

# CANADIAN SYMPOSIUM ON THEORETICAL CHEMISTRY SYMPOSIUM CANADIEN SUR LA CHIMIE THEORIQUE

# INTERNATIONAL CONFERENCE INTERNATIONALE

1989 August 24-30 août

Banff, Alberta

Arvi Rauk Department of Chemistry University of Calgary Calgary, Alberta, Canada T2N 1N4 (403) 220-6247

# SECOND ANNOUNCEMENT

Bruce L. Clarke Department of Chemistry University of Alberta Edmonton, Alberta, Canada T6J 3S3 (403) 432-5739

The 10th Canadian Symposium on Theoretical Chemistry will be held August 24 - 30, 1989 at the Banff Centre, Banff Alberta.

#### TECHNICAL PROGRAM

The program will include invited papers and contributed posters on all areas of theoretical chemistry. The following topics are emphasized:

Electronic Structure Theory and Applications

Density Functional Theory

Quantum Biology and Theoretical Biophysical Chemistry

Algebraic Methods

Theoretical and Solid State Chemistry

Chemisorption and Related Surface Phenomena

**Evolution and Chaos** 

Evolution of Structure in Fluids and Solids

Vibrational Optical Activity

Novel Approaches

#### INVITED SPEAKERS

E. J. Baerends (Amsterdam) A. Bishop (Los Alamos)

T. D. Bouman (SIUE) D. Chandler (UCBerkeley)

C. Fairbridge (CANMET)

D. D. Holm (Los Alamos)

R. E. Kapral (Toronto) P. A. Kollman (UCSF)

V. A. Kostelecky (Indiana)

R. M. Miura (U.B.C.)

L. A. Nafie (Syracuse) M. Randic (Iowa State)

H. F. Schaefer III (Georgia)

E. Shustorovich (Kodak)

P. J. Stephens (UCLA)

T. Ziegler (Calgary)

S. Whittington (Toronto)

A. Becke (Queen's) G. Bluman (U.B.C.)

J. K. Burdett (U. of Chicago)

E. Clementi (IBM)

W. A. Goddard III(Cal. Tech.)

F. Iachello (Yale)

D. J. Klein (Texas A&M) R. Kopelman (Michigan)

W. J. Meath (Western Ontario)

K. Morokuma (Kyoto)

J. A. Pople (Carnegie-Mellon)

D. Rothman (M.I.T.)

P. v. R. Schleyer (Erlangen)

V. H. Smith (Queen's) J. Tuszynski (Alberta)

T. Yamabe (Kyoto)

# **CONTRIBUTED PAPERS**

Contributed papers will be welcomed in all areas of theoretical chemistry. All contributed papers will be given in poster format. If you are contributing a paper to the conference, please fill out the attached Abstract Form. Abstracts should reach Calgary by July 1, 1989.

\*Cascade Inn 762-3311 \$40-\$65

\*Homestead Inn 762-4471 \$45-\$80

Inns of Banff Park 762-4581 1-800-661-1272 \$90-\$105

Irwin's Motor Inn 762-462 \$40-\$70

\*King Edward Hotel 762-2251 \$45-\$80

\*Mount Royal Hotel 762-3331 \$90+

Mountview Village Resort 762-2400 1-800-661-1367 \$90+

Pinewoods Motel & Chalets 762-5515 1-800-661-1272 \$35-\$70

\*Ptarmigan Inn 762-2207 Can. 1-800-661-8310 \$75

\*Rundle Manor Apt. Motel 762-5544 1-800-661-1272 \$60-\$90

Spruce Grove Motel 762-2112 \$60-\$90

Swiss Village Lodge 762-2256 1-800-661-1272 \$90+

\*Traveller's Inn 762-4401 1-800-661-8340 \$60-\$90

Voyager Inn 762-3301 Alta. 1-800-372-9288 \$42-\$80

Woodland Village Inn 762-5521 \$90+

\*Within 15 min walk from Banff Centre

## **MEALS**

Meals are included in the cost of accommodation at the Banff Centre. Off Campus residents who have paid the User Fee have Lunch included. There are many fine restaurants in Banff for those who wish to eat off campus. Meals missed are not refundable. However, the Banff Centre will provide box lunches for those who so desire.

## TRAVEL TO BANFF

Air Canada is the official carrier for the 10th Canadian Symposium on Theoretical Chemistry. Delegates from Canada and the United States may take advantage of reduced rates by arranging their travel as described in the enclosed pamphlet. Please specify the File No 89-0753. The nearest airport to Banff is Calgary, Alberta, from which it is approximately a two hour drive to Banff. Bus service (\$19) is available at 12:30 pm, 3:30 pm and 5:15 pm daily from the Calgary airport to the Banff Centre.

#### **EXPOSITION**

An exposition of computer hardware and software in association with the Conference is planned.

#### REGISTRATION

The registration fee includes full participation in the conference, the book of abstracts, complimentary coffee breaks, the reception on Thursday night and the BBQ on Sunday evening. Registration will take place on Thursday, August 24th 2:00 p.m. to 7:30 p.m. and on Friday, August 25th 8:00 a.m. to 12:00 noon.

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. Please return the completed form to:

10th Canadian Symposium on Theoretical Chemistry Department of Chemistry University of Calgary Calgary, Alberta T2N 1N4 Canada

The 10th Canadian Symposium on Theoretical Chemistry is sponsored by NSERC. The organizers are grateful for additional financial support from the Canadian Society of Chemists and the Faculty of Science of the University of Calgary.

#### **REGISTRATION FEES**

The registration fee is \$200 Cdn if paid before May 1, 1989, and \$250 Cdn after May 1, 1989. Reduced rates are available for post\_doctoral fellows (\$100), graduate students (\$50) and undergraduate students (\$25). The Accompanying Persons registration fee is \$25. The registration fee includes full participation in the conference, the book of abstracts, complimentary coffee breaks, the reception on Thursday night and the conference BBQ on Sunday. A Registration Form is attached to this circular.

## **SOCIAL PROGRAM**

The conference will open with a reception for all delegates and registered accompanying persons at 8:30 p.m. on Thursday, August 24, 1989, followed an Opening Plenary Lecture at 7:30 p.m.

A one day tour of the mountain scenery, The Mountain Lakes and Canyons Tour, is planned for Sunday, August 27, 1989. Tickets may be purchased on the attached Registration Form. The tour provides opportunity for gentle hiking and will return in time for the BBQ.

A western barbecue (BBQ) will be staged at the Banff Centre on Sunday evening, August 27, 1989. The cost of the BBQ is included in the registration fee. Additional tickets may be purchased for \$20 per person.

# GENERAL INTEREST PROGRAM FOR REGISTERED ACCOMPANYING PERSONS

One activity, designed to introduce visitors to the scenic and recreational aspects of the Canadian Rocky Mountains will be offered each day. Some activities will be free of charge for registered accompanying persons. Non-registered persons can be accommodated at a nominal cost. Possible activities include:

- -a tour of, and lunch (extra) at the historic Banff Springs Hotel
- -a gondola ride to Sunshine Village, strolling in alpine meadows
- -a walk on Tunnel Mountain
- -chair lift to the top of Sulphur Mountain
- -a tour of the museums of Banff
- -a recital by a resident artist

Specific events can be booked at the conference and are subject to demand. The general interest program fee includes the opening reception on Thursday night and the BBQ on Sunday.

## ACCOMMODATION

Blocks of rooms have been booked at the Banff Centre, the site of the conference. Please use the attached Accommodation Form to make reservations. Most rooms are of shared type. A limited number of single rooms are available. The room rates, listed on the Accommodation Form, include three meals per day and use of the Sally Borden Recreational Complex. Those who chose not to or are unable to stay on campus will be charged a User Fee of \$17 /day/person which will enable them use of the recreation complex, parking and lunch.

There is no public transportation in Banff. Those wishing to stay off campus may require a car to reach the Banff Centre. Please arrange your own accommodation with the help of a travel agent. A list of Hotels and Motels, with approximate prices, follows (hotels within 15 min. walk of the Banff Centre are marked with an asterisk):

Banff Area Code (403)

Aspen Lodge 762-4418 W. Can. 1-800-661-1238 \$90

Banff Caribou Lodge 762-2713 \$90

\*Banff International Hotel 762-5666 \$90+

Banff International Hostel 762-4122 \$35

\*Banff Park Lodge 762-4433 1-800-661-9266 \$110+

Banff Springs Hotel 762-2211 Can. 1-800-268-9411 \$90+

\*Bow View Motor Lodge 762-2261 \$70-\$110

Bumper's Inn 762-3386 \$42-\$80