Sunday, 28 September

**Session 1**
Chair: Martin Quack, ETH Zürich
19:30 – 20:15
Jürgen Troe, Göttingen
Reaction Dynamics with Wavepackets, Adiabatic Channels and Classical Trajectories
20:15 – 21:00
Martin Jungen, Basel
What is a muon doing in atoms or molecules?

Monday, 29 September

**Session 2**
Chair: Werner Kutzelnigg, Bochum
08:30 – 09:15
Wim Klopper, Karlsruhe
Explicitly correlated calculations of excitation energies
09:15 – 10:00
David Luckhaus, Göttingen
Direct Multi-Arrangement Quantum Dynamics: From Vibrations to Reactions
10:00 – 10:30
Coffee Break

**Session 3**
Chair: Peter Botschwina, Göttingen
10:30 – 11:15
John P. Maier, Basel
Electronic Spectroscopy of Carbon Chains and Such: Relevance to Astrophysics and Nanoscience
11:15 – 12:00
Frédéric Merkt, ETH Zürich
High-Resolution VUV Spectroscopy, Rydberg States and Cations
12:00 – 14:00
Lunch Break

**Session 4**
Chair: Wilfried Meyer, Kaiserslautern
14:00 – 14:45
Hans-Joachim Werner, Stuttgart
Explicitly correlated local wavefunctions: LMP2-R12 with density fitting
14:45 – 15:30
Jeppe Olsen, Aarhus
Coupled Cluster Expansions with Quadruple and Higher Excitations
15:30 – 16:00
Coffee Break

**Session 5**
Chair: Jürgen Hinze, Bielefeld
16:00 – 16:45
Gernot Frenking, Marburg
The Nature of the Chemical Bond - Old Questions, New Answers
16:45 – 17:30
Kimihiko Hirao, Tokyo (PCCP Lecture)
Recent advances in electronic structure theory
18:00 – 19:30
Dinner Break

Mounting of Posters

19:30 – 22:00
Poster Session (EVEN numbered)
Tuesday, 30 September

**Session 6**
Chair: Walter Thiel, Mülheim
08:30 – 09:15
N.N. (Hellmann Prize)

09:15 – 10:00
Tom Rizzo, Lausanne
State-resolved molecule surface reactions - a challenge for theoreticians

10:00 – 10:30
Coffee Break

**Session 7**
Chair: Hans-Peter Lüthi, ETH Zürich
10:30 – 11:15
Roberto Marquardt, Marne-la-Vallée
Vibrational and Rotational Wave Packet Motion in Polyatomic Molecular Systems

11:15 – 12:00
Regina de Vivie-Riedle, München
Analysis and coherent control of ultrafast molecular processes

12:00 – 14:00
Lunch Break

Afternoon: Posters / Discussions / Free / Excursion

19:00
BBQ Dinner

Wednesday, 1 October

**Session 8**
Chair: Dirk Schwarzer, Göttingen
08:30 – 09:15
Sam Leutwyler, Berne
Excited-state H-atom transfer along a hydrogen-bonded "wire"

09:15 – 10:00
Martina Havenith, Bochum
Hydrogen Bonds: New Answers to old Questions

10:00 – 10:30
Coffee Break

**Session 9**
Chair: W.H. Eugen Schwarz, Siegen
10:30 – 11:15
Marius Lewerenz, Paris
Vibrational Dynamics and Structure in Molecular and Ionic Clusters

11:15 – 12:00
Walter Thiel, Mülheim
Ab Initio Vibration-Rotation Spectroscopy

12:00 – 14:00
Lunch Break

**Session 10**
Chair: Frédéric Merkt, ETH Zürich
14:00 – 14:45
Martin Suhm, Göttingen
Vibrational Dynamics of Molecular Handshakes

14:45 – 15:30
Tomasz Wesolowski, Geneva
Electron density partitioning as a route towards accurate multi-scale modeling of complex molecular systems and materials

15:30 – 16:00
Coffee Break
Wednesday, 1 October (continued)

Session 11
16:00 – 16:45 Chair: Kim Baldridge, Zürich
Joachim Sauer, Berlin
Calculations on transition metal oxides - from gas phase clusters to solid catalysts
16:45 – 17:30 Claude Daul, Fribourg
Modelling magnetic and spectroscopical properties of coordination compounds
17:30 – 18:00 Mitgliederversammlung: Arbeitsgemeinschaft für Theoretische Chemie
18:00 – 19:30 Dinner Break

Mounting of Posters

19:30 – 22:00 Poster Session (ODD numbered)

Thursday, 2 October

Session 12
08:30 – 09:15 Chair: Jürgen Stohner, Winterthur
Jürgen Gauss, Mainz
Rovibrational Spectroscopy and Quantum Chemistry
09:15 – 10:00 Markus Reiner, Erlangen
Mode-Tracking: A new method for the calculation of pre-selected molecular vibrations
10:00 – 10:30 Coffee Break

Session 13
10:30 – 11:15 Chair: Ralph Jaquet, Siegen
Lorenz Cederbaum, Heidelberg
Intermolecular decay and ultrafast energy transfer in clusters and weakly bound systems
11:15 – 12:00 William H. Miller, Berkeley
Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations
12:00 – 14:00 Lunch Break

Session 14
14:00 – 14:45 Chair: Dominik Marx, Bochum
Nikos Dotsis, Bochum
Excited state tautomerism of the DNA base guanine
14:45 – 15:30 Michele Parrinello, Zürich/Lugano
Calculation of free energy surfaces in classical and ab-initio molecular dynamics
15:30 – 15:35 Closing of the Meeting

Departure
# 39th Symposium on Theoretical Chemistry
**MOLECULAR SPECTROSCOPY AND DYNAMICS**
**28 September to 2 October 2003**  
Gwatt, Lake Thun, Switzerland

Organized by H.-P. Lüthi, M. Quack and J. Stohner

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<tr>
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