FIRST CANADIAN SYMPOSIUM ON COMPUTATIONAL CHEMISTRY

PREMIER SYMPOSIUM CANADIEN EN CHIMIE COMPUTATIONELLE

Organisateurs: André D. BANDRAUK, André MICHEL
Organizers: Groupe de Chimie Théorique et Modélisation
Université de Sherbrooke, Qué., Canada J1K 2R1

Date: 19-22 mai / May 1991

Lieu: Auberge Chéribourg
Place: Orford, Qué.

Sponsors:
Auspices:

IBM CANADA

NATURAL SCIENCES and ENGINEERING
RESEARCH COUNCIL of CANADA

UNIVERSITÉ de SHERBROOKE

1ST CANADIAN SYMPOSIUM ON COMPUTATIONAL CHEMISTRY

1ER SYMPOSIUM CANADIEN EN CHIMIE COMPUTATIONELLE

19-22 MAI 1991 - ORFORD - QUEBEC

	S-D : 19	M-L : 20	T-M : 21	W-M : 22
Pres.	K. DARVESCH	E. PURISIMA	S. MATTAR	P. KUSALIK
8:20 - 8:30	INTRODUCTION			
8:30 - 9:15	E. CLEMENTI	S. CHIN	D. SALAHUB	G. PATEY
9:15 - 9:45	J.M. ANDRE	A. MICHEL	A.D. BECKE	A.M. TREMBLAY
9:45 - 10:15	M. DUPUIS	H. WEINSTEIN	M. ZERNER	T.F. GEORGE
10:15 - 10:45	BREAK			
Pres.	T. CARRINGTON	H. PRITCHARD	I. HAMILTON	D. WEAVER
10:45 - 11:30	W.H. MILLER	D. KOURI	J. DOLL	R.F.W. BADER
11.30 - 12:00	A. DALGARNO	T. UZER	L. PRATT	V.H. SMITH
12:00 - 12:30	A.D. BANDRAUK	R. KAPRAL	R.J. LEROY	S. HUZINAGA
12:30 - 18:00	LUNCH - FREE	PERIOD		
18:00 - 19:00	DINNER	DINNER	BANQUET	
Pres.	T.T. NGUYEN DANG	M. POIRIER	POSTERS	
19:00 - 19:45	P. BOWEN	B. LIU		
19:45 - 20:15	P. MEZEY	R.J. BOYD		
20:15 - 20:45	D.A. DIXON	F. GREIN		

INVITED LECTURES

1. **Enrico CLEMENTI - IBM Fellow**
   Computational Chemistry - Present and Future.

2. **Jean-Marie ANDRE - (Namur, Belgium).**
   Electronic Properties of Polymers.

3. **Michel DUPUIS - (IBM Kingston, N.Y., USA).**
   The Cope Rearrangement Revisited and Other Quantum Molecular Studies.

4. **William H. MILLER - (UC Berkeley, USA).**
   Recent Developments and Applications of Quantum Mechanical Reactive Scattering Theory.

5. **Alexander DALGARNO - (Harvard-Smithsonian Center for Astrophysics).**
   Collisions of Oxygen and Nitrogen Atoms in the Atmosphere.

6. **André D. BANDRAUK - (Université de Sherbrooke).**
   Molecules in Intense Lasr Fields - Numerical Simulations.

7. **Philip BOWEN - (University of Georgia).**
   Insights into Molecular Structure and Biological Activity.

8. **Paul G. MEZEY - (University of Saskatchewan).**
   Molecular Similarity Measures from 3D Shape Analysis.

9. **David A. ~~DIXON~~ Dobbs - (Dupont Co., Wilmington, USA).**
   Numerical Simulations of Molecular Properties.

10. **Steven CHIN - (IBM Kingston, N.Y.).**
    CHEM-STATION - A General Tool for Computational Chemistry.

11. **André MICHEL (Université de Sherbrooke).**
Characterization of Low Energy Conformational Domains for Peptidic Molecules.

12. **Harel WEINSTEIN - (Mt. Sinai School of Med., N.Y.).**
Computational Simulation of Specificity and Function in Biological Mechanisms.

13. **Donald J. KOURI - (University of Houston).**
Wave Packet Approach to Reactive Scattering.

14. **Turgay UZER - (Georgia Tech.).**
Wave packet Studies of Quantum Dynamics in Atoms, Molecules, and Surfaces.

15. **Raymond KAPRAL - (University of Toronto).**
Chemical Dynamics and Lattice-Gas Automats.

16. **Bowen LIU - (IBM Almaden Res. Cent. San Jose, USA).**
Theoretical Studies of Hyperpolarizabilities.

17. **Russell J. BOYD - (Dalhousie University).**
Computational Tests of Chemical Concepts - A Case Study of Model S_N2 Reactions.

18. **Fritz GREIN - (University of New Brunswick).**
The Anomeric and Reverse Anomeric Effect - Analysis of Ab Initio Results for Acetals and Protonated Acetals.

19. **Dennis R. SALAHUB - (Université de Montréal).**
Density Functional Theory for More and More Complex Systems.

20. **Axel D. BECKE - (Queen's University).**
Density-Functional Thermochemistry.

21. **Michael ZERNER - (University of Florida).**
Use of Intermediate Neglect of Differential Overlap Model for the Structure and Spectroscopy of Transition Metal Complexes.

22. **Jim D. DOLL - (Brown University).**
Stationary Phase Monte Carlo Methods - Interference Effects in Quantum Monte Carlo Dynamics.

23. **Lawrence R. PRATT - (Los Alamos Natl. Lab.).**
Monte Carlo Electron Density Functional Methods and Computer Simulation of Materials.

24. **Robert J. LeROY - (University of Waterloo).**
MD Simulations and the Nture of Melting in Van der Waals Clusters.

25. **Gren PATEY - (University of British Columbia).**
Theory of Liquids and Solutions.

26. **André-Marie TREMBLAY - (Université de Sherbrooke).**
Quantum Monte Carlo Simulations of the 2D Hubbard Model.

27. **Thomas F. GEORGE - (Université of N.Y. - Buffalo).**
Numerical Simulations of Optical Properties of Metallic Fractals.

28. **Richard F.W. BADER - (McMaster University).**
Atoms in Molecules - A Quantum Theory.

29. **Vedene H. SMITH, Jr. - (Queen's University).**
Towards an Understanding of Transition Metal Oxides.

30. **Sigeru HUZINAGA - (University of Alberta).**
Effective Hamiltonian Method for Molecules.

POSTERS

1. **ABOU-RACHID, H., NGUYEN DANG, T.T. (Université Laval).**
Adiabatic Representation for Time-dependent Wave Packets on Molecular Channels coupled by an Arbitrary Laser Pulse.

2. **AMEZIANE-HASSANI, C., MICHEL, A. (Université de Sherbrooke).**
Low Energy Conformational Domains for Met-Eukephalin.

3. **ARTECA, G., MEZEY, P. (University of Saskatchewan).**
Electron Densities in Static External Fields.

4. **AUBANEL, E., BANDRAUK, A.D. (Université de Sherbrooke).**
Pulse Coherences in Two-Photon Molecular Transitions.

5. **BARCLAY, V.J., POLANYI, J. (University of Toronto).**
Simulation of Dynamics of Surface-Aligned Photochemistry: H + HBr on LiF (001).

6. **CHEESEMAN, J.R., BADER, R.F.W. (McMaster University).**
Properties of Atoms in Molecules in Weakly Hydrogenbonded Systems.

7. **CHELKOWSKI, S., BANDRAUK, A.D. (Université de Sherbrooke).**
Pulse Effects in Molecular Photodissociation - Numerical Simulations.

8. **CSAIVNSKY, P. (University of Maine).**
Accuracy of Simpson's Rule in a Variational Density Functional Calculation of Total Atomic Energy.

9. **CULLEN, J. (University of Manitoba).**
Avoiding Basis Set Superposition Errors by a Backward Decomposition of Occupied and Virtual Molecular Orbital Spaces.

10. **CUSTODIO, R., GIORDAN, M., MORGAN, N.G., GODDARD, J.D. (Guelph University).**
Application of an Optimization Technique to Discrete Version of Griffin-Hill-Wheeler-Hartree-Fock Equations.

11. **DARDI, P.S., DAHLER, J.S. (University of Minnesota).**
Phase Shifts, Total Elastic Cross Sections, Resonances in Ar-Ar Scattering.

12. **DICKSON, R.M., BECKE, A.D. (Queen's University).**
Molecular Geometries by a Numerical Density - Functional Technique.

13. **EDGECOMBE, K. (Queen's University).**
Electronic Structure Analysis of Compounds of Interest in Drug Design.

14. **ESQUIVEL, R. (Queen's University).**
Accurate Spin Density and One-Electron Properties for the LiI Isoelectronic Series.

15. **FREEMAN, D.L. (University of Rhode Island).**
Estimation of the Heat Capacity in Quantum Path Integral Monte Carlo Simulations.

16. **FROESE, R., GODDARD, J.D. (University of Guelph).**
Ab Initio Quantum Chemical Studies of CS_3 Potential Energy Surfaces.

17. **GAGNE, S., OOMEN R. (NRC Inst. of Biological Sciences).**
A New Empirical Potential Energy Parameter Set for Carbohydrates: Applicaation to a CHARM Environment.

18. **GALLEGO, N., SUBA, S., WHITEHEAD, M.A. (McGill University).**
Molecular Electronic Structure of Pentastanna Compounds.

19. **GAUTHIER, J.M., BANDRAUK, A.D. (Université de Sherbrooke).**
Laser Induced Avoided Crossings in Ten Photon Photoionization of H_2.

20. **GODBOUT, N., SALAHUB, D. (Université de Montréal).**
Optimization of Orbital Basis Sets for Density Functional Theory - Applications to Organic and Inorganic Systems.

21. **GOODWIN, L., SALAHUB, D. (Université de Montréal).**
Optimized Tight Binding for Group IV Elements: Bulk and Cluster Properties.

22. **HACKEY, M., GREIN, F. (University of New Brunswick).**
Electronic Excited States of H_2CS, an Ab-Initio MRD-SI Study.

23. **HAMILTON, I. (University of Ottawa).**
Vibrational Splitting for Hydrogen Atom Exchange in HO_2.

24. **HO, M. (Queen's University).**
Topological Properties of $\rho(r)$ of the AM1 Wave Functions.

25. **HUNTER, G. (York University).**
a) New Electrostatic Quantum of Action in the Quantum Hall Effects.
b) Significant Digit Arithmetic - Future of Floating Point.

26. **JEANDENANS, C., MICHEL, A. (Université de Sherbrooke).**
Structural Requirements for Cu^{++} Binding Structures as revealed by Low Energy Conformational Domains of Acyclic Peptides.

27. **KEITH, T.A., BADER, R.F.W. (McMaster University).**
Properties of Atoms in Molecules in Electric and Magnetic Fields.

28. **KRISHNAN, S.M., CARRINGTON, T. (Université de Montréal).**
On the Elimination of First Order Coriolis Terms in the RO-Vibrational Hamiltonian.

29. **LAGOWSKI, J., VANSCO, G.J. (University of Toronto).**
Ab-Initio Study of Isopropylbenzene and Phenylbutane. Some Consequences for Chain Conformation of Polystyrene.

30. **LI, X., PALDUS, J. (Univrsity of Waterloo).**
Unitary Group Based Valence Bond and Coupled Cluster Methods for Closed and Open-Shell Systems.

31. **LIU, L. HAMILTON, I. (University of Ottawa).**
Thermal Dissociation of Diatomics - A Nosé Equation Approach.

32. **LUO, X., MEZEY, P. (University of Saskatchewan).**
Theoretical Studies of Molecular Surfaces.

33. **MANDY, M. MARTIN, P.G. (University of Toronto).**
Collisional Excitation of H_2 by H.

34. **MARIOLI, S., NGUYEN DANG, T.T. (Université Laval).**
Laser Induced Resonances and Photodissociation of H_2^+ in an Adiabatic Electronic Field Representation.

35. **MATTAR, S., HAMILTON, W.D. (University of New Brunswick).**
Electronic Structure and Bonding of Sc-Ni Dimer by Local Spin Density LCAO Technique.

36. **McNICHOLS, A., CARRINGTON, T.**
Lanagos Method for Variational Calculation of Energy Levels of Tetraatomic Molecules - Application to H_2CO.

37. **MEI, C. (Queen's University).**
Calculation of Electronic Correlations with Local Ansatz and the Inclusion of One Particle-Excitations.

38. **MIKOSCH, H., SALAHUB, D. (Université de Montréal).**
Theoretical Investigation of $[Mn(CO)_5/CH_4]^+$ Complex.

39. **PANG, L., WHITEHEAD, M.A. (McGill University).**
Prediction of Molecular Orientations, Order-Disorder, Translation-Rotation of CX_3Z Guest Molecules in Dianion's Compounds by Atom-Atom Potential Method.

40. **PANG, L., LUCKEN, E.A., WEBER, J., BERNARDINELLI, G. (McGill and Geneva Universities).**
Investigations and Modeling of Cavities in Clathrates.

41. **PERMANN, D., HAMILTON, I. (University of Ottawa).**
Higher-Order Phase Plots for Forced and WEakly Damped Pendulum.

42. **POIRIER, R.A. (Memorial University of Newfoundland).**
Reaction Mechanism for Deamination of Cytosine.

43. **POULIN, M., CARRINGTON, T. (Université de Montréal).**
Vibrational Analysis of Hydrogen Bonded Systems Using the Adiabatic Approximation.

44. **PRITCHARD, H.O. (York University).**
Computing in the 1950's.

45. **PURISIMA, E.O. (NRC-Biotech. Inst. - Montreal).**
Theoretical Studies of Thromlin Exosite Inhibitors.

46. **RAUK, A., YANG, D. (University of Calgary).**
Vibrational Circular Dichroism Spectra of Substituted Oxiranes and Substituted Thiiranes.

47. **ROZAS, I., MEZEY, P. (University of Saskatchewan).**
Comparative Study of Aromaticity in Five Member Rings Containing S, SO or SO_2 groups.

48. **SCHNIDER, H., SMITH, V.H. (Queen's University).**
Atomic and Molecular Orbitals from Compton Profiles.

49. **SEKIYA, M. (University of Alberta), RICE, J.E., ELLINGER, Y., LIU, B. (IBM Almanden Res. Cent., San Jose).**
Electron Correlation Effects on Hyperpolarizability of Small Molecules.

50. **SHEN, H., BANDRAUK, A.D. (Université de Sherbrooke).**
New Exponential Methods for Solving Time Dependent Schroedinger Equations.

51. **SILBERBACH, H. (E. Merck, Chem. Drug Design, D-6100 - Darnostadt, Germany).**
The Interionic Force.

52. **SIROIS, S., SALAHUB, D. (Université de Montréal).**
Theoretical Study of Adsorption of CO_2 on the 110 Pd Surface.

53. **St-AMAN, A., SALAHUB, D. (Université de Montréal).**
An LCTgO-MCP-DF Study of Hydrogen Adsorption by Ni, Rh, Pd Monomers, Dimers, Trimers.

54. **STYLIANI, C. (Queen's University).**
Electronic States and Transitions of XeH.

55. **VENANT, H., SALAHUB, D. (Université de Montréal).**
Model Potential Calculations for Third-Row Transition Metal Molecules within the Local Spin Density Method.

56. **WANG, J. (Queen's University).**
Spin Densities in Nitroxide Radicals.

57. **WANG, J. BOYD, R.J. (Dalhousie University).**
First Order John-Teller Distortion and Electron Densities.

58. **WEAVER, D.F. BIKKER, J. (Queen's University).**
Computational Conformational Studies of Antiepileptic Dihydropyridine Drugs.

59. **YU, H., BANDRAUK, A.D. (Université de Sherbrooke), SONNAD, V. (IBM - Kingston, N.Y.).**
Finite Element to Multiphoton Processes in Atoms and Molecules at High Laser Intensities.

60. **YUE, S.Y., PURISINRA, E.O., MENARD, R., STORER, A.C. (NRC Biotech. Inst., Montreal).**
Simulation Analysis from the Stability of Papain-E-64 Complex to the Specificity of Papain S_2 Subsite.

61. **ZHANG, Z.C., MEATH, W.J. (University of Western Ontario).**
Nonadditive Interaction Energies and Evaluation of Relevant Integrals.

62. **ZHENG, S., BOYD, R.J. (Dalhousie University).**
Laplacian of Charge Density as a Probe of Reaction Paths and Reactivity - S_N2 Reactions at C and Si.

EXTRA-CURRICULAR ACTIVITIES

1. TENNIS (FREE)

2. INDOOR SWIMMING POOL (FREE)

3. EXERCISE ROOM (FREE)

4. GOLF COURSE ($22/DAY)

5. EXCURSION - MT ORFORD
   1/2 HOUR WALK TO SKI-CENTER

6. CASH BARS - 2 (ENTRANCE; OUTSIDE CONFERENCE ROOM).

OFFICIAL APOLOGY

In the course of the organization of this symposium, an unfortunate error occurred due to a communication breakdown between the organizers and sponsors. Thus the names of **M. KARPLUS** and **P. JORGENSEN** appeared on the first circular, since we were first lead to believe that they had been contacted by sponsors. This turned out not to be the case as they had previous commitments.

To these two eminent scientists and all the participants who were looking forward to their presence, we present our sincerest apologies for this unfortunate error.

1 C.C.C.C. Orford, Québec. May 19-22nd 1991. List of Attendees.

Abou-Rachid, Hakima
Université Laval

Ameziane-Hassani, Chakib
Université de Sherbrooke

André, Jean-Marie
F.N.D.P. Namur (Belgique)

Arteca, Gustave
University of Saskatchewan

Aubanel, Éric
Université de Sherbrooke

Bader, Richard F.W.
McMaster University

Bandrauk, André D.
Université de Sherbrooke

Barday, Victoria
University of Toronto

Becke Axel D.
Queen's University

Bikker, Jack A.
Queen's University

Blair, Mark
University of Toronto

Boulay Gaston
Université de Sherbrooke

Bowen, Philip J.
University of Georgia

Boyd, Russell J.
Dalhousie University

Bredin Nathalie
Université de Sherbrooke

Brisson, Josée
Université Laval

Bundgen, Peter
University of New-Brunswick

Carrington Jr, Tucker
Université de Montréal

Cheeseman, James R.
McMaster University

Chelkowski, Sczephan
Université de Sherbrooke

Chin, Steven
IBM Corporation, Kingston

Clementi, Enrico
IBM Corporation, Kingston

Csaivnsky, Peter
University of Maine

Cullen, John M.
University of Manitoba

Custodio, Roferio
University of Guelph

Dalgarno, Alexander
Harvard-Smithsonian Center
for Astrophysics

Dardi, Peter S.
University of Minnessota

Darvesh, Kathy
Mt.St.Vincent University

Dewez Nadine
Université de Sherbrooke

Dickson, Ross M.
Queen's University

Dion Claude
Université de Sherbrooke

Dixon, David A.
Dupont U.S.A.

Doll, Jim D.
Brown University

Drouin Marc
Université de Sherbrooke

Dupuis, Michel
IBM Corporation, Kingston

Edgecomde, Ken
Queen's University

Esquivel, Rodolfo
Queen's University

Font, José L.
Monsanto Company

Freeman, David L.
University of Rhode Island

Froese, Robert
University of Guelph

Gagné, Stephanne
NRC-Institute Bialof.Sc.

Gallego, Nuria
McGill University

Gauthier, Jean-Marc
Université de Sherbrooke

George, Thomas F.
State University of New-York

Gervais, Jacques
IBM Canada Ltée

Godbout, Nathalie
Université de Montréal

Goldstein Solo
Université de Sherbrooke

Goodwin, Leif
Université de Montréal

Grein, Fritz
University of New-Brunswick

Hachey, Michel
University of New-Brunswick

Hamilton, Ian
University of Ottawa

Ho, Minhhoy
Queen's University

Huber, Lee M.
Dow Chemical Corporation

Hunter, Geoffrey
York University

Huzinaga, Sigeru
University of Alberta

Jeandenans, Catherine
Université de Sherbrooke

Kapral, Raymond
University of Toronto

Keith, Todd A.
McMaster University

Kouri, Donald J.
University of Houston

Krishnan, Sunder M.
Université de Montréal

Kusalick, Peter
Dalhousie University

Lagowski, Jolanta
University of Toronto

LeRoy, Robert J.
University of Waterloo

Li, Xiangzhu
University of Waterloo

Liu, Li
University of Ottawa

Liu, Bowen
IBM Corporation, San Jose

Luo, Xincai
University of Saskatchewan

Mandy, Margot E.
University of Toronto

Manoli, Sohiel
Université Laval

Mattar, Saba M.
University of New-Brunswick

McNichols, André
Université de Montréal

Mei, Changjiang
Queen's University

Mezey, Paul G.
University of Saskatchewan

Michel, André G.
Université de Sherbrooke

Mikosch, H.
Université de Montréal

Miller, William H.
University of California

Montcalm, Thierry
Université de Sherbrooke

Nguyen-Dang, Tunf T.
Université Laval

Pang, Li
McGill University

Patey, G.
University of British Columbia

Permann, Delmar
University of Ottawa

Pisanty, Alexandro
National Univiversity
Mexico

Poirier, Raymond A.
Memorial University

Popelier, Paul
McMaster University

Poulin, Martin
Université de Montréal

Pratt, Lawrence R.
Los Alamos Natl. Laboratory

Pritchard, H.O.
York University

Purisima, Enrico O.
NRC Biotechnoly Research Institute

Rozas, Isabel
University of Saskatchewan

Salahub, Dennis R.
Université de Montréal

Schmider, Hartmut
Queen's University

Scott, Jim
Cray Research Inc

Sekiya, Masahiro
University of Alberta

Shen, Hai
Université de Sherbrooke

Silberbach, Heinrich
Merck, Germany

Sirois, Suzanne
Université de Montréal

Smith Jr, Vedene H.
Queen's University

St-Amant, Alain
Université de Montréal

Stacey, Jim A.
Ontario Center for Large
Scale Computing

Styliani, Constas
Queen's University

Tremblay, André-Marie
Université de Sherbrooke

Trudel Yolaine
Université de Sherbrooke

Uzer, Turgay
Georgia Tech.

Venant, Hitimana
Université de Montréal

Villeneuve Gérald
Université de Sherbrooke

Wang, Jran
Dalhousie University

Wang, Jraker
Queen's University

Weaver, Robert
University of Toronto

Weaver, Donald F.
Queen's University

Weinstein, Harel
Mt Sinai School of Medecine

Wheatley, R.F.
University of Western Ontario

Yang, Danya
University of Calgary

Yu, Hengtai
Université de Sherbrooke

Yue, Shi-Hi
NRC Biotechnology Research Institut

Zerner, Michael
University of Florida

Zhang, Z.C.
University of Western Ontario

Zheng, Shi
Dalhousie University

SUBJECTS — CONFERENCES — SUJETS

1. COLLISIONS / DYNAMICS
COLLISIONS / DYNAMIQUE

A. Dalgarno (Harvard); A.D. Bandrauk (Sherbrooke); R. Kapral (Toronto); D. Kouri (Houston); W.H. Miller (Berkeley); T. Uzer (Georgia Tech.)

2. DENSITY FUNCTIONALS /THEORETICAL INORGANIC CHEMISTRY
DENSITE FONCTIONELLE / CHIMIE INORGANIQUE THEORIQUE

A.D. Becke (Queen's); D. Salahub (Montréal); V.H. Smith (Queen's); M. Zerner (Florida).

3. THEORETICAL ORGANIC CHEMISTRY
CHIMIE ORGANIQUE THEORIQUE

R.F.W. Bader (McMaster); R.J. Boyd (Dalhousie); F. Grein (New Brunswick); B. Liu (IBM, San Jose).

4. MOLECULAR MODELLING / RECOGNITION
MODELISATION / RECONNAISSANCE MOLECULAIRE

S. Chin (IBM, Kingston); A. Michel (Sherbrooke); P. Bowen (Georgia); D.A. Dixon (Dupont, U.S.A.); P. Mezey (Saskatchewan); H. Weinstein (Mt. Sinai, N.Y.).

5. QUANTUM CHEMISTRY / METHODS
CHIMIE QUANTIQUE / METHODOLOGIE

J.M. André (Namur); M. Dupuis (IBM, Kingston); E. Clementi (IBM, Kingston); T.F. George (Suny, Buffalo); S. Huzinaga (Alberta); G Malli (Simon Fraser).

6. MONTE CARLO METHODS / STATISTICAL MECHANICS
METHODES MONTE CARLO / MECANIQUE STATISTIQUE

J. Doll (Brown); R.J. LeRoy (Waterloo); G. Patey (British Columbia); L. Pratt (Los Alamos); A.M. Tremblay (Sherbrooke).