

## Provisional Programme

### Faraday Discussion 150: Frontiers in Spectroscopy 6 – 8 April 2011 Basel, Switzerland

Wednesday 6 April

11:30	<b>Registration</b> <i>Foyer, Department of Chemistry, University of Basel, St. Johannis – Ring 19</i> <a href="http://www.chemie.unibas.ch/visitors/sitemap.html">http://www.chemie.unibas.ch/visitors/sitemap.html</a>
12:00	<b>Networking and sandwich lunch</b> – all delegates welcome <i>Foyer, Department of Chemistry, University of Basel</i>
13:00	<b>Welcome and introductions</b> <i>Large Auditorium, Department of Chemistry, University of Basel</i>
13:15 <b>Paper 1</b>	<b>Introductory lecture</b> <b>Spectroscopy and astronomy</b> Takeshi Oka <i>University of Chicago, USA</i>
<b>Session 1</b>	<b>Precision spectroscopy</b> Session chair: Gerard Meijer, <i>Fritz-Haber-Institut der MPG, Berlin, Germany</i>
14:15 <b>Paper 2</b>	<b>Optical frequency comb spectroscopy</b> A Foltynowicz, P Maslowski, T Ban, F Adler, K C Cossel, T C Briles and J Ye* <i>University of Colorado at Boulder, USA</i>
<b>Paper 3</b>	<b>Tailored molecular samples for precision spectroscopy experiments</b> Melanie Schnell* and Jochen Küpper <i>Max-Planck Advanced Study Group at the Center for Free-Electron Laser Science, Germany</i>
15:15	<b>Afternoon tea</b> <i>Foyer, Department of Chemistry, University of Basel</i>
15:45 <b>Paper 4</b>	<b>Towards measuring the ionization and dissociation energies of molecular hydrogen with sub-MHz accuracy</b> Daniel Sprecher, Christian Jungen, Wim Ubachs and Frédéric Merkt* <i>ETH Zürich, Switzerland</i>
<b>Paper 5</b>	<b>Synchrotron-based highest resolution Fourier transform infrared spectroscopy of naphthalene (C<sub>10</sub>H<sub>8</sub>) and indole (C<sub>8</sub>H<sub>7</sub>N) and its application to astrophysical problems</b> Siegward Albert*, Karen Keppler Albert, Philippe Lerch and Martin Quack <i>ETH Zürich, Switzerland</i>
<b>Paper 6</b>	<b>Spectroscopy of molecules in very high rotational states using an optical centrifuge</b> Liwei Yuan, Carlos Toro, Mack Bell and Amy S Mullin* <i>University of Maryland, USA</i>
17.15	<b>Close of session</b>
18.00 – 18.30	<b>Welcome Drinks (Poster presenters put up posters)</b> – all delegates welcome <i>Hotel Bildungszentrum 21</i> <a href="http://www.bildungszentrum-21.ch">www.bildungszentrum-21.ch</a>
18.30 – 20.30	<b>Poster session with drinks and light snacks</b> <i>Hotel Bildungszentrum 21</i> <a href="http://www.bildungszentrum-21.ch">www.bildungszentrum-21.ch</a>

Thursday 7 April

<b>Session 2</b>	<b>Biomolecules</b> Session chair: John Simons, <i>University of Oxford, UK</i>
08.30 <b>Paper 7</b>	<b>Potential for the detection of molecular complexes and determination of interaction geometry by 2DIR: Application to protein sciences</b> Rui Guo, Margherita Miele, Elizabeth M Gardner, Frederic Fournier, Kathryn M Kornau and David R Klug* <i>Imperial College, London, UK</i>
<b>Paper 8</b>	<b>State-resolved THz spectroscopy and dynamics of crystalline peptide-water systems</b> Zeeshan Ahmed, Shin Grace Chou, Karen Siegrist and David F Plusquellic* <i>National Institute of Standards and Technology, USA</i>
<b>Paper 9</b>	<b>Exploring hydrophobicity by THz absorption spectroscopy of solvated amino acids</b> Gudrun Niehues, Matthias Heyden, Diedrich A Schmidt, and Martina Havenith* <i>Ruhr Universität-Bochum, Germany</i>
10:00	<b>Morning coffee</b> <i>Foyer, Department of Chemistry, University of Basel</i>
10.30 <b>Paper 10</b>	<b>Single-conformation spectroscopy and population analysis of model <math>\gamma</math>-peptides: New tests of amide stacking</b> Evan G Buchanan, William H. James III, Anna Gutberlet, Jacob C Dean, Li Guo, Samuel H Gellman and Timothy S Zwier* <i>Purdue University, USA</i>
<b>Paper 11</b>	<b>Structural studies of biomolecules in the gas phase by chirped-pulse Fourier transform microwave spectroscopy</b> Amanda L Steber, Justin L Neill, Daniel P Zaleski, Brooks H Pate, Alberto Lesarri, Ryan G Bird, Vanesa Vaquero-Varac and David W Pratt* <i>University of Pittsburgh, USA</i>
<b>Paper 12</b>	<b>Spectroscopy of mobility-selected biomolecular ions</b> Georgios Papadopoulos, Annette Svensden, Oleg V Boyarkin and Thomas R Rizzo* <i>École Polytechnique Fédérale de Lausanne, Switzerland</i>
12:00	<b>Close of session and transfer to lunch/poster session</b> – all delegates welcome <i>Auditorium, Hotel Bildungszentrum 21</i>

<b>Session 3</b>	<b>Theoretical Spectroscopy</b> Session chair: James T Hynes, <i>Ecole Normale Supérieure, France and University of Colorado at Boulder, USA</i>
14:00 <b>Paper 13</b>	<b>Time-resolved photoelectron spectroscopy from first principles: Excited state dynamics of benzene</b> Alexis L Thompson and Todd J Martínez* <i>Stanford University, USA</i>
<b>Paper 14</b>	<b>The effect of microhydration on ionization energies of thymine</b> Kirill Khistyev, Ksenia B Bravaya, Eugene Kamarchik, Oleg Kostko, Musahid Ahmed and Anna I Krylov* <i>University of Southern California, USA</i>
<b>Paper 15</b>	<b>Quantitative vibronic coupling calculations. The visible spectrum of propadienylidene</b> John F Stanton* <i>The University of Texas at Austin, USA</i>
15:30	<b>Afternoon tea</b> <i>Foyer, Department of Chemistry University of Basel</i>
16:00 <b>Paper 16</b>	<b>Charge-transfer and the hydrogen bond: Spectroscopic and structural implications from electronic structure calculations</b> Eloy Ramos-Cordoba, Daniel S Lambrecht and Martin Head-Gordon* <i>University of California, Berkeley, USA</i>
<b>Paper 17</b>	<b>Application of time-independent cumulant expansion to calculation of Franck-Condon profiles for large molecular systems</b> Joonsuk Huh and Robert Berger* <i>Johann Wolfgang Goethe-Universität, Frankfurt, Germany</i>
<b>Paper 18</b>	<b>Structural characterization of spectroscopic substates in carbonmonoxy neuroglobin</b> Stephan Lutz and Markus Meuwly* <i>University of Basel, Switzerland</i>
17:30	<b>Close of session</b>
19.30	<b>Conference dinner with concert</b> – ticket holders only <i>Safran Zunft</i> <a href="http://www.safran-zunft.ch/">www.safran-zunft.ch/</a>  <b>Concert detail: <i>Flora wilt thou torment mee?</i></b> A collection of English and Italian duets blending the comic and tragic sides of love

Friday 8 April

<b>Session 4</b>	<b>Spectroscopy for dynamics</b> Session chair: Mike Ashfold, <i>University of Bristol, UK</i>
09:00 <b>Paper 19</b>	<b>Non-Born-Oppenheimer wavepacket dynamics in polyatomic molecules: vibrations at conical intersections in DABCO</b> Andrey E Boguslavskiy, Michael S Schuurman, Dave Townsend and Albert Stolow* <i>National Research Council, Canada</i>
<b>Paper 20</b>	<b>Linking photochemistry in the gas and condensed phase: S-H bond fission in <i>p</i>-methylthiophenol following UV photoexcitation</b> Thomas A A Oliver, Yuyuan Zhang, Michael N R Ashfold and Stephen E Bradforth* <i>University of Southern California, USA</i>
<b>Paper 21</b>	<b>Robustness of electronic coherence in the Fenna–Matthews–Olson complex to vibronic and structural modifications</b> Dugan Hayes, Jianzhong Wen, Gitt Panitchayangkoon, Robert E Blakeship and Gregory S. Engel* <i>University of Chicago, USA</i>
10:30	<b>Morning coffee</b> <i>Foyer, Department of Chemistry, University of Basel</i>
11:00 <b>Paper 22</b>	<b>Quantum state resolved velocity-map imaging spectroscopy: A new tool for collision dynamics at gas/self-assembled monolayer interfaces</b> Joseph R Roscioli and David J Nesbitt* <i>University of Colorado at Boulder, USA</i>
<b>Paper 23</b>	<b>Photoelectron–photofragment coincidence studies of NO -X clusters (X = H<sub>2</sub>O, CD<sub>4</sub>)</b> Berwyck L J Poad, Christopher J Johnson and Robert E Continetti* <i>University of California, San Diego, USA</i>
<b>Paper 24</b>	<b>The structure and terahertz dynamics of water confined in nanoscale pools in salt solutions</b> David A Turton, Carmelo Corsaro, Marco Candelaresi, Angela Brownlie, Ken R Seddon, Francesco Mallamace and Klaas Wynne* <i>University of Strathclyde, UK</i>
12:30 <b>Paper 25</b>	<b>Concluding remarks</b> Martin Quack <i>ETH Zürich, Switzerland</i>
13:00	<b>Acknowledgements</b>
13:15	<b>Close of meeting</b>

\* denotes presenting author, to whom affiliation applies