



SOFTWARE TOOLS FOR EPR SPECTROSCOPY – CAPABILITIES AND DEMONSTRATIONS
JULY 26-27, 2018
SNOWBIRD, UTAH, USA

ORGANIZATION

Gary Gerfen (Chair)

Sponsored by SharedEPR



AGENDA

THURSDAY, JULY 26, 2018

1:30 PM	Welcome. Stefan Stoll
1:40 PM	mtsslSuite - Interpreting PELDOR/DEER Distance Distributions in Terms of Macromolecular Structure. Gregor Hagelueken, University of Bonn
2:10 PM	Site-directed in Silico Spin Labeling and Structure Modelling with MMM 2018. Gunnar Jeschke, ETH Zürich
2:40 PM	Software for Advanced and Global Analysis of EPR Data: GloPel and SpecProFi. Stephan Rein, University of Freiburg
3:10 PM	SpecMan4EPR: Connecting Spectrometers to People. Boris Epel, University of Chicago
3:40 PM	<i>Break</i>
4:00 PM	Streamlining Lineshape Fitting of Spin Labels in the Slow-motion Regime. David Budil, Northeastern University
4:30 PM	Model-based and Global Analysis of DEER Data using DD and GLADDvu. Eric Hustedt, Vanderbilt University
5:00 PM	Using Wavelet Transforms to Denoise and Obtain Accurate cw and Pulse ESR Results. Madhur Srivastava, Cornell University, ACERT

FRIDAY, JULY 27, 2018

8:30 AM	EasySpin - An Extensive Toolbox for Simulation and Fitting of CW and Pulse EPR Spectra. Stefan Stoll, University of Washington
9:00 AM	SpinFit and Anisotropic SpinFit. Kalina Rangelova and Ralph Weber, Bruker
9:30 AM	Simulation of Rotamer Structure of Spin Labels and its Implication for DEER. Peter Fajer, Florida State University
10:00 AM	<i>Break</i>
10:20 AM	Simulation of DEER, RIDME, SIFTER, (MAS) DNP, CIDNP and Other Time-domain Processes. Ilya Kuprov, University of Southampton
10:50 AM	Full-featured LabVIEW Programs to Derive Distance Probability Distributions from Dipolar Interaction Data (DEER, CW). Christian Altenbach, UCLA
11:20 AM	Assessing and Interpreting Distance Distributions with DeerAnalysis 2018. Gunnar Jeschke, ETH Zürich
11:50 AM	Closing. Gary Gerfen