



## **12th Canadian Symposium on Theoretical Chemistry**

**12e Symposium  
Canadien sur la  
Chimie Théorique**

**August 6-11, 1995  
Fredericton, NB  
Canada**

**An international  
conference devoted to a  
broad range of topics in  
theoretical chemistry**

First announcement

### **General Information**

The 12th Canadian Symposium on Theoretical Chemistry will be held in Fredericton, NB, August 6- 11, 1995 under the co-chairmanship of William J. Meath (University of Western Ontario) and Ajit J. Thakkar (University of New Brunswick).

The topics selected for emphasis are:

- Structure, properties and dynamics of weakly interacting systems
- Condensed phases from clusters to solids and from dynamics to bulk properties
- Laser-molecule interactions: dynamics to spectroscopy
- Kinetics and reaction dynamics
- Molecular properties
- Surfaces and interfaces
- Materials design
- Computer simulation and statistical mechanics
- Quantum chemistry: methods and applications
- Novel computational and mathematical techniques
- Biochemical systems

The Symposium will feature invited speakers and poster presentations.

If you wish to present a poster, please submit a half-page abstract before June 1, 1995 to:

Dr. A.J. Thakkar  
Department of Chemistry  
Univ. of New Brunswick  
Fredericton, NB  
Canada E3B 6E2  
Fax: (506)-453-4599  
Internet: [ajit@unb.ca](mailto:ajit@unb.ca)

### **Registration**

Fees before March 1, 1995

Normal: \$275  
PDFs: \$150  
Graduate students: \$ 50  
Undergraduates: \$ 25  
• \$50 surcharge later

### **Accommodations**

Accommodations will be available at the University of New Brunswick Residences and at various hotels. More details will be given in the second announcement.

### **Future mailings**

To receive the next mailing, return the questionnaire by mail,

Fax or e-mail to:

Dr. W.J. Meath  
Department of Chemistry  
Univ. of Western Ontario  
London, ON  
Canada N6A 5B7  
Fax: 519-661-3022  
Internet: [a1043@nve.uwo.ca](mailto:a1043@nve.uwo.ca)



# 12th Canadian Symposium on Theoretical Chemistry 12ième Symposium Canadien sur la Chimie Théorique

Fredericton, 6-11 August/Août 1995

Co-chairmen: William J. Meath and Ajit J. Thakkar

The 12th Canadian Symposium on Theoretical Chemistry will be held August 6-11, 1995 at the Wu Conference Centre, University of New Brunswick, Fredericton, NB, under the co-chairmanship of William J. Meath (University of Western Ontario) and Ajit J. Thakkar (University of New Brunswick). The program will include invited papers and contributed posters in all areas of theoretical chemistry. The topics selected for emphasis are:

- Structure, properties and dynamics of weakly interacting systems
- Condensed phases from clusters to solids and from dynamics to bulk properties
- Laser-molecule interactions: dynamics to spectroscopy
- Kinetics and reaction dynamics
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- Surfaces and interfaces
- Materials design
- Computer simulation and statistical mechanics
- Quantum chemistry: methods and applications
- Novel computational and mathematical techniques
- Biochemical systems

## Invited Speakers

J.M. Andre (Belgium)  
A.D. Bandrauk (Canada)  
R.J. Bartlett (U.S.A.)  
D.M. Bishop (Canada)  
P. Botschwina (Germany)  
P.W. Brumer (Canada)  
D. Ceperley (U.S.A.)  
E.R. Davidson (U.S.A.)  
C.E. Dykstra (U.S.A.)  
J.T. Hynes (U.S.A.)  
B. Jeziorski (Poland)  
W.L. Jorgensen (U.S.A.)  
R.E. Kapral (Canada)  
H.J. Kreuzer (Canada)  
R.J. LeRoy (Canada)  
W. Meyer (Germany)  
P.G. Mezey (Canada)  
W.H. Miller (U.S.A.)  
D.J. Moore (Switzerland)

## Invited Speakers

J.N. Murrell (England)  
J. Oddershede (Denmark)  
S.D. Peyerimhoff (Germany)  
P. Pyykko (Finland)  
H.A. Rabitz (U.S.A.)  
M.A. Ratner (U.S.A.)  
A. Rauk (Canada)  
S.A. Rice (U.S.A.)  
D.R. Salahub (Canada)  
P. Saxe (U.S.A.)  
H.A. Scheraga (U.S.A.)  
K.C. Showalter (U.S.A.)  
J. Simons (U.S.A.)  
D.W. Sumners (U.S.A.)  
D.G. Truhlar (U.S.A.)  
D.M. Wardlaw (Canada)  
K.B. Whaley (U.S.A.)  
W. Yang (U.S.A.)

## Session chairs

R.J. Boyd (Canada)  
T. Carrington, Jr. (Canada)  
R.S. Dumont (Canada)  
I.P. Hamilton (Canada)  
W.G. Laidlaw (Canada)  
T.T. Nguyen-Dang (Canada)  
J. Paldus (Canada)  
G.N. Patey (Canada)  
R.A. Poirier (Canada)  
S.M. Rothstein (Canada)  
B.C. Sanctuary (Canada)  
V.H. Smith, Jr. (Canada)  
S.G. Whittington (Canada)  
J.S. Wright (Canada)  
M.C. Zerner (U.S.A.)  
T. Ziegler (Canada)

Contributed papers are welcome in all areas of theoretical chemistry. All contributed papers will be given in poster format. For registration forms, contact the Conference Secretary, 12th CSTC, Department of Chemistry, University of New Brunswick, Fredericton, NB E3B 6E2, Canada. Fax: 506-453-4981. Internet: coy@unb.ca



# 12th Canadian Symposium on Theoretical Chemistry 12ième Symposium Canadien sur la Chimie Théorique

Fredericton, 6-11 August/Août 1995

## Co-Chairs

**William J. Meath**  
Department of Chemistry  
University of Western Ontario  
London, ON  
Canada N6A 5B7

**Ajit J. Thakkar**  
Department of Chemistry  
University of New Brunswick  
Fredericton, NB  
Canada E3B 6E2

## SECOND ANNOUNCEMENT

The 12th Canadian Symposium on Theoretical Chemistry will be held August 6-11, 1995 at the Wu Conference Centre, University of New Brunswick, Fredericton, NB. The program will include invited papers and contributed posters in all areas of theoretical chemistry. The topics selected for emphasis are:

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- Kinetics and reaction dynamics
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### Invited Speakers

J.M. Andre (Belgium)  
A.D. Bandrauk (Canada)  
R.J. Bartlett (U.S.A.)  
D.M. Bishop (Canada)  
P. Botschwina (Germany)  
P.W. Brumer (Canada)  
D. Ceperléy (U.S.A.)  
E.R. Davidson (U.S.A.)  
C.E. Dykstra (U.S.A.)  
J.T. Hynes (U.S.A.)  
B. Jeziorski (Poland)  
W.L. Jorgensen (U.S.A.)  
R.E. Kapral (Canada)  
H.J. Kreuzer (Canada)  
R.J. LeRoy (Canada)  
W. Meyer (Germany)  
P.G. Mezey (Canada)  
W.H. Miller (U.S.A.)  
D.J. Moore (Switzerland)

### Invited Speakers

J.N. Murrell (England)  
J. Oddershede (Denmark)  
S.D. Peyerimhoff (Germany)  
P. Pyykko (Finland)  
H.A. Rabitz (U.S.A.)  
M.A. Ratner (U.S.A.)  
A. Rauk (Canada)  
S.A. Rice (U.S.A.)  
D.R. Salahub (Canada)  
P. Saxe (U.S.A.)  
H.A. Scheraga (U.S.A.)  
K.C. Showalter (U.S.A.)  
J. Simons (U.S.A.)  
D.W. Sumners (U.S.A.)  
D.G. Truhlar (U.S.A.)  
D.M. Wardlaw (Canada)  
K.B. Whaley (U.S.A.)  
W. Yang (U.S.A.)

### Session chairs

R.J. Boyd (Canada)  
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W.G. Laidlaw (Canada)  
T.T. Nguyen-Dang (Canada)  
J. Paldus (Canada)  
G.N. Patey (Canada)  
R.A. Poirier (Canada)  
S.M. Rothstein (Canada)  
B.C. Sanctuary (Canada)  
V.H. Smith, Jr. (Canada)  
S.G. Whittington (Canada)  
J.S. Wright (Canada)  
M.C. Zerner (U.S.A.)  
T. Ziegler (Canada)

**Contributed papers** are welcome in all areas of theoretical chemistry. All contributed papers will be given in poster format. If you are contributing a poster, please send an abstract before June 15, 1995 preferably by e-mail to coy@unb.ca or mail it to Conference Secretary, 12th CSTC, Chemistry Department, University of New Brunswick, Fredericton, NB E3B 6E2, Canada. The abstract should begin with the title, authors' names and bylines with the presenting author indicated. The body of the abstract should be no more than 15 lines and, if mailed, should be prepared in a 12 point Times Roman font.

**Registration Fee:** The fee covers full participation in the conference, the book of abstracts, complimentary refreshment breaks, the Sunday night reception and the Thursday evening barbecue. The fee schedule is shown on the enclosed registration form. Note that there will be a surcharge for registrations received after June 1, 1995. Please complete the attached registration form and mail it, together with a bank draft, money order, or cheque, payable in Canadian funds to the *Canadian Association of Theoretical Chemists*, to Conference Secretary, 12th CSTC, Chemistry Department, University of New Brunswick, Fredericton, NB E3B 6E2, Canada.

### **Social Program**

The conference will open with a reception for all participants and guests on Sunday, August 6 at 8:00 p.m. On Wednesday afternoon, there will be a trip to the King's Landing Historical Settlement. Buses will be hired for transportation. The cost of the bus trip and admission will be \$10 per person. There will be a barbecue on Thursday (August 10) evening. The conference ends at 1:00 p.m. on Friday, August 11.

There are no other social programs planned during the conference. However, a conference rate has been organized for a whale watching trip in the Bay of Fundy on Saturday, August 12. The cost of the day trip is \$100 per person including a four hour boat trip to spot whales, lunch and bus transportation from Fredericton to St. Andrews (100 km) and back. Tickets will be available on a first come, first serve basis. All registered participants will be sent a tour reservation form.

### **Travel to Fredericton**

There are flights from all major Canadian centres to Fredericton. The airport is about a 20 minute taxi ride (\$17) from the University of New Brunswick campus. There is also shared limousine service available at the airport at a lower cost.

### **Accommodations**

Accommodations will be available at the University of New Brunswick (UNB) Residences and at various hotels. A form is enclosed for reserving a room at the UNB residences.

Those not wishing to stay on campus should also arrange their own accommodation. Some hotels within a short (and relatively cheap) taxi ride of the conference centre are listed below with their telephone numbers, and corporate rates. Remember to ask for the UNB corporate rate.

Carriage House Inn, (20 minute walk from conference centre). (506)-452-9924  
\$70 (\$75)/night for 1 (2) person(s) in a room with private bathroom.  
\$55 (\$59)/night for 1 (2) person(s) in a room with access to a shared bathroom.  
Rates include breakfast. Taxes extra.

Fredericton Inn, (30 minute walk from conference centre). (506)-455-1430  
Single room: \$57/night plus taxes. Double room: \$67/night plus taxes.

Keddy's Inn, (506)-454-4461 or 1-800-561-7666 (toll free)  
Single room: \$50.95/night plus taxes. Double room: \$56.95/night plus taxes.

Lord Beaverbrook Hotel, (506)-455-3371 or 1-800-561-7666 (toll free), downtown by the river.  
Single room: \$72/night plus taxes. Double room: \$77/night plus taxes.