



## ESF Research Conferences

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Final  
Programme

# ESF-FWF Conference in Partnership with LFUI **Biomolecules** **From Gas Phase Properties to Reactions relevant in Living Cells**

Universitätszentrum Obergurgl (Oetz Valley, near Innsbruck) • Austria • 24-29 June 2006

**Chairs:** Nigel J. Mason • The Open University, Milton Keynes, UK  
& Eugen Illenberger • Freie Universität Berlin, DE

[www.esf.org/conferences/pc06200](http://www.esf.org/conferences/pc06200)

<b>Saturday 24 June</b>	16.00 onwards	Registration at ESF-RC desk	
	20.00	Dinner	
	21.00	<b>Welcome Drink</b>	
<b>Sunday 25 June</b>	09.00-10.00	<b>Conference Opening</b> <b>Chair:</b> Tilmann Märk • University of Innsbruck, AT	
	10.00-11.00	<b>Plenary Lecture</b> <b>Robert Huber</b> • MPI für Biochimie, Martinsried, DE (Nobel Laureate 1988) <b>Chair:</b> Nigel J. Mason • The Open University, UK	<i>Protein structures, innovations for science and medicine</i>
	11.00-11.30	Coffee break	
	<b>Session 1 • Biomolecular Structure and Spectroscopy I</b> Chair: Eugen Illenberger • Freie Universität Berlin, DE		
	11.30-12.00	<b>Timothy Zwier</b> • Purdue University, US	<i>Laser probes of isomerisation in flexible biomolecules and complexes: valley-to-valley searches for molecular scale mountain passes</i>
	12.00-12.30	<b>Karl Kleinermanns</b> • Universität Düsseldorf, DE	<i>Excited states of biomolecules</i>
	12.30-13.00	<b>Hanspeter Helm</b> • Universität Freiburg, DE	<i>Terahertz spectroscopy of biomolecules</i>
<b>Session 2 • Biomolecular Sources and Novel Techniques</b> Chair: Lars H. Andersen • University of Aarhus, DK	13.00	Lunch	
	15.00-15.30	<b>Gert von Helden</b> • Fritz-Haber-Institut der MPG, Berlin, DE	<i>Probing gas-phase biomolecules by IR spectroscopy</i>
	15.30-16.00	<b>Bernhard Brutschy</b> • Universität Frankfurt/Main, DE	<i>Detection of biomolecules from liquid droplets</i>
	16.00-16.30	<b>Oddur Ingólfsson</b> • University of Iceland, Reykjavik, IS	<i>MALDI with biomolecules</i>
	16.30-17.00	<b>Klaus Dreisewerd</b> • Universität Münster, DE	<i>MALDI: fundamentals and major applications</i>
	17.00-17.30	Coffee break	
	<b>Short oral presentations</b> Chair: Jean-Pierre Schermann • Université Paris Nord, FR		
	17.30-17.50	<b>Lavina Cornelia Snoek</b> • Oxford University, UK	<i>Molecular recognition in the gas phase; pi-bonding in carbohydrate-aromatic interactions</i>
	17.50-18.10	<b>Nick Polfer</b> • FOM, Nieuwegein, NL	<i>Gas phase reactions of biomolecules probed by infrared spectroscopy</i>
	18.10-18.30	<b>Valérie Gabelica</b> • Liège University, BE	<i>Electron detachment and subsequent fragmentation of multiply charged DNA ions under UV-visible irradiation</i>
	19.30	Dinner	
	21.00	Poster session 1	

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### Session 3 • Collisions with Biomolecules

Chair: Francesco Gianturco • Università La Sapienza, Rome, IT

09.00-09.30	<b>Léon Sanche</b> • Université de Sherbrooke, CA	<i>Electron damage in DNA</i>
09.30-10.00	<b>Tilmann D. Märk</b> • Universität Innsbruck, AT	<i>Electron attachment to biomolecules</i>
10.00-10.30	Coffee break	
10.30-11.00	<b>Thomas Schlathölter</b> • Groningen University, NL	<i>Ion interactions with Watson Crick pairs</i>
11.00-11.30	<b>Michael A. Huels</b> • Université de Sherbrooke, CA	<i>Ion collisions with biomolecules</i>
11.30-12.00	<b>Robert Abouaf</b> • Université Paris-Sud, FR	<i>Electron spectroscopy of biomolecules</i>
12.00-12.30	<b>E. Krishnakumar</b> • Tata Institute Mumbai, IN	<i>Site selective bond cleavage in organic molecules</i>
12.30	Lunch	

### Session 4 • Electron Interactions with Biomolecules I

Chair: E. Krishnakumar • Tata Institute of Fundamental Research, Mumbai, IN

15.30-16.00	<b>Francesco A. Gianturco</b> • Universita di Roma, IT	<i>Electron and positron interactions with biomolecules</i>
16.00-16.30	<b>Jimena Gorfinkel</b> • The Open University, UK	<i>Theoretical studies of electron interactions with biologically relevant molecules.</i>
16.30-17.00	Coffee break	
17.00-17.30	<b>Jack Simons</b> • University of Utah, US	<i>Theoretical studies of mechanisms for low energy electron damage to DNA</i>
17.30-18.00	<b>Bernd Giese</b> • University of Basel, CH	<i>Electron transfer in DNA and peptides</i>

### Short oral presentations

Chair: Jack Simons • University of Utah, US

18.00-18.20	<b>Ilko Bald</b> • Freie Universität Berlin, DE	<i>Dissociative electron attachment to DNA/RNA building blocks</i>
18.20-18.40	<b>Sylwia Ptasinska</b> • Sherbrooke University, CA	<i>Electron irradiation of biocomplexes</i>
19.30	Dinner	
21.00	Poster session 2	

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### Session 5 • Biomolecular Structure and Spectroscopy II

Chair: Hanspeter Helm • University of Freiberg, DE

09.00-09.30	<b>Pavel Hobza</b> • Academy of Sciences Praha, CZ	<i>Structure, energetics and dynamics of DNA base pairs and amino acid pairs</i>
09.30-10.00	<b>Neil Macleod</b> • University of Oxford, UK	<i>Conformational landscapes of neutral and protonated biomolecules in the gas phase and in solution</i>
10.00-10.30	Coffee break	
10.30-11.00	<b>Roman Zubarev</b> • University of Uppsala, SE	<i>Mass Spectrometry of biomolecules</i>
11.00-11.30	<b>Rainer Weinkauf</b> • Heinrich-Heine-U., Düsseldorf, DE	<i>Laser spectroscopy of peptides</i>
11.30-12.00	<b>Lars H. Andersen</b> • University of Aarhus, DK	<i>Probing proteins by photo-absorption studies at an electrostatic storage ring</i>
12.00-12.30	<b>Tom Rizzo</b> • EPFL, Lausanne, CH	<i>IR and UV photofragment spectroscopy of cold, biomolecular ions</i>
12.30	Lunch	

<p><b>Wednesday 28 June</b></p>	<b>Session 6 • Electron Interactions with Biomolecules II</b>		
	Chair: Robert Abouaf • Université Paris-Sud, Orsay, FR		
	15.30-16.00	<b>Andrzej L. Sokalski</b> • Polish Acad. of Sc., PL	<i>Hydrogen bonds - a key for photostability of biomolecular systems</i>
	16.00-16.30	<b>Ron Naaman</b> • Weizmann Institute, Rehovot, IL	<i>Electron transmission through monolayers of short DNA oligomers</i>
	16.30-17.00	<b>Tihomir Solomun</b> • Freie Universität Berlin, DE	<i>Electron interactions with immobilised oligonucleotides</i>
	17.00-17.30	Coffee Break	
	<b>Short oral presentations</b>		
	Chair: Thomas Schlathölter • Groningen University, NL		
	17.30-17.50	<b>John R. Sabin</b> • University of Florida, US	<i>Theoretical investigation of fragmentation and energy deposition cross sections for proton impact on biomolecules</i>
	17.50-18.10	<b>Iwona Dabkowska</b> • Gdańsk University, PL	<i>Electron induced proton transfer</i>
	18.10-18.30	<b>Karol Marek Langner</b> • Wrocław University of Technology, PL	<i>The significance of electrostatic interactions in nucleic acid base stacking complexes</i>
	19.30	Dinner	
	21.00	Poster session 3	
	<b>Session 7 • Biomolecular Anions</b>		
	Chair: Léon Sanche • University of Sherbrooke, CA		
	09.00-09.30	<b>Thomas Schultz</b> • MBI Berlin, DE	<i>Electronic relaxation in isolated and micro-hydrated DNA base pairs</i>
	09.30-10.00	<b>Jens Michaelis</b> • LMU Munich, DE	<i>Mechanism of force generation of a viral DNA packaging motor</i>
	10.00-10.30	Coffee break	
	10.30-11.00	<b>Anne Lafosse</b> • Université Paris-Sud, Orsay, FR	<i>Electron interactions with thin films of organic acids</i>
	11.00-11.30	<b>Jean-Pierre Schermann</b> • Université Paris-Nord, FR	<i>Structures of biomolecular complexes from dipole-bound anion formation</i>
	<b>Short oral presentations</b>		
	Chair: John Sabin • University of Florida, US		
	11.30-11.50	<b>Nina Morgner</b> • Goethe University, Frankfurt /Main, DE	<i>Biomolecules in liquid droplets</i>
	11.50-12.10	<b>Linan Yang</b> • Purdue University, US	<i>Radical reactions with oligonucleotides evaporated by laser induced acoustic desorption (LIAD) in the gas phase</i>
	12.10-12.30	<b>Sandrine Lacombe</b> • Paris Sud University, FR	<i>Role of radiosensitizers in hadrontherapy</i>
	12.30	Lunch	
	<b>Session 8 • New directions and New Opportunities</b>		
	Chair: Nigel J. Mason • The Open University, UK		
	<b>Short oral presentations</b>		
	Chair: Pavel Hobza • Academy of Sciences Praha, CZ		
	16.00-16.20	<b>Bogdan C. Ibanescu</b> • Fribourg University, CH	<i>Site and selective chemistry in DEA to compounds with amino and hydroxyl groups</i>
	16.20-16.40	<b>Martine N. Blom</b> • FOM, Nieuwegein, NL	<i>Stepwise solvation of isolated amino acids</i>
	16.40-17.00	<b>Marcello Coreno</b> • CNR-IMIP, Trieste, IT	<i>Photoionisation mass spectrometry and photoemission of amino acids</i>

<b>Thursday 29 June</b>	17.00-17.20	<b>Samuel Eden</b> • Nuclear Physics Institute Lyon, FR	<i>Proton impact ionisation of gas phase DNA bases and water molecules</i>
	17.20-17.45	Coffee break	
	17.45- 19.00	Forward Look Plenary Discussion	
	20.00	<b>Reception followed by Conference Dinner</b>	
Breakfast & Departure			

**Abstracts, posters and short talks:**

There will be no **short talks** other than those announced on the programme.  
 All other abstracts are accepted as **posters**.