CHIMIA **2005**, *59*, No. 7/8

The Organizing and Scientific Committees gratefully acknowledge **financial support from:**

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Swiss Academy of Sciences

Swiss Academy of Engineering Sciences

Swiss National Science Foundation

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Conférence Universitaire de Suisse Occidentale (3ème Cycle en Chimie)

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SCIENTIFIC PROGRAM

CHIMIA **2005**, *59*, No. 7/8

PROGRAM IN DETAIL

SUNDAY, SEPTEMBER 11, 2005

MAIN HALL (ground floor)
Uni Mail Building
University of Geneva
40 Boulevard du Pont-d'Arve
CH-1205 Geneva, Switzerland

16h00–20h00 **REGISTRATION**

18h00–20h00 **WELCOME RECEPTION**

MONDAY, SEPTEMBER 12, 2005

Auditorium R380, Ground floor of the Uni Mail Building, University of Geneva,
40 Boulevard du Pont-d'Arve, CH-1205 Geneva, Switzerland

Legend
I: *invited lecture*
C: *oral contribution*
P: *poster*

OPENING CEREMONY

8h45–9h00 ***J. Weber***, *Chairman of the Organizing Committee*
A. Hurst, *Rector of the University of Geneva*
M. Tornare, *Mayor of the City of Geneva*

MORNING SESSION I

Chairperson: J. Weber (CH)

9h00–9h45 I1 ***W. Kohn***
Department of Physics, University of California, Santa Barbara, USA
'Nearsightedness of Electronic Matter'

9h45–10h30 I2 ***A. Savin***
Laboratory of Theoretical Chemistry, Paris VI University, France
'Model Hamiltonians for Better Approximations'

10h30 – 11h00 **COFFEE BREAK**

MORNING SESSION II

Chairperson: D.J. Tozer (UK)

11h00–11h45 I3 ***H.J. Freund***
Department of Chemical Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
'Models in Heterogeneous Catalysis at the Atomic Level'

11h45–12h10 C1 ***A. Michalak***
Department of Theoretical Chemistry, Jagiellonian University, Cracow, Poland
'DFT Modeling of the Polymerization and Co-Polymerization Processes Catalyzed by the Late-Transition Metal Complexes'

12h10–12h35 C2 ***P. Cortona***
SPMS Laboratory, Paris Central School, Châtenay-Malabry, France
'New Correlation Energy Functional: A Modified Colle-Salvetti Approach'

12h45–14h00 **LUNCH**

AFTERNOON SESSION I

Chairperson: P. Geerlings (B)

14h00–14h45 I4 ***J.L. Brédas***
School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia, USA
'Electrical and Optical Properties of π-Conjugated Materials: A DFT Perspective'

14h45–15h10 C3 ***J.A. Aramburu***
Department of Earth Sciences and Condensed Matter Physics, University of Cantabria, Santander, Spain
'Off-Centre Instabilities of Impurities in Solids Explained Through *ab initio* Calculations'

AFTERNOON SESSION II Chairperson: U. Röthlisberger (CH)

15h10–15h35 C4 ***C. Gossens***
Laboratory of Computational Chemistry and Biochemistry, Swiss Federal Institute of Technology, Lausanne, Switzerland
'DNA-Binding of Ruthenium-Arene Anticancer Drugs'

15h35–16h00 C5 ***A.N. Bondar***
Computational Molecular Biophysics, University of Heidelberg, Germany
'Quantum Mechanical/Molecular Mechanical Investigation of Bacteriorhodopsin Proton Pumping'

16h15–18h00 **POSTER SESSION I**
Methodology and Applications
Posters P1 – P137

TUESDAY, SEPTEMBER 13, 2005

Auditorium R380, Ground floor of the Uni Mail Building, University of Geneva,
40 Boulevard du Pont-d'Arve, CH-1205 Geneva, Switzerland

Legend
I: *invited lecture*
C: *oral contribution*
P: *poster*

MORNING SESSION I Chairperson: E.J. Baerends (NL)

Dedicated to the Memory of Professor Laurens Jansen

9h00–9h45 I5 ***E.V. Ludeña***
Center of Chemistry, IVIC, Caracas, Venezuela
'The Kinetic Energy Functional in DFT: Exact Results for Model Systems and Plausible Approximations for Actual Ones'

9h45–10h30 I6 ***P.M.W. Gill***
Research School of Chemistry, Australian National University, Canberra, Australia
'Post-DFT: Beyond the One-Particle Density'

10h30–11h00 **COFFEE BREAK**

MORNING SESSION II Chairperson: A. Theophilou (GR)

11h00–11h45 I7 ***A. Görling***
Laboratory of Theoretical Chemistry, Erlangen-Nürnberg University, Germany
'DFT and Time-Dependent DFT Methods with State- and Orbital-Dependent Functionals'

11h45–12h10 C6 ***S.D. Chakarova***
Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden
'Non-Local Interactions in Naphthalene, Anthracene, and Pyrene Dimers'

12h10–12h35 C7 ***A.M. Köster***
Chemistry Department, CINVESTAV, Mexico
'Density Functional Methods with Auxiliary Functions'

12h45–14h00 **LUNCH**

AFTERNOON SESSION I Chairperson: J. Garcia De La Vega (SP)

14h00–14h45 I8 ***F. Neese***
Max-Planck-Institut für Bioanorganische Chemie, Mülheim an der Ruhr, Germany
'Calculation of EPR Parameters for Radicals and Transition Metal Complexes. Density Functional Theory versus Simplified Correlated *ab initio* Methods'

14h45–15h30 I9 ***C. Adamo***
Laboratory of Electrochemistry and Analytical Chemistry, ENSCP, Paris, France
'Molecular Photoelectrochemical Processes: A DFT Point of View'

16h00 **EXCURSIONS**

WEDNESDAY, SEPTEMBER 14, 2005

Auditorium R380, Ground floor of the Uni Mail Building, University of Geneva,
40 Boulevard du Pont-d'Arve, CH-1205 Geneva, Switzerland

Legend
I: *invited lecture*
C: *oral contribution*
P: *poster*

MORNING SESSION I Chairperson: R. Nalewajski (PL)

9h00–9h45 I10 ***R.J. Bartlett***
Quantum Theory Project, University of Florida, Gainesville, Florida, USA
'Progress and Problems in *ab initio* DFT for Ground and Excited States'

9h45–10h30 I11 ***M. Challacombe***
Theoretical Division, Los Alamos National Laboratory, New Mexico, USA
'New Developments in Linear Scaling Density Functional Theory: The Perturbed Projector for *ab-initio* Response Theory and Hybrid HF/DFT for the Condensed Phase'

10h30–11h00 **COFFEE BREAK**

MORNING SESSION II Chairperson: M. Parrinello (CH)

11h00–11h45 I12 ***J. Hutter***
Physical Chemistry Institute, University of Zurich, Switzerland
'Large-Scale Condensed Matter Calculations with the Gaussian and Augmented Plane-Wave Method'

11h45–12h10 C8 ***N.N. Lathiotakis***
Institute of Theoretical Physics, Free University Berlin, Germany
'Applications of the Reduced Density Matrix Functional Theory to Periodic Systems and Open Shell Finite Systems'

12h10–12h35 C9 ***F. De Angelis***
CNR Institute of Molecular Science and Technology, University of Perugia, Italy
'A Time-Dependent DFT Study of $[Fe(CN)_6]^{4-}$ and Ruthenium-Polypyridyl Complexes Sensitization of TiO_2 Nanoparticles'

12h45–14h00 **LUNCH**

AFTERNOON SESSION I Chairperson: A. Bencini (I)

14h00–14h45 I13 ***D.A. Case***
Department of Molecular Biology, The Scripps Research Institute, La Jolla, California, USA
'Analysis of Spin-Spin Interactions in Transition Metal Clusters of Biochemical Interest'

14h45–15h10 C10 ***V.G. Malkin***
Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovak Republic
'Relativistic Unrestricted Two-Component Calculations of Electronic g-Tensors and Hyperfine Structure'

AFTERNOON SESSION II Chairperson: H. Chermette (F)

15h10–15h35 C11 ***T. Heine***
Institute of Physical Chemistry and Electrochemistry, TU Dresden, Germany
'The Tensorial Magnetic Shielding Function in DFT – Background and Applications'

15h35–16h00 C12 ***D.J. Tozer***
Department of Chemistry, University of Durham, UK
'Semi-Empirical Exchange-Correlation Functionals in Kohn-Sham Theory'

16h15–18h00 **POSTER SESSION II**
Applications
Posters P201–P337

18h30–20h00 **COCKTAIL RECEPTION**
20h00–24h00 **CONFERENCE DINNER**
Maison Communale de Plainpalais, Ground-floor room, 52 rue de Carouge, CH-1205 Geneva

THURSDAY, SEPTEMBER 15, 2005

Auditorium R380, Ground floor of the Uni Mail Building, University of Geneva,
40 Boulevard du Pont-d'Arve, 1205 Geneva, Switzerland

Legend
I: *invited lecture*
C: *oral contribution*
P: *poster*

MORNING SESSION I Chairperson: D.R. Salahub (CA)

9h00–9h45 I14 ***A.D. Becke***
Department of Chemistry, Queen's University, Kingston, Ontario, Canada
'Real-Space Correlation Models'

9h45–10h30 I15 ***F. De Proft***
Department of General Chemistry, Free University Brussels, Belgium
'Recent Developments in Conceptual Density Functional Theory: Theory and Applications'

10h30–11h00 **COFFEE BREAK**

MORNING SESSION II Chairperson: E.K.U. Gross (D)

11h00–11h45 I16 ***K. Burke***
Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, New Jersey, USA
'Rigorous Treatment of Single-Molecule Transport in Density Functional Theory'

11h45–12h10 C13 ***T. Saue***
Laboratory of Quantum Chemistry and Molecular Modeling, Louis Pasteur University, Strasbourg, France
'4-Component Relativistic TD-DFT: Properties and Excited States'

12h10–12h35 C14 ***K. Pernal***
Section Theoretical Chemistry, Free University Amsterdam, The Netherlands
'An Effective Potential For the Natural Spinorbitals'

12h35–13h00 **CONCLUDING REMARKS**

13h00 **LUNCH**