

Regional Symposium on
CHEMICAL PHYSICS
October 23-25, 1987
at the University of Waterloo

REGISTRATION begins at 6 p.m.

SESSION I: *Friday, October 23, 1987* *Optometry 347*
Chairman: K.T. Leung

- 7:30 - 8:10 P. Norton (University of Western Ontario).
Phase Transitions and Surface Reactivity.
- 8:10 - 8:30 K. Maynard and M. Moskovits (University of Toronto).
Surface Enhanced Raman Spectroscopy of CO on Alkali Metal
Pre-Dosed Silver Surfaces.
- 8:30 - 8:50 J.S. Suh and K.H. Michaelian (University of Toronto).
Surface Enhanced Raman Scattering as a Probe of Surface
Geometry Effects on the Polymerization of Acrylic Acid and
Acrylamide on Silver.
- 8:50 - 9:10 A. Rochefort and D.R. Salahub (Universite de Montreal).
An LCGTO-LSD-MP Study: Effect of the Addition of Tin to Rh,
Pd(111) Clusters on Chemisorption and Diffusion of Hydrogen.
- 9:10 - 9:30 M. Menzinger, A. Giraudi and P. Jankowski (University of
Toronto). Stirring Effects in Nonlinear Dynamics.

SESSION II: *Saturday, October 24, 1987 A.M.* *Optometry 347*
Chairman: J.J. Sloan

- 9:00 - 9:40 R.J.D. Miller (University of Rochester).
Picosecond Dynamics of Surface Mediated Electron Transfer
Processes at Single Crystal Semiconductor Interfaces.
- 9:40 - 10:00 S.-P. Lee, S. Deshmukh and E.W. Rothe (Wayne State
University). Characteristics of Pulsed Laser-induced
Optogalvanic (LOG) Effect: Detection of OH Radical and
Resonance Enhanced Multi-Photon Ionization of NH₃.
- 10:00 - 10:20 S.M. Deshmukh, E.W. Rothe and G.P. Reck (Wayne State
University). Laser Photoablation Induced Chemiluminescence
of POLYCARBONATE and PVA.
- 10:20 - 10:40 **Coffee Break**

- 10:40 - 11:20 B. Schlegel (Wayne State University).
Spin Projection and Moller-Plesset Perturbation Theory.
- 11:20 - 11:40 R. Fournier, J. Andzelm and D.R. Salahub (Universite de Montreal). Energy Gradient for the LCGTO-LSD Method.
- 11:40 - 12:00 A. St.-Amant and D.R. Salahub (Universite de Montreal).
Optimisation of the Molecular Geometry within the LCGTO-HF Method Using the Simulated Annealing Technique of Car and Parrinello.
- 12:10 - 1:45 **Lunch** Optometry 347

SESSION III: Saturday, October 24, 1987 P.M.
Chairman: J.W. Hepburn

- 2:00 - 3:00 D. Herschbach (Harvard University).
Electronic Structure in Strange Dimensions.
- 3:00 - 3:20 M. Shen and J.M. Farrar (University of Rochester).
Photodissociation of Mass-Selected Cluster Ions: $\text{Sr}^+(\text{H}_2\text{O})$.
- 3:20 - 3:40 L.E. Fried and G.S. Ezra (Cornell University).
Classical Perturbation Theory Provides a Route to the Semiclassical Quantization of Molecular Vibrations.
- 3:40 - 4:00 E.E. Aubane and D.M. Wardlaw (Queen's University).
Semiclassical Treatment of the Vibrational Spectroscopy of OCS.

SESSION IV: Saturday, October 24, 1987 P.M. Festival Room-SCH
POSTER SESSION

- 1) J.D. Goddard (University of Guelph). Tests of Several Quantum Chemical Approaches for the Energies and Geometries of the Ground and Lowest Excited Electronic States of Some Sulphur Containing Free Radicals.
- 2) G. Corey (Universite de Montreal) and M. Alexander (University of Maryland). A Theoretical Study of Alignment Effects in Collisions of N_2 with an Ag Surface.
- 3) J.E. Black (Brock University). The Vibration Modes of A Two Dimensional Fractal.
- 4) E.W. Rothe (Wayne State University), T. Seelemann and P. Andresen (Max-Planck-Inst. fur Stromungsforschung). Resonance Enhanced Multiphoton Ionization of Vibrationally-Excited State-Selected NH_3 . Spectroscopy and Collisional State Transfer.
- 5) C. Getino-Gonzalez, J. Santamaria (Universidad Complutense de Madrid, Spain) and G.S. Ezra (Cornell University). Classical Trajectory Study of Overtone Induced Dissociation of HOOH and HOOD .

- 6) B.G. Sumpter and G. Ezra (Cornell University). Intramolecular Dynamics of Rotating Polyatomic Molecules: Mode Energy Transfer and Semiclassical Quantization.
- 7) J.T. Stuckless and M. Moskovits (University of Toronto). 1 & 2 Photon Laser Induced Electron Emission From Silver Surfaces.
- 8) W. Jaworski and D.M. Wardlaw (Queen's University). Time Delay in Tunneling. Transmission and Reflection Time Delays.
- 9) W. Jaworski and D.M. Wardlaw (Queen's University). On the Concept of a Time-of-Sojourn Operator.
- 10) R.H. Judge, D.J. Clouthier and D.C. Moule (Brock University). Single-Triplet Excitation Spectrum of the Short-Lived Species Selenoformaldehyde.
- 11) F. Ioannoni, J.D. Goddard, D.J. Clouthier and D.C. Moule (Brock University). Spectroscopic Identification and Theoretical Considerations of trans- and cis-Dithioformic Acid, HCSSH.
- 12) K.D. Bier, T.L. Haslett, A.D. Kirkwood and M. Moskovits (University of Toronto). The Resonance Raman and Visible Absorbance Spectra of Matrix Isolated Mn₂ and Mn₃.
- 13) D.W. Blue, K.R. Helwig and M. Moskovits (University of Toronto). A SERS Study of the Diffusion of C₂H₄ Through Thin Pyrazine Films on Rough Ag Surfaces.
- 14) T.L. Haslett, A.D. Kirkwood, M. Moskovits and A.L. Weitzman (University of Toronto). Dissociation Energies of Transition Metal Dimers.
- 15) C.C. Tung, G.P. Reck and E.W. Rothe (Wayne State University). Crossed Beam Study of Na (²P_{3/2}) + O₂ -> Na⁺ + O₂⁻. The Dependence of the Total Cross Section Upon Na Alignment.
- 16) G.P. Reck, L. Hitchcock, C.C. Tung, E.W. Rothe and M. Modi (Wayne State University). Temperature Measurement Via 2 + 1 REMPI of H₂.
- 17) F. Schlenker, I.M. Waller, F. Bouchard, D. Cyr and J.W. Hepburn (University of Waterloo). Dynamics of Organometallic Photochemistry.
- 18) S.R. Vande Linde, (Wayne State University)
- 19) M. Davies and R.J. Le Roy (University of Waterloo). Calculation of Frequency Shifts for H₂ in Inert Gas Matrices.

7:00 P.M.

DINNER

Laurel Room - SCH

SESSION V: Sunday, October 25, 1987
Chairman: T.E. Gough

Optometry 347

- 9:00 - 9:40 J. Reid (McMaster University).
Optically Pumped NH₃ Laser: A New Approach To Stable Lasers.
- 9:40 - 10:00 T.R. Rizzo, X. Luo and P. Rieger (University of Rochester).
Double Resonance Reactant Preparation for State-Selective
Unimolecular Reaction Studies.
- 10:00 - 10:20 E. Altendorf and W.K. Liu (University of Waterloo).
Energy Transfer and Trapping of Atoms by Solid Surfaces.
- 10:20 - 10:40 **Coffee Break**
- 10:40 - 11:20 P. Brumer (University of Toronto).
Chaotic Intramolecular Energy Transfer.
- 11:20 - 11:40 D. Wardlaw and W. Jaworski (Queen's University).
Quantum Chaos in Scattering: Study of an Unusual Model
System.
- 11:40 - 12:00 B.I. Niefer, E.J. Kruus and J.J. Sloan (NRC, Ottawa).
The State-Resolved Dynamics of O(1D) Reactions with Hydride
Molecules.