

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** Chair: Kim Baldrige, Zürich
16:00 – 16:45 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** Chair: Jürgen Stohner, Winterthur
08:30 – 09:15 Jürgen Gauss, Mainz
Rovibrational Spectroscopy and Quantum Chemistry
09:15 – 10:00 Markus Reiher, Erlangen
Mode-Tracking: A new method for the calculation of pre-selected molecular vibrations
10:00 – 10:30 Coffee Break

Session 13 Chair: Ralph Jaquet, Siegen
10:30 – 11:15 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 Chair: Dominik Marx, Bochum
14:00 – 14:45 Nikos Doltsinis, 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

	Time	Sunday, 28 Sep	Monday, 29 Sep	Tuesday, 30 Sep	Wednesday, 1 Oct	Thursday, 2 Oct	Time
Morning Session 8:30-12:00	8:30-9:15		Klopper Luckhaus	N.N. (Hellmann Lecture) Rizzo	Leutwyler Havenith	Gauss Reiher	8:30-9:15 9:15-10:00
	10:00-10:30 10:30-11:15 11:15-12:00 12:00-14:00 14:00-14:45 14:45-15:30 15:30-16:00 16:00-16:45 16:45-17:30 17:30-18:00	Arrival and Registration (from 3 pm)	Maier Merkel Werner Olsen C o f f e e Frenking Hirao (PCCP Lecture)	Marquardt de Vivie-Riedle L u n c h Excursion or free	Lewerenz Thiel B r e a k Suhm Wesolowski C o f f e e Sauer Daul AGTC Meeting D i n n e r Poster Session (odd numbered)	Cederbaum Miller Doltsinis Parrinello Departure	10:00-10:30 10:30-11:15 11:15-12:00 12:00-14:00 14:00-14:45 14:45-15:30 15:30-16:00 16:00-16:45 16:45-17:30 17:30-18:00
Afternoon Session 14:00-18:00	18:00-19:30 19:30-20:15 20:15-21:00	Troe Jurgen	D i n n e r Poster Session (even numbered)	BBQ D i n n e r			18:00-19:30 19:30-20:15 20:15-21:00
	Evening Session 19:30-22:00						

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