student and PostDoc level is another valuable outcome. Due to the unexpectedly large fraction of biologists among the students, we also expect that the school will spread awareness among biologists of the new opportunities in structural biology that have arisen by the development of advanced EPR techniques during the past few years.