**Scientific & Social Program**

### Monday, 16 August 2010

*Location: Entry Hall and Lecture Room A140 Campus Pérolles II*

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<td>16:00 - 20:00</td>
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| 17:00 - 18:00 | **Opening Ceremony**  
Welcome by Claude Daul  
Musical interlude by Donaflor feat. Claude Schneider (Switzerland/Brazil)  
In Memory of Philip Tregenna-Piggott by Hansueli Guedel and Hoegni Weihe  
Final words by Isaac Bersuker |
| 18:00 - 20:00 | Welcome Reception - Botanical Garden                               |

### Tuesday, 17 August 2010

*Location: Entry Hall and Lecture Room A140 Campus Pérolles II*

<table>
<thead>
<tr>
<th>Time</th>
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<tr>
<td>08:00 - 16:00</td>
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| 08:30 - 09:15 | **Horst Koeppel** (Heidelberg, Germany)  
| 09:15 - 09:40 | **Lluis Blancafort** (Girona, Spain)  
Connectivity of seam of intersection segments related by permutational symmetry in benzene. |
| 09:40 - 10:05 | **Spiridoula Matsika** (Philadelphia, USA)  
Conical intersections in non-isolated chromophores. |
| 10:05 - 10:35 | Coffee Break                                                       |
| 10:35 - 11:20 | **Viktor Polinger** (Seattle, USA)  
Vibronic Origin of Ferroelectricity. |
| 11:20 - 11:45 | **Pablo Garcia-Fernandez** (Santander, Spain)  
Origin of octahedral tilting in the perovskites. |
| 11:45 - 12:10 | **Randy S. Fishman** (Oak Ridge, USA)  
Inverse Jahn-Teller Transition in Bimetallic Oxalates. |
12:10 - 13:20  Lunch Break

3rd Session (Chair: Arnout Ceulemans)
13:20 - 13:45  Michael Kaplan & George Zimmerman (Boston, USA)
Virtual Phonon Exchange Influence of magnetic properties of Jahn-Teller Crystals.

13:45 - 14:10  Heinz Barentzen (Stuttgart, Germany)
Intrinsic Interaction between Ee Complexes in Jahn-Teller Crystals.

14:10 - 14:35  Dennis Clougherty (Burlington, USA)
Berry-Phase Approach to Electric Polarization and Charge Fractionalization.

14:35 - 15:00  Daniel I. Khomskii (Cologne, Germany)
Orbital ordering, spin gaps and metal-insulator transitions in oxides.

15:00 – 15:25  Hiroyasu Koizumi (Tsukuba, Japan)
Local lattice distortion and spin-vortices in cuprates: how to interpret ARPES, EXAFS, and neutron scattering results.

15:25 - 15:50  Kliment Kugel (Moscow, Russia)
Effect of electron-lattice interaction on the phase separation in strongly correlated systems with Jahn-Teller ions.

15:50 – 16:20  Coffee Break

4th Session (Chair: Michael Atanasov)
16:20 - 16:45  Hua Wu (Cologne, Germany)
Orbital order in La_{0.5}Sr_{1.5}MnO_4: failure of the standard Jahn-Teller physics.

16:45 - 17:10  Charles J. Simmons (Hawaii, USA)
Evidence for a Thermal Equilibrium Between Copper(II) Complexes with Tetragonally Elongated and Compressed Geometries.

17:10 - 17:35  Alexander Levin (Moscow, Russia)
Pseudospin-phonon coupling influence on the phase transition temperature of KDP-like ferroelectrics.

17:35 - 18:00  Gerry Lucovsky (NC, USA)
Spectroscopic detection of spin-polarized bands and mixed valence in GdSc1-xTixO3 alloys.

18:00 - 18:25  Wim Maaskant (Burgerveen, Netherlands)
The C-M_2O_3 sesquioxide structure as a subgroup of fluorite type crystals.

Special session (Chair: Wolfgang Domcke)
21:00 – 22:00  Special session dedicated to Horst Koeppel's 60th birthday
Speakers: Susanta Mahapatra and a panel of Junior Scientists
Wednesday, 18 August 2010
Location: Entry Hall and Lecture Room A140 Campus Pérolles II

08:00 - 16:00  REGISTRATION DESK

5th Session (Chair: Frederic Merkt)
08:30 - 09:15  Hideki Uschio (Tokyo, Japan)
On the Interplay of Jahn-Teller physics and Mott physics in the mechanism of high Tc superconductivity.

09:15 - 09:40  Wolfgang Domcke (Munich, Germany)
The Relativistic Jahn-Teller Effect.

09:40 - 10:05  Wolfgang E. Ernst (Graz, Austria)
Jahn-Teller Effect and Spin-Orbit Coupling in Heavy Alkali Trimers.

10:05 - 10:35  Coffee Break

6th Session (Chair: Isaac Bersuker)
10:35 - 11:20  Alex Mueller (Zurich, Switzerland)
Fermi Glass versus High-Temperature Superconductivity Behavior.

11:20 - 11:45  Annette Bussman-Holder (Stuttgart, Germany)
Evidence for Jahn-Teller polaron formation in cuprate superconductors from isotope and local probe experiments.

11:45 - 12:10  Takashi Kato (Nagasaki, Japan)
Unified Theory of the Role of Vibronic Interactions in Micro- and Macroscopic Sized Superconductivity.

12:10 - 13:20  Lunch Break

7th Session (Chair: Sam Leutwyler)
13:20 - 13:45  Satrajit Adhikari (Kolkata, India)
Ab - initio calculations on the excited states of Na3 cluster to explore beyond Born - Oppenheimer theories: adiabatic to diabatic PESs and nuclear dynamics.

13:45 - 14:10  Maja Gruden-Pavlovic (Belgrade, Serbia)
Density Functional Theory for the study of the multimode Jahn-Teller effect.

14:10 - 14:35  Susanta Mahapatra (Hyderabad, India)
(B +Exb)x e Jahn-Teller and pseudo-Jahn-Teller Effects in the Spiropentane Radical Cation.

14:35 - 15:00  Janette L. Dunn (Nottingham, UK)
C60 molecules on surfaces: the role of Jahn-Teller effects and surface interactions.

15:00 - 15:25  Arnout Ceulemans (Leuven, Belgium)
Frustration in Jahn-Teller System.

15:25 - 15:50  Martin Breza (Bratislava, Slovakia)

15:50 - 16:20  Coffee Break
8th Session (Chair: Boris Tsukerblat)

16:20 - 16:45  **Benjamin Lasorne** (Montpellier, France)
The Electronic Excited States of Ethylene and Large-Amplitude Deformations: a Dynamical Symmetry Group Investigation.

16:45 - 17:10  **Fanica Cimpoesu** (Bucharest, Romania)
The Vibronic Approach to Molecular Dynamics and Supramolecular Cooperativity.

17:10 - 17:35  **Vladimir Hizhnyakov** (Tartu, Estonia)
Anomalous vibronic coupling in doped quantum 3He droplets.

17:35 - 18:00  **Dimiter Alexandrov** (Ontario, Canada)
Interactions of Hydrogen Ions with 2-D Clusters of Nitride Semiconductors.

18:00 - 18:25  **Vladimir Gudkov** (Ekateringburg, Russia)
Vibronic constants, force constants, and adiabatic potentials in ZnSe:Cr and ZnSe:Fe reconstructed in an ultrasonic experiment.

18:25 - 18:50  **Grace G. Morgan** (Dublin, Ireland)
Structural and Magnetic Bistability in Mononuclear Manganese(III)Complexes.

19:00 - 21:00  Poster Session with Buffet Dinner

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Thursday, 19 August 2010

Location: Entry Hall and Lecture Room A140 Campus Pérolles II

08:00 - 16:00  REGISTRATION DESK

9th Session (Chair: Janette Dunn)

08:30 - 09:15  **Sophia Klokishner** (Kishinev, Moldova)
Origin of Magnetic Anisotropy in Single Molecule and Single Chain Magnets Containing Ions with Unquenched Orbital Angular Momenta.

09:15 - 09:40  **Samuel Leutwyler** (Berne, Switzerland)
Excitonic Splittings and Vibronic Coupling in Jet-Cooled Molecular Homodimers.

09:40 - 10:05  **Wolfgang Eisfeld** (Bielefeld, Germany)
A new approach to anharmonicity and dissociation in vibronically coupled systems.

10:05 - 10:35  Coffee Break

10th Session (Chair: Vladimir Hizhnyakov)

10:35 - 11:20  **Miguel Moreno** (Santander, Spain)
Jahn-Teller and pseudo Jahn-Teller problems in doped insulators: What can we learn from ab initio calculations?

11:20 - 11:45  **Naoya Iwashara** (Kyoto, Japan)
Photoelectron spectrum and vibronic couplings in C_{60}.

11:45 - 12:10  **Tohru Sato** (Kyoto, Japan)
Vibronic coupling density analysis.
12:10 - 13:30  Lunch Break

13:30  Departure for Sightseeing “Gruyères”

17:30  Arrival in Fribourg, possibility to refresh at the hotel

19:00  Departure Surprise Apero & Conference Dinner with Special Guest

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**Friday, 20 August 2010**

*Location: Entry Hall and Lecture Room A140 Campus Pérolles II*

**11th Session (Chair: Tohru Sato)**

09:00 - 09:45  Mark Riley (Queensland, Australia)
   The dynamic Jahn-Teller Effect in Cu(II)/MgO.

09:45 - 10:10  Boris Tsukerblat (Beer-Sheeva, Israel)
   A Symmetry-Adapted Approach to the Dynamic Jahn-Teller Problem.

10:10 - 10:40  Coffee Break

**12th Session (Chair: Daniel Khomskii)**

10:40 - 11:25  Isaac Bersuker (Texas, USA)

11:25 - 11:50  Antonio Varandas (Coimbra, Portugal)
   Cyclic phases in Jahn-Teller systems.

11:50 - 12:15  Monika Gruetter (Zurich, Switzerland)
   The E x e Jahn-Teller effect in the presence of a tunable spin-orbit interaction: Rotationally resolved photoelectron spectra of CH3X+ (X=F,Cl,I).

12:15 - 12:40  Dirk Reinen (Marburg, Germany)
   The modulation of Jahn-Teller coupling by elastic and binding strains - a novel concept and examples from solid state chemistry

12:40 - 12:45  Closing remarks

12:45 - 14:00  Lunch Break

14:00  Departure