DIRECTIONS IN

THEORETICAL CHEMISTRY

A workshop supported by the National Science Foundation

Snowbird, Utah

April 22-24, 1986

Organizer:

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I. The Workshop Format and Findings

During the week of April 21-25, 1986 a scientific conference was held at Snowbird, Utah. The so-called SNOWBEL conference was focused on "the interface between electronic structure and chemical dynamics". This meeting was held under the auspices of the Sanibel Symposium organization, Professors P. O. Lowdin, Y. Ohrn and J. Simons served as its coorganizers. More than one hundred individuals (representing theoretical and experimental chemistry as well as computer and materials science and funding agencies) took part as registered participants. Scientists from industry, government laboratories, academic institutions and foreign research institutes were present. Ph.D. students, postdoctorals, and independent junior and established research workers were broadly represented in the participant list which is shown below. The scientific program schedule is reproduced on pg. 7.

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Final Snowbird Conference Schedule

Sessions are held in the Cottonwood Conference Center. There are three sessions per day: A: 8:15-10:30 a.m., B: 3:30-6:30 p.m., C: 8:30-11:00 p.m. The time between sessions is free for informal get togethers, meals, skiing, etc.

Monday 8:00-8:15 Opening Remarks

Session A

Thom Dunning, "Reaction Paths for Chemical Reactions"
Per Siegbahn, "The calculation of potential energy surfaces for homogenous and heterogenous catalytic processes"
Bill Lester, "Quantum Monte Carlo for Molecules: Energies and Other Properties"

Session B

Jan Almlof, "The Calculation of Accurate Infrared Vibrational Intensities"
Rod Bartlett, "Analytical Derivative Methods and Coupled Cluster Theory"
Ed McCullough, "MCSCF and MCSCF-CI Calculations on Transition Metal Diatomics Using Numerical Basis Sets"
Rich Martin, "Model Studies of the Epoxidation of Ethylene on Silver"

Session C Poster Session #1

Tuesday

Session A

Ken Jordan, "Temporary Anion Resonances in Polyatomic Molecules"
David Yarkony, "Recent Advances in the Theoretical Treatment of Nonadiabatic Processes"
Michael Allan, "Some recent experiments on inelastic electron-molecule collisions at low energies"

Session B

David Chandler, "Field Theoretic Approaches to Solvation"
Mark Ratner, "Semiclassical Self-Consistent Field Calculations of Vibrational Dynamics"
Casey Hynes, "Dynamical Aspects of Reactions in Solution"
Jules Moscowitz, "Monte-Carlo Green's Function Methods in Electronic Structure"
Eric Heller, "Chaos, Quantum Mechanics, and the Mexico City Earthquake"

Session C NSF Workshop Session #1

Wednesday

Session A

Steve Leone, "Dynamics of Ion-molecule Reactions"
Jean Futrell, "Reaction Dynamics of Low Energy Charge Transfer Reactions"
Carl Lineberger, "Photodetachment Probes of Electronic Structure and Vibration, Rotation-Electronic Coupling in Anions"

Session B

Bill Breckenridge, "Half-Collision Versus Full-Collision Dynamics: Van der Waal's Complexes of Electronically Excited Atoms"
Don Truhlar, "Electronic Structure and Dynamics Calculations: Inelastic and Reactive Collisions"
George Schatz, "The Dynamics of Reactions which Produce Highly Excited Intermediates or Products: The Need for Better Global Potential Surfaces"
Bob Wyatt, "Dynamics of the Li + HF Reaction"

Session C NSF Workshop Session #2

Thursday

Session A

Curt Wittig, "Reactions in Clusters"
Jim Doll, "Theoretical Studies of Hydrogen Diffusion"
John Tully, "Dynamics of Gas-Surface Interactions"

Session B

Ken Janda, "Measurements and Calculations on the Vibrational Predissociation of $NeCl_2$"
George Lie and Enrico Clementi, "Global Computations: Quantum Chemistry, Statistical Mechanics and Continuum Mechanics"
Randy Shirts, "Intramolecular Vibrational Rotational Dynamics on Model Potential Surfaces"
Andy Komornicki, "Ab Initio Vibrational Spectroscopy: Computational Aspects and Applications"

Session C NSF Workshop Session #3

Friday

Session A

Yngve Ohrn, "Dynamics of Nuclei and Electrons Using the AGP Coherent State"
Jan Linderberg, "Reactive Scattering in Hyperspherical Coordinates"
Bill Hase, "Potential Energy Surface Properties and Intramolecular Vibrational Energy Relaxation in Benzene"

Session B

Per-Olov Lowdin, "Towards a Theory of Chemical Reactions"
Sally Chapman, "Proton transfer reactions: Heavy-Light-Heavy dynamics in ionic systems"
Howard Taylor, "Energy Localization in Molecules: Dynamic Causation and Spectroscopic Consequences"
David Micha, "Extensions of the time-dependent Hartree-Fock Method and applications to atomic collisions"

As an integral part of the Snowbel conference, a three-session National Science Foundation funded workshop was held on Tuesday, Wednesday and Thursday evenings. It's primary purposes were to examine and make constructive recommendations concerning the status and state of health of theory within chemistry and of chemistry within science and society. To focus the discussion of the workshop, at least initially, a set of eight questions were posed for consideration. These eight questions are listed below.

1. **What is the present state of health of theory within chemistry?**

2. **Where has theory contributed substantially and significantly to research in chemistry and in related disciplines?**

3. **Where should theoretical chemistry be focusing its efforts so as to have greater impact in science and technology?**

4. **What steps can be taken to so focus theory's efforts and what resources are needed to achieve this?**

5. **What is the present image of chemistry in society?**

6. **What should and can be done to improve this image?**

7. **In what directions should chemistry research be evolving so as to maximize both innovation and its impact on related disciplines?**

8. **What improvements are needed in our educational process to better prepare our students for productive careers in theory?**

The NSF workshop began on Tuesday evening with a forty minute introductory and overview session in which the workshop organizer Jack Simons outlined to the more than one hundred participants the format, scope, and goals of the workshop. Subsequently, the participants were divided into eleven working groups of approximately ten persons per group. For the remainder of the Tuesday session, these working groups met individually to discuss the above eight questions. During the first working group meetings all participants responded to a questionnaire consisting of twenty-five written statements which were designed to provide further directions to their initial discussions. The twenty-five statements along with numerical data summarizing the responses of all participants are displayed below.

Questionnaire Response Summary

Statement	Ave[a]	Std[b]
1. Chemistry is a "central science" which generates new spin-offs and impacts many other disciplines.	7.17	0.62
2. Theory is maturing and, as a result, contributing more to chemistry than it did ten to twenty years ago.	6.75	1.35
3. Theoretical chemistry plays much the same role in chemistry as theoretical physics does within physics.	-3.50	1.26

4.	Chemists should carry out more of their work in centralized interdisciplinary research centers.	-2.08	2.32
5.	Theoretical chemists should develop closer ties with scientists in the chemical, biotechnological, and materials industry.	5.58	1.10
6.	The NSF funded supercomputer initiative is a good idea which greatly benefits theoretical chemistry.	4.17	1.57
7.	Theoretical chemists need to develop centers for work in theory much like the Santa Barbara theoretical physics institute.	3.67	1.57
8.	Computer programs developed for research by theoretical chemists should be more openly circulated to the general chemistry research community.	3.83	2.53
9.	Theoretical models and concepts should be emphasized to a larger extent than at present in the undergraduate chemistry curriculum.	5.57	1.86
10.	The public thinks of Bhophal, acid rain, and chemical and nuclear waste when they think of "chemistry".	5.33	1.37
11.	The NSF's new initiatives (e.g., supercomputers, computational mathematics, life processes, etc.) provide net benefit to the basic research effort which NSF is supposed to fund.	4.33	1.37
12.	The following constitute major intellectual frontiers: understanding chemical reactivity, chemical catalysis, chemistry of life processes, chemistry around us, chemical behavior under extreme conditions.	5.67	1.11
13.	Priority should be given to the following research frontiers: understanding chemical reactivity, chemical catalysis, chemistry of life processes, chemistry around us, chemical behavior under extreme conditions.	3.17	2.11
14.	New mechanisms and new incentives should be sought for strengthening links between industrial and academic research.	5.67	0.94
15.	Industry should increase its support for university fundamental research in the chemical sciences.	6.17	0.90
16.	The federal investment in chemistry should be raised to be commensurate with the practical importance of chemistry, both economic and societal, and with the outstanding opportunities it now offers.	7.00	1.83
17.	Within molecular dynamics, areas of major importance are: fast chemical processes in real time, energy	6.33	1.25