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19. ABSTRACT (Continue on reverse if necessary and identify by block number) The objective has been to develop theoretical models and computational codes to describe chemical and physical phenomena associated with clusters, microstructures and surfaces, in order to gain a better understanding of surface/solid-state chemistry and its role in applied areas such as catalysis and microelectronics. The approach has been to examine topics relevant to this objective, using techniques appropriate for molecular dynamics, spectroscopy and electronic structure. The following nine topics have been studied: (1) clusters, with emphasis on geometry, stability, spectroscopy and reactions; (2) infrared-laser-excited adspecies with emphasis on energy and phase relaxation and desorption; (3) ultraviolet-laser-induced chemical vapor deposition; (4) resonance fluorescence at flat metallic surfaces; (5) photochemistry at structured metallic surfaces, with emphasis on gratings and thin films; (6) phase-conjugated surfaces; (7) laser-induced reactions in solid matrices; (8) nonlinear optical processes in polymeric systems; and (9) molecular dynamics simulations.				
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Summary

The objective under the current ONR contract has been to develop theoretical models and computational codes to describe chemical and physical phenomena associated with clusters, microstructures and surfaces, in order to gain a better understanding of surface/solid-state chemistry and its role in applied areas such as catalysis and microelectronics. The approach has been to examine topics relevant to the above objective, using theoretical techniques appropriate for molecular dynamics, spectroscopy and electronic structure. Various topics are listed below, with one or two sentences describing a representative accomplishment and/or result for each topic.

I. Clusters

A. Geometry and Stability

- Extended Hückel molecular orbital calculations along with graph theory have been used to determine relative stabilities and geometries of alkali metal clusters (neutrals, cations and anions) for sizes up to fourteen atoms, and an analysis has been made with respect to trends in orbital energies, shell structures, ionization potentials and extrapolation to the bulk limit.
- A non-Cartesian coordinate system has been developed which permits the vibrational motions of Buckminsterfullerene (C_{60}) to be expressed in terms of four force constants, where a 180×180 matrix is diagonalized to yield the complete vibrational spectrum.

B. Spectroscopy

A comprehensive treatment of classical decay rates for a molecule in the vicinity of a spherical metallic surface has been carried out, where results have been obtained for both radiative and nonradiative transfer when the molecule is located outside or inside the surface.

C. Reactions

Using a tight-binding calculation to determine the geometry and charge distribution of Si_n^+ for n ranging from 30 to 45, a hypothesis has been verified that large silicon clusters are arranged in a cylindrical shape as stacked quasigraphite rings, which seems to explain the experimental observation of periodic variations in reactivity of Si_n with NH_3 and CH_3OH as n is varied.

II. Infrared-Laser-Excited Adspecies

A. Energy and Phase Relaxation

- The Born and Markov approximations for phonon relaxation and coherent excitation of adsorbed species have been shown to be invalid for CO adsorbed on Ni or Cu (a strongly-bound physisorbed system) but valid for the weakly-bound system of Ar on W.
- A master equation approach which includes electron-hole excitations in the substrate reveals that the probability of finding a laser-driven adsorbed CO molecule on a Cu surface in its first excited vibrational state is 0.03, which is encouraging for experiments on laser-stimulated surface reactions involving CO.
- The vibrational dephasing rate for OH on SiO_2 has been found to be considerably faster than the energy relaxation rate, and the calculated value of 4 ps for the dephasing relaxation time (corresponding to a linewidth of 1.3 cm^{-1}) is in good agreement with experiments.

B. Desorption

A master equation approach shows that a pulsed laser does not lead to a dramatic increase in the rate of desorption, and in the high-intensity limit, resonant heating and desorption reach the same saturation limit for a pulsed laser and for a continuous-wave laser.

III. Ultraviolet-Laser-Induced Chemical Vapor Deposition

Using the Rayleigh hypothesis and determining all components of the electromagnetic field (incident laser, reflected field, image field and surface plasmon field), the dynamics of periodic structured growth of Cd on Si, resulting from photolysis of gaseous $\text{Cd}(\text{CH}_3)_2$, has been calculated in order to explain experimental results.

IV. Resonance Fluorescence at Flat Surfaces

A rigorous quantum theory of atomic resonance fluorescence near a flat metallic surface has been derived which allows for polarization-dependent detection involving specific transitions between degenerate substrates.

V. Photochemistry at Structured Surfaces

A. Gratings

The photodissociation of I_2 above a Ag grating surface has been calculated semiclassically, where there is an optimal distance of the molecule from the surface at which dissociation is a maximum. The reason for this is that the enhancement due to the surface plasmon field as the molecule is brought closer to the surface is offset by a diminution due to line-broadening effects.

B. Thin Films

Due to cross-coupling into long- and short-range surface plasmons and the different coupling nature between radiations from an incident laser and from the molecular dipole to a corrugated thin metallic film substrate, it has been shown that enhanced photoabsorption may be achieved through control of the various film parameters.

VI. Phase-Conjugated Surfaces

An atom near a phase conjugator behaves quite differently than an atom in empty space or in the vicinity of an ordinary (linear) surface, and it is shown with nonlinear optics that an atom in its ground state can fluoresce if it is sufficiently close to a phase conjugator. This

phenomenon opens the door to new and novel types of surface spectroscopy.

VII. Laser-Induced Reactions in Solid Matrices

To describe recent experiments on laser-induced chemical reactions in HCl - and Cl_2 -doped xenon solid, a semiempirical approach called the diatomics-in-ionic systems (DIIS) method has been developed which accounts for the coupling between ionic and neutral species and charge delocalization among host rare-gas atoms. Calculations have been carried out by treating 66 Xe matrix atoms via pairwise interactions, including polarization, with the remaining part of the matrix treated as a continuum, and it has been shown that the positive charge in the ionic activated complex is distributed most often between several Xe atoms forming, in general, a $\text{Xe}_{12}^+\text{Cl}^-$ molecule. A theoretical prediction of the excitation spectrum of Xe_{12}Cl has been confirmed experimentally (after annealing, such that Cl is at a substitutional site).

VIII. Nonlinear Optical Process in Polymeric Systems

The transient behavior of the nonlinear optical susceptibility of polydiacetylene induced by an ultrafast pump field is investigated. Spectral hole burning, optical nutation and optical bistability are observed theoretically.

IX. Molecular Dynamics Simulations

A semiclassical wavepacket method has been developed for studying the dynamics of various nonequilibrium statistical processes in condensed phases. The development is based on the construction of a Gaussian density matrix satisfying the maximum entropy principle.

Research Personnel

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Dr. Henk F. Arnoldus	Villanova University
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Dr. Peter Leung	Portland State University
Dr. Devaraj Sahu	Computer Sciences Corporation, Maryland
Dr. Sander van Smaalen	University of Groningen, The Netherlands

Publications

Each manuscript listed below corresponds by number to the Technical Report previously submitted to the Office of Naval Research for Contract N00014-86-K-0043. The major portion of these are refereed journal articles, and the remainder are invited book chapters and conference proceedings.

1. D. Agassi and T. F. George, "Surface Plasmon Dispersion Relation and Local Field Enhancement Distribution for a Deep Sinusoidal Grating," *Surf. Sci.* 172, 230-56 (1986).
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