



Annual Report 2000

Theory, Modeling, and Simulation

September 2001

**Pacific Northwest
National Laboratory**

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Cover Photo: $C^\alpha-H\cdots O=C$ hydrogen bonds in the β -sheet formed by the protein called *Achromobacter protease I*. Numbers indicate estimated distances (in angstroms) between the hydrogen atoms (white) and oxygen atoms (red). Carbon atoms are shown in gray and nitrogen atoms in blue. High-level *ab initio* calculations provide a lower limit of -2.1 kcal/mol for the $C^\alpha-H\cdots O=C$ hydrogen bond. The magnitude of this interaction, roughly one-half the strength of the $N-H\cdots O=C$ hydrogen bond, suggests that $C^\alpha-H\cdots O=C$ hydrogen bonding may represent a hitherto unrecognized contribution to protein conformation.

This collaborative research effort among scientists in the Theory, Modeling, and Simulation (TM&S) directorate and the Universidad Autónoma Metropolitana - Iztapalapa exemplifies the effective use of high performance computers in developing accurate force field parameters to provide a more quantitative understanding of complex biological systems. The TM&S directorate also operates the Molecular Science Computing Facility (MSCF), a national user resource, in support of environmental molecular research projects.

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Annual Report 2000

**Theory, Modeling,
and Simulation**

D. A. Dixon, Associate Director
and the Staff of the Theory, Modeling,
and Simulation Program

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Contents

1. Introduction

Theory, Modeling, and Simulation
Program..... 1-3

2. Applied Mathematics Group

Hybrid Multiscale Full-Physics Solvers
*J. B. Jones-Oliveira and
J. S. Oliveira*..... 2-2

NWGrid and NWPhys – NorthWest Grid
Generation and Physics Codes
*H. E. Trease, L. L. Trease, and
J. Nieplocha*..... 2-5

NWPhys Parallel Computing
Performance
*H. E. Trease, J. Nieplocha, and
L. L. Trease*..... 2-7

Virtual Lung Project
*R. Corley, D. A. Dixon, C. Timchalk,
H. E. Trease, K. R. Minard,
L. L. Trease, J. Kimbell, and
J. D. Fowler*..... 2-9

Virtual Cell Project
*H. E. Trease, J. H. Miller, D. A. Dixon,
L. L. Trease, A. D. Rasmussen,
J. Shiff, and J. D. Fowler*..... 2-10

Virtual Fish Project
*M. C. Richmond, H. E. Trease, C. L.
Rakowski, L. L. Trease, C. B. Cook,
and J. D. Fowler*..... 2-11

Reconnection for the Free-Lagrange
Method
*H. E. Trease, D. Fraser, B. Hotchkiss,
and M. Sahota*..... 2-13

Mathematical Modeling of Molecular
Surfaces Using Unstructured Mesh
Techniques
*J. B. Jones-Oliveira, J. S. Oliveira,
G. K. Schenter, and H. E. Trease* 2-14

Invariant Discretization Methods for
n-Dimensional Nonlinear Reactive
Transport Models
*J. S. Oliveira, H. E. Trease,
J. M. Malard, and C. G. Bailey*..... 2-16

Algebraic-Combinatorial Models of
Emerging Biochemical Reaction
Pathways for Cell Signaling
*J. S. Oliveira, J. B. Jones-Oliveira,
and C. G. Bailey*..... 2-20

Algorithm for Analysis of Tandem Mass
Spectrometry Data
W. R. Cannon 2-24

DNA Replication
W. R. Cannon 2-25

Radical SAM: Data Mining of the
Protein Databases with New
Bioinformatics Approaches
*H. J. Sofia, G. Chen, B. G. Hetzler,
J. F. Reyes-Spindola, and N. E. Miller*.... 2-26

First-Order System Least-Squares Finite-
Element Solution of the Material Form of
Maxwell's Equations
A. A. El-Azab..... 2-28

Lattice Boltzmann Algorithm for
Simulating Thermal Two-Phase Flow
B. J. Palmer and D. A. Rector..... 2-30

Classification and Computational
Solution Methods for Nonlinear
Hyperbolic Stochastic PDEs
K. D. Jarman..... 2-31

3. Extensible Computational Chemistry Environment

Extensible Computational Chemistry
Environment
*G. D. Black, J. M. Chase, D. K. Gracio,
E. R. Jurrus, D. J. Nordwall, B. J. Palmer,
K. L. Schuchardt, E. G. Stephan, and
E. R. Vorpagel*..... 3-1

Extensible Computational Chemistry Environment New Development <i>G. D. Black, D. K. Gracio, E. R. Jurrus, D. J. Nordwall, B. J. Palmer, K. L. Schuchardt, E. G. Stephan, and E. R. Vorpagel</i>	3-3	Contaminant-Organic Complexes, Their Structure and Energetics in Surface Decontamination Processes <i>B. P. Hay, D. A. Dixon, C. C. Ainsworth, K. N. Raymond, J. Garza, and R. Vargas</i>	4-5
Extensible Computational Chemistry Environment Data Management Development <i>E. G. Stephan, G. D. Black, J. M. Chase, C. S. Lansing, B. J. Palmer, and K. L. Schuchardt</i>	3-6	Study of C-H...O Hydrogen Bonds in N,N'-Dimethylformamide Dimers.....	4-7
Extensible Computational Chemistry Environment Molecular Dynamics Development <i>B. J. Palmer, G. D. Black, E. R. Jurrus, and K. L. Schuchardt</i>	3-10	Conformational Analysis of N, N, N', N'- Tetramethylsuccinamide.....	4-8
4. Computational Structure and Reactivity Group		HostBuilder: A Tool for the Combinatorial Generation of Host Molecules <i>B. P. Hay and J. B. Nichola</i>	4-8
Computational Thermochemistry	4-1	Computational Materials Design	4-9
Predicting the Heats of Formation of Model Hydrocarbons up to Benzene <i>D. F. Feller and D. A. Dixon</i>	4-2	Isomerization of Fluorophors on a Treated Silicon Surface <i>J. L. Gole and D. A. Dixon</i>	4-9
Evidence for a Lower Enthalpy of Formation of Hydroxyl Radical and a Lower Gas-Phase Bond Dissociation Energy of Water <i>B. Ruscic, D. F. Feller, D. A. Dixon, K. A. Peterson, L. B. Harding, R. L. Asher, and A. F. Wagner</i>	4-2	Theoretical Calculation of Photoabsorp- tion of Various Polymers in the Extreme Ultraviolet Region <i>N. N. Matsuzawa, H. Oizumi, S. Mori, S. Irie, S. Shirayone, E. Yano, S. Okazaki, A. Ishitani, and D. A. Dixon</i>	4-11
The Molecular Structures and Energetics of Cl ₂ CO, ClCO, Br ₂ CO, and BrCO <i>D. A. Dixon, K. A. Peterson, and J. S. Francisco</i>	4-3	Time-Dependent Density Functional Theory Calculations of Photoabsorption Spectra in the Vacuum Ultraviolet Region <i>N. N. Matsuzawa, A. Ishitani, D. A. Dixon, and T. Uda</i>	4-12
The Molecular Structure and Ionization Potential of Si ₂ : The Role of the Excited States in the Photoionization of Si ₂ <i>D. A. Dixon, D. Feller, K. A. Peterson, and J. L. Gole</i>	4-4	Computational Inorganic Chemistry.....	4-13
Ligand Design.....	4-5	Tetrachloro- and Tetrabromoarsonium(V) Cations: Raman and ⁷⁵ As, ¹⁹ F NMR Spectroscopic Characterization and X-ray Crystal Structures of [AsCl ₄][As(OTeF ₅) ₆] and [AsBr ₄][AsF(OTeF ₅) ₅] <i>M. Gerken, P. Kolb, A. Wegner, H.P.A. Mercier, H. Borrmann, D. A. Dixon, and G. J. Schrobilgen</i>	4-13

<p>Syntheses and Structures of TcOF₅ and the Tc₂O₂F₉⁺ Cation and the Formation of the TcOF₄⁺ Cation in Solution <i>N. LeBlond, H.P.A. Mercier, D. A. Dixon, and G. J. Schrobilgen</i> 4-14</p>	<p>Periodic Density Functional LDA and GGA Study of CO Adsorption at the (001) surface of MgO <i>J. A. Snyder, D. R. Alfonso, J. E. Jaffe, Z. Lin, A. C. Hess, and M. Gutowski</i> 4-22</p>
<p>Fluoride-Ion Donor Properties of TcO₂F₃ and ReO₂F₃: the X-Ray Crystal Structures of MO₂F₃×SbF₅ (M = Tc, Re) and TcO₂F₃×XeO₂F₂, and the Raman and NMR Spectroscopic Characterization of MO₂F₃×PnF₅ (Pn = As, Sb), [ReO₂F₂(CH₃CN)₂][SbF₆] and [Re₂O₄F₅][Sb₂F₁₁] <i>D. A. Dixon, N. LeBlond, and G. J. Schrobilgen</i> 4-17</p>	<p>Opposite Rumpling of the MgO and CaO (100) Surfaces: an All-Electron Density Functional Theory Study <i>D. R. Alfonso, J. A. Snyder, J. E. Jaffe, A. C. Hess, and M. Gutowski</i>..... 4-23</p>
<p>[Xe₂F₃][AsF₆] and a Density Functional Theory Study of the Xe₂F₃⁺ Cation <i>B. A. Fir, M. Gerken, B. E. Pointner, H.P.A. Mercier, D. A. Dixon, and G. J. Schrobilgen</i> 4-17</p>	<p>LDA and GGA Calculations for High-Pressure Phase Transitions in ZnO and MgO <i>J. E. Jaffe, J. A. Snyder, Z. Lin, and A. C. Hess</i> 4-23</p>
<p>Development of New Density Functional Theory Approaches 4-19</p>	<p>High-Coverage Adsorption of Alkali Metals at the CaO and MgO (100) Surfaces <i>D. R. Alfonso, J. E. Jaffe, A. C. Hess, and M. Gutowski</i> 4-23</p>
<p>The Role of the Local-Multiplicative Kohn-Sham Potential on the Description of Occupied and Unoccupied Orbitals <i>J. Garza, J. A. Nichols, and D. A. Dixon</i> 4-19</p>	<p>Formation of the c(1x1) Cu Monolayer on CaO(100): A Theoretical Study <i>D. R. Alfonso, J. E. Jaffe, A. C. Hess, and M. Gutowski</i> 4-24</p>
<p>Orbital Energy Analysis with Respect to LDA and Self-Interaction Corrected Exchange-only Potentials <i>J. Garza, R. Vargas, J. A. Nichols, and D. A. Dixon</i> 4-20</p>	<p>Negative Ion Chemistry 4-24</p>
<p>Computational Surface Science/Solid State Chemistry 4-21</p>	<p>The Importance of Exchange Effects in Three-Body Interactions: The Lowest Quartet State of Na₃ <i>J. Higgins, T. Hollebeek, J. Reho, T.-S. Ho, K. K. Lehmann, H. Rabitz, G. Scoles, and M. Gutowski</i> 4-25</p>
<p>First-Principles Studies of Adsorption of CO on Na Surface <i>D. R. Alfonso, J. A. Snyder, J. E. Jaffe, A. C. Hess, and M. Gutowski</i> 4-21</p>	<p>(MgO)_n⁻ (n=1-5) Clusters: Multipole-Bound Anions and Photodetachment Spectroscopy <i>M. Gutowski, P. Skurski, X. Li, and L. S. Wang</i> 4-25</p>
<p>Comparison of Embedded-Atom Models and First-Principles Calculations for Al Phase Equilibrium <i>J. E. Jaffe, R. J. Kurtz, and M. Gutowski</i> 4-22</p>	<p>Bi-Dipole-Bound Anions <i>M. Gutowski, P. Skurski, and J. Simons</i> 4-26</p>

Dipole-Bound Anions of Glycine Based on the Zwitterion and Neutral Structures <i>M. Gutowski, P. Skurski, and J. Simons</i>	4-26	Coupled-Cluster Methods <i>J. van Lenthe, D. E. Bernholdt, J. A. Nichols, and R. J. Harrison</i>	5-4
Excited Electronic States of the Anion of 7,7,8,8-tetracyanoquinodimethane (TCNQ) <i>P. Skurski and M. Gutowski</i>	4-26	Accurate Numerical Grids for Density-Functional Calculations of Large Systems <i>E. Aprà and J. Nichols</i>	5-4
How to Choose a One-Electron Basis Set to Reliably Describe a Dipole-Bound Anion <i>P. Skurski, M. Gutowski, and J. Simons</i>	4-27	The Rys Quadrature Revisited: A Novel Formulation for the Efficient Computation of Electron Repulsion Integrals Over Gaussian Functions <i>M. Dupuis and A. Marquez</i>	5-6
An <i>Ab Initio</i> Study of $(\text{H}_3\text{B} \leftarrow \text{NH}_3)^-$ a Dipole-Bound Anion Supported by the Dative Charge Transfer Bond in the Neutral Host <i>R. Barrios, P. Skurski, J. Rak, and M. Gutowski</i>	4-27	Implementation of the Conductor-like Screening Model (COSMO) Solvation Model in NWChem <i>M. Dupuis</i>	5-7
Computational Biology	4-27	Analytic HF and DFT Second Derivatives <i>B. G. Johnson and T. L. Windus</i>	5-7
Cellular Signal Regulation by Endocytic Trafficking	4-27	Parallel Douglas-Kroll Energy and Gradients in NWChem, and the Development of Douglas-Kroll Contracted Basis Sets. <i>W. A. de Jong and R. J. Harrison</i>	5-8
The Epidermal Growth Factor Receptor System	4-28	Capabilities Added to the PSPW Module in NWChem <i>E. J. Bylaska</i>	5-8
Molecular Dynamics Simulation of the RasGTP:RasGAP Complex <i>J. H. Miller, T. P. Straatsma, and H. Resat</i>	4-29	Relativistic Methods Development for Actinides <i>K. Dyllal</i>	5-10
Dosimetry Calculations for Single-Cell Irradiation by Electrons <i>J. H. Miller, H. E. Trease, and W. E. Wilson</i>	4-31	Fast Numerical Methods for All-Electron Calculations <i>R. J. Harrison and G. I. Fann</i>	5-10
5. High-Performance Computational Chemistry		NWChem 4.0.1 Infrastructure Updates	5-10
High-Performance Computational Chemistry Group.....	5-1	Windows NT Port of NWChem <i>B. G. Johnson</i>	5-10
NWChem New Algorithms and Methods Developments	5-4	Improved Distribution and Support of NWChem <i>T. Windus, R. Wattenburger, and J. Nichols</i>	5-12
		Investigations of Actinide Systems.....	5-12

Density Functional Study of Uranyl Hydration: Structures and Binding Energies <i>T. L. Windus and Z. Zhang</i>	5-12	Gaussian Basis Sets for Use in Correlated Molecular Calculations: IX. The Atoms Aluminum through Argon Revisited <i>T. H. Dunning Jr., K. A. Peterson, and A. K. Wilson</i>	6-3
Density Functional Study of the Excited States of Aqua Anion UO_2^{2+} Complexes <i>Z. Zhang and R. J. Harrison</i>	5-13	Cooperativity and Hydrogen Bonding Network in Water Clusters <i>S. S. Xantheas</i>	6-3
Spin-Orbit CI Calculation of the Low Lying Excited States of UO Spectra <i>Z. Zhang and R. J. Harrison</i>	5-13	Spectroscopic Observation of Ion-Induced Water Dimer Dissociation in the $\text{X}(\text{H}_2\text{O})_2$ ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$) Clusters <i>P. Ayotte, S. B. Nielsen, G. H. Weddle, M. A. Johnson, and S. S. Xantheas</i>	6-7
Density Functional Study of UF_6 Hydrolysis <i>Z. Zhang and R. J. Harrison</i>	5-13	Quantum Statistical Mechanics of Ion-Water Vibrational Dynamics <i>G. K. Schenter, B. C. Garrett, and G. A. Voth</i>	6-8
Testing/Benchmarking of New Capabilities	5-13	A First Principles Study of the Acetylene-Water Interaction <i>D. Tzeli, A. Mavridis, and S. S. Xantheas</i>	6-9
Benchmark of Molecular DFT Calculations on Massively Parallel Machines <i>E. Aprà</i>	5-13	Rotationally Resolved Spectroscopy of a Librational Fundamental Band of Hydrogen Fluoride Tetramer <i>T. A. Blake, S. W. Sharpe, and S. S. Xantheas</i>	6-11
Additional Application Problems.....	5-15	Binding Affinities of Benzene for the Alkali Cations <i>D. Feller, D. A. Dixon, and J. B. Nicholas</i>	6-13
Modeling of the Rough LPS Membrane of <i>Pseudomonas aeruginosa</i> <i>T. P. Straatsma and R. D. Lins</i>	5-15	Binding Enthalpies for Alkali Cation-benzene Complexes <i>D. F. Feller, D. A. Dixon, and J. B. Nicholas</i>	6-14
Modeling the Structural Dynamics of the $\text{p}21^{\text{RAS}}$ Molecular Switch II <i>T. P. Straatsma, T. A. Soares, and J. H. Miller</i>	5-18	Novel Binding Modes in Tetramethoxycalix[4]arene and Its Implication for Ligand Design <i>B. P. Hay, J. B. Nicholas, and D. Feller</i>	6-15
Multiwavelet Methods for Viscous Flow Simulations <i>G. I. Fann and G. Beylkin</i>	5-22		
6. Molecular Theory and Modeling Group			
Approximating the Basis Set Dependence of Coupled Cluster Calculations: Evaluation of Perturbation Theory Approximations for Molecules <i>T. H. Dunning Jr. and K. A. Peterson</i>	6-1		

Solvation Effects Upon Reactions of OH⁻ with Chlorinated Hydrocarbons
E. E. Arcia, Y. A. Borisov, M. Dupuis, and B. C. Garrett..... 6-16

Proton Transfer in Polar Solution. Variational Transition State Theory Evaluation of the Rate Constant
R. P. McRae, G. K. Schenter, B. C. Garrett, S. Hammes-Schiffer, and D. G. Truhlar..... 6-19

The Role of Collective Solvent Coordinates and Nonequilibrium Solvation in Charge Transfer Reactions
G. K. Schenter, B. C. Garrett, and D. G. Truhlar..... 6-21

Water/Graphite Interactions
D. Feller and K. D. Jordan..... 6-22

A Mechanism for Ion Transport Across the Water/Dichloromethane Interface: A Molecular Dynamics Study Using Polarizable Potential Models
L. X. Dang 6-23

Molecular Dynamics Study of Benzene – Benzene and Benzene-Potassium Ion Interactions Using Polarizable Potential Models
L. X. Dang 6-26

Electrostatic Potential of Ion Transport Across Interfaces
G. K. Schenter, K. Wu, M. J. Iedema, and J. P. Cowin 6-31

Mechanisms of Atomic Clustering in Alkali Silicate Glasses
B. Park and L. R. Corrales..... 6-32

Threshold Displacements in Zircon
B. Park, W. J. Weber, and L. R. Corrales 6-34

Excitons in Silica
R. M. VanGinhoven, J. Song, H. Jónsson, and L. R. Corrales 6-35

An Accurate Global *Ab Initio* Potential Energy Surface for the X¹A' Electronic State of HOBr
K. A. Peterson 6-36

Thermal Rate Constant Calculations for Radical Reactions Involving OH + Ethylene, Butadiene, and Isoprene
S. M. Kathmann, M. Dupuis, and B. C. Garrett..... 6-38

Dynamical Nucleation Theory: Sensitivity Analysis of Nucleation Kinetics
S. M. Kathmann, G. K. Schenter, and B. C. Garrett..... 6-39

Dynamics of Water Condensation and Evaporation
G. K. Schenter, S. M. Kathmann, and B. C. Garrett..... 6-40

7. Molecular Science Computing Facility

MSCF Resources 7-1

MSCF Organization and Staff 7-2

MSCF Use 7-3

User Computing in the MSCF 7-3

A Computational Approach to Understanding Oxidant Chemistry and Aerosol Formation in the Troposphere
B. C. Garrett, M. Dupuis, D. A. Dixon, L. X. Dang, S. M. Kathmann, G. K. Schenter, S. S. Xantheas, J. S. Francisco, J. T. Hynes, A. Morita, R. Bianco, B. Gertner, T. J. Lee, K. A. Peterson, and J. H. Seinfeld 7-6

Dynamical Nucleation Theory 7-6

Theory of Sum Frequency Generation (SFG) Spectroscopy for Surfaces Important for Heterogeneous Reactions of Atmospheric Significance..... 7-8

<p>List of Significant Methods/Routines or Codes Developed 7-8</p> <p>Computational Thermochemistry and Benchmarking of Reliable Method <i>D. Feller, D. A. Dixon, T. H. Dunning Jr., M. Dupuis, D. McClemore, K. A. Peterson, S. Xantheas, D. E. Bernholdt, T. Windus, G. Chalasinski, R. Fosada, J. Olguim, K. Dobbs, D. Frurip, W. J. Stevens, N. Rondan, J. Chase, and J. Nichols</i> 7-9</p> <p>The Binding Energy of Water to Single-Layer Graphite 7-10</p> <p>Heats of Formation of Furan, Tetrahydrofuran (THF) and Several THF-Derived Radicals 7-10</p> <p>Binding Enthalpies of the Alkali Cations to Benzene 7-11</p> <p>Binding Enthalpies of the Alkali Cations to 15-crown-5 7-11</p> <p>Study of C-H...O Hydrogen Bonds in N,N'-Dimethylformamide Dimers 7-12</p> <p>Conformational Analysis of N, N, N', N'-Tetramethylsuccinamide 7-12</p> <p><i>Ab Initio</i> Study of Rotational Barriers in N-Methylbenzamide and Benzylamide Systems 7-12</p> <p>Stretching and Torsional Potential Energy Surfaces of [Fe(III)(catecholate)₃]³⁻ 7-13</p> <p>A Database of Alkane Structural Information Based on Density Functional Theory 7-13</p> <p>Isodesmic Reactions for Thermochemistry 7-13</p> <p>Accurate Determination of the Binding Energies of the First Few Water Clusters 7-14</p>	<p>Computational Chemistry for Nuclear Waste Characterization and Processing: Relativistic Quantum Chemistry of Actinide <i>R. J. Harrison, J. A. Nichols, R. A. Kendall, D. A. Dixon, T. L. Windus, W. A. de Jong, Z. Zhang, J. Nieplocha, G. I. Fann, R. L. Shepard, J. L. Tilson, A. F. Wagner, R. Stevens, M. Minkoff, A. T. Wong, P. J. Hay, R. L. Martin, L. R. Pratt, G. Schreckenbach, W. Ermler, K. Dyllal, R. Pitzer, B. E. Bursten, J. Li, D. Bernholdt, C. Marsden, and N Ismail-Büchner</i> 7-15</p> <p>Douglas-Kroll in NWChem: Parallel Energy and Gradient Calculations, and Douglas-Kroll Contracted Basis Sets <i>W. A. de Jong and R. J. Harrison</i> 7-15</p> <p>Relativistic Calculations on the Electric Field Gradients and NMR Chemical Shifts of Uranyl Carbonate Complexes <i>W. A. de Jong, H. H. Cho, and G. Schreckenbach</i> 7-15</p> <p>Accurate <i>Ab Initio</i> Calculation of the Ground State ²P_{1/2}-²P_{3/2} Spin-Orbit Splitting in SiF <i>W. A. de Jong, Z. Zhang, and R. J. Harrison</i> 7-16</p> <p>Relativistic Calculations on the Potential Energy Curves of the Cl₂ Molecule <i>W. A. de Jong, S. Xantheas and T. N. Kitsopoulos</i> 7-17</p> <p>The Structure of AnX₂²⁺ Ions (An = U, Pu and X = S, Se, Te) Valence-Isoelectronic with AnO₂²⁺ and the Nature of Actinyl-Phosphate Binding <i>W. A. de Jong, N. Ismail-Büchner, and C. Marsden</i> 7-17</p>
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<p>Parallelization of the MOLFDIR Program Package <i>W. A. de Jong, M. Pernpointer, and L. Visscher</i> 7-17</p>	<p>Structure and Spectra of UO_2F_2 <i>Q. Wang and R. M. Pitzer</i> 7-22</p>
<p>Spin-Orbit DFT in NWChem <i>Z. Zhang</i>..... 7-18</p>	<p>“Fast” Methods of Correlated Calculations: A Study of the RI-MP2 Approach Applied to Tetramethoxycalix[4]arene <i>D. E. Bernholdt, J. B. Nicholas, and B. P. Hay</i> 7-23</p>
<p>Density Functional Study of the Ground States of Aqua Anion UO_2^{2+} Complexes <i>Z. Zhang</i>..... 7-18</p>	<p>List of Significant Methods/Routines or Codes Developed 7-24</p>
<p>Density Functional Study of the Excited States of Aqua Anion UO_2^{2+} Complexes <i>Z. Zhang</i>..... 7-18</p>	<p>Mechanistic Process Modeling for Subsurface Remediation <i>G. I. Fann, J. Malard, D. R. Rector, H. Trease, B. D. Wood, S. Yabusaki, G. P. Flach, J. P. Holland, R. S. Maier, K. E. Jordan, S. L. Bryant, M. F. Wheeler, A. F. B. Tompson, W. E. Soll, S. Chen, and W. G. Gray</i> 7-24</p>
<p>Spin-Orbit Density Functional Study of Actinyls <i>Z. Zhang</i>..... 7-19</p>	<p>Significant Methods/Routines or Codes Developed 7-32</p>
<p><i>Ab Initio</i> Study of the Low-Lying Electronic States of UO <i>Z. Zhang</i>..... 7-19</p>	<p>Chemical Fate of Contaminants in the Environment Chlorinated Hydrocarbons in the Groundwater <i>B. C. Garrett, T. H. Dunning Jr., M. Dupuis, E. E. Arcia, T. P. Straatsma, D. G. Truhlar, J. Thompson, C. J. Cramer, J. Gao, K. Morokuma, W. J. Stevens, and Y. A. Borisov</i>..... 7-33</p>
<p>Relativistic DFT Studies of Organoactinide Complexes <i>J. Li and B. E. Bursten</i>..... 7-19</p>	<p>Metal Oxides in the Environment <i>H. Jonsson, L. René Corrales, J. F. Haw, R. R. Irani, J. B. Nicholas, K. Tsemekhman, M. Neurock, Shluger, J. Song, P. Gabriel, R. van Ginhoven, and G. Henkelman, 7-40</i></p>
<p>Calculations of the Vibrational Frequencies and Intensities of Laser-Abated Products of Th+CO 7-20</p>	<p>List of Significant Methods/Routines or Codes Developed 7-40</p>
<p>Calculations of the Vibrational Frequencies and Intensities of Laser-Abated Products of Th/U+CO₂ 7-20</p>	<p>Computational Studies of the Self-Trapped Exciton in Silica <i>H. Jonsson, L. R. Corrales, J. Song, R. M. Van Ginhoven, and K. Tsemekhman</i> 7-40</p>
<p>Matrix Effects to the Ground-State Reversal of CUO..... 7-21</p>	
<p>Geometries and Electronic Structures of An(OR)₄ (An = Th-Am; R = H, Me, Ph) 7-21</p>	
<p>Development of Relativistic Basis Sets and Relativistic Approximations <i>K. Dyall</i> 7-21</p>	
<p>Molecular Structure, Spin-Orbit Coupling, and Other Relativistic Effects With Applications to Electronic States of RuO, EuO₂₂⁺, and AmO₂₂⁺ <i>W. C. Ermler and J. W. Pan</i> 7-22</p>	

The STE in Quartz-Like Clusters: Wave Function Based <i>Ab Initio</i> Calculations.....	7-41	The Electrostatic Potential and Molecular Dynamics of Bacterial S-Form LPS from <i>Salmonella Typhimurium</i> <i>T. P. Straatsma and R. D. Lins</i>	7-53
STE States at a Crystalline Surface.....	7-44	Molecular Dynamics of the Outer Membrane of <i>Pseudomonas Aeruginosa</i> <i>T. P. Straatsma and R. D. Lins</i>	7-54
Solid Metal Oxide Acids and Green Chemistry.....	7-45	Aqueous Hydrolysis Reactions.....	7-55
Methanol-to-Gasoline (MTG) Chemistry in ZSM-5.....	7-45	Trivalent Ion Hydrolysis Reactions: A Linear Free-Energy Relationship Based on Density Functional Electronic Structure Calculations <i>J. R. Rustad, D. A. Dixon, K. M. Rosso, and A. R. Felmy</i>	7-55
Acid-Base Reactions on ZSM-5.....	7-46	Understanding the Formation of Polymerized Species Under Extreme Conditions <i>J. R. Rustad, D. A. Dixon, and A. R. Felmy</i>	7-55
Deprotonation Energies for Chabazite.....	7-48	Environmental Redox Chemistry.....	7-57
Adsorption Properties and Acidity of Sulfated Zirconia.....	7-48	The Free Energies of Reactions of Chlorinated Methanes with Aqueous Chlorinated Methanes with Aqueous Monovalent Anions: Application of <i>Ab Initio</i> Electronic Structure Theory <i>E. J. Bylaska, D. A. Dixon, and A. R. Felmy</i>	7-57
Methane to Olefin (MTO) Chemistry on HSAPO-34.....	7-49	Implementing Free-Space Boundary Conditions Into Plane-Wave Methods <i>E. J. Bylaska, J. R. Rustad, R. Kawai, and J. H. Weare</i>	7-57
Biomolecular Interfaces: Simulation of Sedimentation of Biomolecular Assemblies <i>B. M. Pettitt, S. S. Akhtar, B. W. Beck, G. C. Lynch, T. C. Rogala, and K. Wong</i>	7-49	Mixed Hamiltonian (PW/MM) Methods for Geochemical Electronic Structure Studies <i>E. J. Bylaska, J. R. Rustad, and M. Dupuis</i>	7-59
Multiscale Computations of Biological and Non-Biological Assemblies <i>S. S. Akhtar, B. W. Beck, G. C. Lynch, T. C. Rogala, K. Wong, and B. M. Pettitt</i>	7-49	Parallel Projector Augmented-Wave Code <i>E. J. Bylaska, M. Valiev, and J. H. Weare</i>	7-60
Computational Studies in Molecular Geochemistry and Biogeochemistry <i>A. R. Felmy, J. Rustad, D. Dixon, M. Dupuis, T. P. Straatsma, K. M. Rosso, E. Bylaska, G. A. Voth, J. H. Weare, R. Kawai, D. Yuen, W. Halley, and P. E. Smith</i>	7-51		
Microbial Surface Mediated Processes.....	7-52		
Background.....	7-52		
FY 2000 Progress.....	7-53		

Significant Methods/Routines or Codes
Developed 7-60

Parallel Projector Augmented-Wave Code
*E. J. Bylaska, M. Valiev,
and J. H. Weare* 7-60

Implementing Free-Space Boundary
Conditions Into Plane-Wave Methods
*E. J. Bylaska, J. R. Rustad,
R. Kawai, and J. H. Weare* 7-61

Simulation of Climate Forcing by
Aerosols
*S. J. Ghan, G. Fann, R. C. Easter,
X. Bian, R. Zaveri, E. G. Chapman,
S. C. Kothari, and Y. Zhang* 7-61

Overview of the Past Year's
Accomplishments and Activities 7-61

Significant Methods/Routines or Codes
Developed 7-62

First Principles Methods for Predicting
the Chemistry of Environmentally
Relevant Systems
*T. Cagin, G. Wang, W. A. Goddard
III, R. Martin, R. Friesner,
B. Gherman, B. Dunietz, E. Batista,
H. Stern, F. Ritter, G. Kaminski,
M. Diallo, J. H. Johnson,
J-C. Faulon, R. Murphy,
and M. Beachy* 7-62

Overview of Accomplishments 7-62

Catalytic Mechanism of Methane
Monooxygenase 7-62

Polarizable Force Field Development
From *Ab Initio* Quantum Chemistry 7-63

Parameter Development from Quantum
Chemical Calculations 7-63

Development of Polarizable Models for
Pure Liquid Simulations 7-65

Studies of Iron Oxide Surfaces 7-66

Molecular Modeling of Hydrophobic
Organic Contaminants Uptake and
Sequestration by Soil Organic Matter 7-67

Atomistic Models of
Hydrodesulfurization Catalysts over
Co/MoS₂ 7-68

Dendrimers: A New Class of High
Capacity Chelating Agents for Metals
Ions 7-68

Code Development 7-69

Parallelization of Jaguar 7-69

Development of QM/MM Methods 7-69

Development of a Polarizable Force Field
Simulation Code 7-69

8. MSCF Operation Report

MSCF Operation Report 8-1

MSCF Expanded Computer System
Management 8-1

Silver Meta Scheduler
*D. B. Jackson, S. M. Jackson,
G. D. Black, and E. Apra* 8-1

Qbank 2.8
S. M. Jackson 8-4

Maui Scheduler
D. B. Jackson, and S. M. Jackson 8-5

SP-XXL
*S. M. Jackson, J. Nieplocha, J. Mauth,
D. Cowley, J. White, and R. Eades* 8-6

TrackNodes V2
R. Braby and R. Wescott 8-6

Logit
*C. Place, G. Skouson, and
R. Braby* 8-6

Linux Cluster
*S. Jackson, R. Braby, G. Skouson,
 and D. Jackson* 8-7

9. Scientific Consulting Group

Workshops
*Visualization and User
 Services Group* 9-1

Web Page Development
*D. R. Jones, J. C. White, G. Elliott,
 A. K. Lebold, S. W. Matsumoto,
 M. C. Perkins, A. Schur, and
 A. R. Vorpagel* 9-2

Computational Science and Engineering
 Initiative
*D. R. Jones, J. C. White, K. L. Manke,
 A. K. Lebold, M. C. Perkins,
 C. A. Peterson, and N. L. Prince* 9-3

Graphics and Visualization Laboratory
 Research and Development Activities –
 IBM Scalable Graphics Engine for the
 MSCF
D. R. Jones and K. A. Perrine 9-4

SGE/Mesa
D. R. Jones and K. A. Perrine 9-5

SGE MPEG Player
D. R. Jones and K. A. Perrine 9-5

Graphics and Visualization Laboratory
 Video, Animation, and Simulation
 Development 9-5

Oocyte Response to Heat Shock
 Animation
D. R. Jones and K. A. Perrine 9-5

Oocyte Response to Heat Shock
 Animation
D. R. Jones and K. A. Perrine 9-5

Bubble Growth Simulation
B. Palmer and D. Rector 9-6

Simulation of Solid Oxide Fuel
 Cell Start-up
K. Recknagle 9-6

NWGrid/NWPhys Simulations
*H. Trease, L. Trease, J. Kimbell, and
 K. Perrine* 9-6

Membrane Modeling of *Pseudomonas
 Aeruginosa*
*R. D. Lins, T. P. Straatsma, and
 K. Perrine* 9-7

Single-Molecule/Ultrafast Spectroscopy
P. Lu, M. Perkins, and D. R. Jones 9-7

Scaleable Graphics Engine Demonstrations
D. R. Jones and K. A. Perrine 9-7

Spent Nuclear Fuel Project Animation
*M. C. Perkins, K. Perrine,
 and D. R. Jones* 9-8

Ras-Raf Binding Simulation
K. Perrine and D. R. Jones 9-8

PNNL Visualization Demo Video
D. R. Jones and K. A. Perrine 9-8

10. Appendix

Theory, Modeling and Simulation Staff 10-1

Associate Director's Office 10-1

Applied Mathematics Group 10-1

Computational Chemistry
 Environment Group 10-1

Computational Structure and
 Reactivity Group 10-1

High-Performance Computational
 Chemistry Group 10-1

Molecular Theory and Modeling Group 10-1

Molecular Science Computing Facility
 Scientific Consulting 10-1

Molecular Science Computing Facility		Publications and Presentations	10-9
Computer Operations	10-2	Honors and Recognition	10-21
Staff Biosketches	10-2	Collaborations.....	10-22
Postdoctoral Fellows.....	10-7	Workshops/Conferences	10-30
Visiting Scientists	10-8	Acronyms and Abbreviations	10-31
Graduate Students	10-9	Where TM&S Fits in PNNL.....	10-34
Undergraduate Students	10-9		