Meeting Report: The Third International Synchrotron Radiation Circular Dichroism Spectroscopy Meeting

17-20 May 2015

Bad Honnef, Germany

The International Synchrotron Radiation Circular Dichroism (SRCD) Spectroscopy Meeting was held at the Physikzentrum, Bad Honnef, Germany on 17-20 May 2015, as the 590th WE-Heraeus-Seminar. It was the third in the series of SRCD Workshops, following on the first one held at the Daresbury Synchrotron (UK) in 2001, and the second at the Beijing Synchrotron Radiation Facility (BSRF) and the Institute of High Energy Physics (IHEP) in 2009. SRCD2015 was organised by Dr. Jochen Bürck, Prof. Anne Ulrich and Dr. Dirk Windisch (all of Institute of Biological Interfaces (IBG-2), Karlsruhe Institute of Technology, Germany) and Prof. Bonnie Ann Wallace (Birkbeck College, University of London, UK). It was aimed at both synchrotron SRCD beamline scientists and scientific users of the beamlines, and included participants from 14 countries. For the first time, representatives of all operational SRCD beamlines worldwide were present at the same meeting, and scientists developing two new SRCD beamlines also participated.

The meeting was opened by Professor Ulrich, who welcomed all participants. This was followed by a keynote address presented by Prof. John Sutherland (East Carolina University, USA) who described his creation of the early SRCD beamlines at the NSLS (USA) and the subsequent instrumentation advances over the years that were now leading to many exciting new scientific achievements internationally.

The first session on day 2 focused on applications of SRCD spectroscopy in biology, most specifically for studies of proteins and peptides, and how insights into structure and function could be gained by the complementary use of SRCD spectroscopy and other methods. They included talks by Prof. Wallace on studies of voltage-gated sodium channels, Dr. Heather Findlay (Kings College, London, UK) on the folding and unfolding of transporter proteins in membranes, Dr. Robert Janes (Queen Mary University of London, UK) on the dental protein statherin, Dr. Jose Luiz Lopes (University of Sao Paulo, Brazil) on intrinsically disordered proteins, and Prof. Martin Ulmschneider (Johns Hopkins University, USA) on combining molecular dynamics simulations with SRCD spectroscopy to study peptides in membranes.

The next sessions were devoted to reports on the current capabilities and future plans for existing SRCD beamlines, presented by Drs. Søren Vronning Hoffmann and Nyk Jones (ISA, Denmark), Jochen Bürck (ANKA, Germany), Frank Wien (Soleil, France), Koichi Matsuo (HiSor, Japan), Ye Tao (BSRF, China), Giuliano Siligardi (Diamond Light Source, UK), Wei-Ning Huang (NSRRC, Taiwan), and Peter Baumgärtel (Bessy II). Each discussed the different designs, performance characteristics, and unique features of their beamlines, including “periscope” sample chambers, oriented SRCD, high throughput sampling devices, and stopped flow and continuous flow for dynamic measurements. These were followed by “flash talks” given by Drs. Douglas Galante (LNLS, Brazil) and Salvador Ferrer (ALBA, Spain) on new beamlines in planning and development stages. It was clear that the field had matured greatly since the previous international meetings, with beamlines now very effectively functioning as user facilities whilst continuing to develop new innovations and improvements in instrumentation.

These sessions were followed by talks on related methods, including linear dichroism spectroscopy using synchrotron radiation by Profs. Alison Rodger (Warwick University, UK) and Tim Dafforn

(Birmingham University, UK), theoretical calculations of spectra by Prof. Jonathan Hirst (Nottingham University, UK), and time resolved conventional CD spectroscopy by Francois Hache, (CNRS, France). The combination of SRCD with neutron scattering and crystallography was discussed by Prof. Petri Kursula (University of Bergen, Norway), with solid state NMR by Dr. Dirk Windisch (Karlsruhe Institute of Technology, Germany), and with other synchrotron-based techniques such as SAXS by Dr. Inari Kursula (University of Oulu, Finland). Finally, validation and analyses of spectra (Dr. Andrew Miles, Birkbeck College, University of London, UK), new bioinformatics methods for determining secondary structures from SRCD spectra (Dr. József Kardos, Eötvös Lorand University, Hungary) and the Protein Circular Dichroism Data Bank (PCDDB) resource (Dr. Lee Whitmore, Birkbeck College, UK) rounded out the talks. Several sessions were devoted to an excellent set of posters, which showed the breadth of current and potential applications of SRCD spectroscopy ranging from biophysics to astrobiology, chemistry and material science. In addition, it was clear from the posters that SRCD spectroscopy was effective for examining samples in the gas phase, in solutions, films, solids, and lipid membranes.

An important component of the meeting, following the example of the first two international workshops, was the more informal "roundtable" discussion amongst beamline scientists and developers, that was held on the afternoon of the third day (during which time other meeting participants had the opportunity to take a walking tour of the nearby Burg Drachenfels). This roundtable enabled comparisons of design features, data collection procedures and calibration standards, means of avoiding radiation damage (including confirmation that the early estimates of the threshold flux that would initiate the process – Wien et al, JSR, 2005 – had proven to be correct), as well as common data formats and software, and access mechanisms. It was noteworthy that so many of the technical issues focused on at the previous roundtables had been resolved (in large part by inter-beamline cooperative studies at different synchrotrons, and through regular local meetings involving, for example, European beamline scientists). That meant that the beamlines were now moving on to new and novel instrumentation for exploring new types of samples and conditions such as thermal and dynamic changes. In closing the session, Dr. Janes urged all beamline scientists to encourage their users to deposit their spectral and metadata in the PCDDB, as this was rapidly becoming a highly used resource for both conventional and SR circular dichroism studies and bioinformatics developments, with >500 entries and >300,000 downloads having been undertaken already.

On the final day, Prof. B.A. Wallace gave the concluding address, during which she summarised the state of the field and its growth and development since the first SRCD meeting in 2001, talked about her experiences at all of the SRCD beamlines worldwide, and speculated on the potential advances for the future in both instrumentation and in applications for biology and material science. Poster prizes were awarded to J.-D. Savoie (Université Laval, Canada), C. Meinert (Université de Nice Sophia Antipolis, France), and L. Steger (Karlsruhe Institute of Technology , Germany). The meeting concluded with participants expressing their appreciation to the scientific organising committee for a wonderful meeting, to the Physikzentrum Bad Honnef for technical and administrative support and especially to the Wilhelm und Else Heraeus-Stiftung (WE-Heraeus Foundation) for hosting and administrative organisation of the meeting, and for its financial support.

B.A. Wallace[1] and Jochen Bürck[2]

[1]Institute of Structural and Molecular Biology, Birkbeck College, University of London, UK
[2]Institute of Biological Interfaces (IBG-2), Karlsruhe Institute of Technology, Germany

Photo:

Participants in the 3rd International SRCD Spectroscopy Meeting (590th WE-Heraeus-Seminar) at the Physikzentrum, Bad Honnef, Germany