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13. ABSTRACT *(Maximum 200 words)*

The objective of this work was to develop a broad array of methods for electronic structure theory, with special emphasis on improved parallel codes. A new highly scalable code for frozen core second order perturbation theory (MP2) gradients for closed and open shell molecules has been devel9ped and is on-line for general use at several IBM SP2 and Cray T3E systems. The key element of this approach is our distributed data interface (DDI) that facilitates distribution of very large arrays across all available nodes. This code has been ported tot he cluster environment, so it can now be used on cluster of PCs or Macs running Linux, as well as on clusters of high performance workstations. The development of analogous codes for molecules with unpaired electrons has been completed and is in the most recent GAMESS release. The derivation for the preferred restricted open shell ZAPT method is complete and a paper describing this method has been published. The corresponding code is now in GAMESS. The code for implementing Hartree-Fock with DDI has been completed, and a paper describing this code has been published. We are now turning to analogous developments for MCSCF and CI codes. A scalable code for the multi-reference second order perturbation theory has been completed, a paper published, and the code is in GAMESS. Other important developments include: the derivation of gradients for multi-reference second order perturbation theory, further developments of our effective fragment potential (EFP) method for studying solvation and liquid behavior, the development of molecular dynamics and Monte Carlo methods to facilitate the study of solvation and liquid behavior, the development and implementation of a new method for producing global energy surfaces from (cont. below)

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sets of ab initio points, the development and implementation of both grid-based and gridless approaches to destiny functional theory, and the development and implementation of several MCSCF-based approaches to spin-orbit coupling.

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AFOSR FINAL REPORT

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Design of New Materials Using Computational Chemistry and Materials Science (CHSSI)

AFOSR F49620-02-1-0203

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2. Objectives: **No Change in Objectives**

3. Status of effort: A brief statement of progress towards achieving the research objectives. (Limit to 200 words.)

The objective of this work was to develop a broad array of methods for electronic structure theory, with special emphasis on improved parallel codes. A new highly scalable code for frozen core second order perturbation theory (MP2) gradients for closed and open shell molecules has been developed and is on-line for general use at several IBM SP2 and Cray T3E systems. The key element of this approach is our distributed data interface (DDI) that facilitates distribution of very large arrays across all available nodes. This code has been ported to the cluster environment, so it can now be used on clusters of PCs or Macs running Linux, as well as on clusters of high performance workstations. The development of analogous codes for molecules with unpaired electrons has been completed and is in the most recent GAMESS release. The derivation for the preferred restricted open shell ZAPT method is complete and a paper describing this method has been published. The corresponding code is now in GAMESS. The code for implementing Hartree-Fock with DDI has been completed, and a paper describing this code has been published. We are now turning to analogous developments for MCSCF and CI codes. A scalable code for the multi-reference second order perturbation theory has been completed, a paper published, and the code is in GAMESS. Other important developments include: the derivation of gradients for multi-reference second order perturbation theory, further developments of our effective fragment potential (EFP) method for studying solvation and liquid behavior, the development of molecular dynamics and Monte Carlo methods to facilitate the study of solvation and liquid behavior, the development and implementation of a new method for producing global potential energy surfaces from sets of *ab initio* points, the development and implementation of both grid-based and gridless approaches to density functional theory, and the development and implementation of several MCSCF-based approaches to spin-orbit coupling.

4. Accomplishments/New Findings: Describe research highlights, their significance to the field, their relationship to the original goals, their relevance to the AF's mission, and their potential applications to AF and civilian technology challenges.

The objective of this work is to develop a broad array of methods for electronic structure theory, with special emphasis on improved parallel codes. Progress has been made in many areas.

Parallel Developments. A highly scalable code for frozen core second order perturbation theory gradients for closed shell molecules has been developed and is on-line for general use at several MSRC sites. This new code uses the Distributed Data Interface (DDI) so that the large arrays do not have to be replicated. This means that much larger molecules

can be studied using geometries based on correlated wavefunctions. The code scales very well for as many as 512 nodes and has already been applied to several challenging compounds. The development of analogous codes for molecules with unpaired electrons, using unrestricted wavefunctions, has been completed. The corresponding method for spin restricted wavefunctions has been completed. The unrestricted second order perturbation theory parallel code under DDI has been completed and tested, and a paper on this has been published. A paper on the restricted open-shell derivation has been published, and the development of the parallel code has been completed. A general overview paper on second order perturbation theory derivatives has been published. A paper on a DDI implementation of the SCF method has also been published. Improved parallel MCSCF codes have been completed, and a distributed parallel full CI code has been implemented and a paper published. The multi-reference perturbation theory code (MCQDPT) has now been implemented under DDI. The effective fragment potential (EFP) code has been made scalable under DDI. In an important related development, parallel GAMESS now runs on clusters of PCs and Macs (running Linux) and high end workstations. This is more challenging than self-contained massively parallel computers, since the overhead due to inter-node communications is more complex. This issue has been solved to some extent by using a Gigabit Ethernet switch with large data packets. We are also exploring alternative communications solutions, such as Myrinet, SCI, and Infiniband. These developments and their applications have been enhanced by the construction of a new 32-node, 128-CPU IBM Power3+ cluster using funds provided by a DURIP grant. As for all other GAMESS developments, we will make our experiences in developing scalable clusters available to all users.

Condensed Phase Methods. We have already shown that our effective fragment potential (EFP) method for solvation is excellent for water, in a variety of applications. We are now working on extending the capabilities of the method in several ways. We have developed a new approach for incorporating dispersion, charge transfer and other higher order terms into the method. Such terms are particularly important for nonpolar solvents. The model has been developed in such a way that it is equally applicable and accurate for any solvent. The derivation of an expression for the analytic gradient for the EFP-*ab* initio interaction term is in progress. A very important new development (by co-worker Jan Jensen) is a new method for using EFPs across covalent bonds. This will facilitate the representation of large substituents, as well as the treatment of large biological molecules. We have also interfaced the EFP method with two continuum methods, the simple Onsager reaction field and the more sophisticated polarizable continuum model (PCM).

As the number of solvent molecules in the system increases, the number of configurations to be considered increases rapidly, and traditional small molecule geometry optimization methods are not effective. We are therefore developing both molecular dynamics and Monte Carlo simulation codes so that the configurational space can be probed more effectively, not only for minima, but for transition states and reaction paths as well. This is also an important first step in the development of methods based on the EFP model for predicting bulk properties and super-critical behavior. We are therefore incorporating Ewald summations into our MD method. Related to these dynamical methods is our development and implementation of a method for converting the large numbers of points

generated in *ab initio* trajectories into a global potential energy surface, using a modified Shepard interpolation approach.

Major James Shoemaker's Ph.D dissertation in Engineering Physics at the Air Force Institute of Technology focused on the development and applications of an embedded cluster model for treating surface chemistry. A paper on the theoretical method, called SIMOMM, has been published in the Journal of Physical Chemistry. Several papers applying this method have now been published or submitted, and a manuscript that describes applications to silicon carbide surfaces is in progress. Extensions of this method to transition metal catalysts are planned; however, molecular mechanics is not likely to be a viable approach for the bulk, since electrons in such systems are too delocalized. To overcome this potential problem, we have begun to explore fast multipole methods (FMM) that scale linearly and are also highly parallel, so that the bulk part of the system can be treated by quantum mechanics. One preliminary paper has been published and the first FMM paper has been published. The parallel efficiency of the FMM method has been greatly improved, and gradients have recently been developed and implemented.

Other developments There are many problems that involve species for which one cannot write one simple Lewis structure. Such species must be treated with multi-configurational (MCSCF) wavefunctions. However, the computational demands for MCSCF calculations are very high. So, we have developed a set of methods for converging such wavefunctions that range from very rapid convergence with high CPU and disk requirements to methods that converge more slowly but have very modest computational demands. The advantage of the latter is that much larger molecules than normal can be treated with this method.

For species that must be treated with MCSCF wavefunctions, non-traditional methods are also needed to recover the dynamic correlation. One method that has been implemented into GAMESS is multi-reference second order perturbation theory. The gradient formulas for this method have been derived, and the implementation into GAMESS is in progress.

There are many problems that involve multiple electronic states on multiple potential energy surfaces. Since such surfaces can cross and therefore induce radiationless transitions, it is important to have the capability to predict non-adiabatic coupling among these surfaces. One origin of non-adiabatic interactions among surfaces is spin-orbit coupling. Spin-orbit coupling matrix elements must be calculated using multi-reference wavefunctions, but until recently, there have been no generally available codes for the computation of these matrix elements using all electrons and any arbitrary MCSCF wavefunction for any arbitrary set of spin states. We have now developed and implemented such a method. It will be particularly valuable for the study of high energy density materials and for the study of any processes involving transition metals, since both types of species involve multiple electronic states. Since such all-electron calculations are very demanding, two alternative approaches to this problem have also been develop and implemented into GAMESS for use with larger molecules. One of

these is called the Z_{eff} method, in which the two electron term is ignored and a fitted empirical parameter is introduced into the one-electron part of the Hamiltonian. While this is a very efficient approach, its accuracy is limited. However, there is an intermediate method, in which only those matrix elements connecting orbitals in the active space with each other are neglected. We have shown that in this case excellent agreement with the all electron method is obtained, without any need for fitted parameters. We have also implemented the RESC (relativistic elimination of the small component) method for calculating spin-orbit coupling interactions, complete with analytic gradients.

Density functional theory (DFT) has become extraordinarily popular in recent years, because it has the same computational requirements as Hartree-Fock theory, but often has a level of accuracy that is comparable to second order perturbation theory. We have developed and implemented a gridless approach to DFT, by using the resolution of the identity to evaluate the complicated integrals. This procedure requires the use of auxiliary basis sets to resolve the identity. After extensive analysis of the convergence of several molecular properties as a function of basis set, we have recommended a series of auxiliary basis sets for use with the first row in the periodic table. The next step will be to extend this basis set development to heavier elements. We have also implemented a more traditional grid-based DFT method, including all of the most popular functionals.

Another approach that is very important for large molecules, especially molecules that contain heavier elements, is the effective core potential (ECP) method. This method replaces inner shell electrons by model potentials, making the calculations much more efficient. These potentials include relativistic corrections for the heavier elements. To make these calculations more useful, we have developed much more efficient methods for obtaining the first and second energy derivatives; that is, the gradients and hessians. The increase in speed is a factor of 5-10, and the method has been implemented to take advantage of parallel computers.

As calculations on larger and larger species are made feasible by advances in parallel programs and other innovative algorithms, it becomes increasingly important to develop graphical methods for interpreting the results of complex calculations. This has led to the continuing development of MacMolPlt, a graphical interface for GAMESS. MacMolPlt provides the ability to visualize (and rotate in real time) orbitals, wavefunctions, electron densities and electrostatic potentials in two and three dimensions. We are now in the process of developing a Windows based version of this code.

We have also been exploring alternatives and extensions to the popular G2 and G3 methods developed by Pople and co-workers for the accurate prediction of such theormodynamic properties as heats of formation, ionization potentials and electron affinities. One limitation of these methods is that they are applicable only to species that are adequately described by single configuration wavefunctions. This eliminates many transition metal compounds, diradicals and most transition states. We have therefore initiated, in collaboration with the Radom group, the development of multi-reference analogs of the G2 and G3 methods. The multi-reference methods are based on CASSCF

wavefunctions, instead of Hartree-Fock, followed by multi-reference perturbation theory (instead of MP2) and finally multi-reference CI. The initial paper describing this method has been published.

5. Personnel Supported: List professional personnel (Faculty, Post-Docs, Graduate Students, etc.) supported by and/or associated with the research effort.

Dr. Michael W. Schmidt, Senior Research Associate
Ms. Christine Aikens, graduate student
Mr. Yuri Alexeev, graduate student
Dr. Pradipta Bandyopadhyay, postdoctoral research associate
Dr. Brett Bode, graduate student, postdoctoral research associate
Dr. Galina Chaban, graduate student, postdoctoral research associate
Dr. Cheol Ho Choi, postdoctoral research associate
Mr. Dmitri Fedorov, graduate student
Dr. Graham Fletcher, postdoctoral research associate
Dr. Kurt Glaesemann, graduate student, postdoctoral research associate
Professor Jan Jensen, University of Iowa
Professor Shiro Koseki, Mie University
Dr. Haruyuki Nakano, Tokyo University
Ms. Heather Netzloff, graduate student
Mr. Ryan Olson, graduate student
Dr. Walter Stevens, NIST

6. Publications: Peer-reviewed publications submitted and/or accepted during the 12-month period starting the previous 1 October.

PUBLICATIONS

1. G. Chaban, M.W. Schmidt, and M.S. Gordon, "Approximate Second Order Method for Orbital Optimization of SCF and MCSCF Wavefunctions", Theor. Chem. Accts., 97, 88 (1997).

2. J.H. Jensen and M.S. Gordon, "An Approximate Formula for the Intermolecular Pauli Repulsion Between Closed Shell Molecules. II. Application to the Effective Fragment Potential Method", J. Chem. Phys., 108, 4772 (1998).

3. H. Nakano, K. Hirao and M.S. Gordon, "Analytic Energy Gradients for Multiconfigurational Self-Consistent Field Second-Order Quasidegenerate Perturbation Theory (MC-QDPT)", J. Chem. Phys., 108, 5660 (1998).

4. K.R. Glaesemann and M.S. Gordon, "Investigation of a Grid-Free Density Functional Theory (DFT) Approach", J. Chem. Phys., 108, 9959 (1998).

5. T. Takata, T. Taketsugu, K. Hirao and M. S. Gordon, "*Ab initio* potential energy

surface by modified Shepard interpolation: Application to the $CH_3 + H_2 \rightarrow CH_4 + H$ reaction", J. Chem. Phys., 109, 4281 (1998).

6. . G.N. Merrill and M.S. Gordon, "A Study of Small Water Clusters Using the Effective Fragment Potential (EFP) Method, J. Phys. Chem. A, 102, 2650 (1998).

7. M.S. Gordon, M.W. Schmidt, G.M. Chaban, K. R. Glaesemann, W.J. Stevens, and C. Gonzalez, "A Natural Orbital Diagnostic for Multiconfigurational Character in Correlated Wavefunctions", J. Chem. Phys., 110, 4199 (1999).

8. K.R. Glaesemann and M.S. Gordon, "Evaluation of Gradient Corrections in Grid-Free Density Functional Theory", J. Chem. Phys., 110, 6580 (1999).

9. J. Shoemaker, L.W. Burggraf and M.S. Gordon, "SIMOMM: An Integrated Molecular Orbital/Molecular Mechanics Optimization Scheme for Surfaces", J. Phys. Chem. A, 103, 3245 (1999).

10. . B.M. Bode and M.S. Gordon, "MacMolPlt: A Graphical User Interface for GAMESS", J Molec. Graphics., 16, 133(1999).

11. G.D. Fletcher, M.W Schmidt, and M.S. Gordon, "Developments in Parallel Electronic Structure Theory", Adv. Chem. Physics (invited), 110, 267 (1999).

12. S. Koseki, M.W. Schmidt and M.S. Gordon, "Effective Nuclear Charges for the First- Through Third-Row Transition Metal Elements in Spin-Orbit Calculations, J. Phys. Chem., 102, 10431 (1998).

13. G. Merrill and M.S. Gordon, "On the Question of Empirical Corrections in *Ab Initio* Model Chemistries", J. Chem. Phys., 110, 6154 (1999).

14. C.H. Choi, J. Ivanic, M.S. Gordon, and K. Ruedenberg, "Direct Recurrence Relations for the Rapid and Stable Determination of Rotation Matrices between Spherical Harmonics", J. Chem. Phys., 111, 8825 (1999).

15. D.G. Fedorov, M. Evans, Y. Song, M.S. Gordon and C.Y. Ng, "An Experimental and Theoretical Study of the Spin-orbit Interaction for $CO^+(A^2\prod_{3/2,1/2}, v^+=0\text{-}41)$ and O_2^+ $(X^2\prod_{3/2,1/2}, v^+=0\text{-}38)$", J. Chem. Phys., 111, 6413 (1999).

16. B.M. Bode and M.S. Gordon, "Fast Computation of Analytical Second Derivatives with Effective Core Potentials: Application to Si_8C_{12}, Ge_8C_{12} and Sn_8C_{12}", J. Chem. Phys., 111, 8778 (1999).

17. J. Shoemaker, L.W. Burggraf, and M.S. Gordon, "An Ab Initio Study of the Structure of the Si(100) Surface", J. Chem. Phys., 112, 2994 (2000).

18. D.G. Fedorov and M.S. Gordon, "A Study of the Relative Importance of One and

Two Electron Contributions to Spin-Orbit Coupling", J. Chem. Phys., 112, 5611 (2000).

19. M.W. Schmidt, G.D. Fletcher, B.M. Bode and M.S. Gordon, "The Distributed Data Interface in GAMESS", Computer Physics Communications (INVITED), 128, 190 (2000).

20. M.A. Freitag, M.S. Gordon, J.H. Jensen and W.J. Stevens, "Evaluation of charge penetration between distributed multipolar expansions", J. Chem. Phys., 112, 7300 (2000).

21. Bandyopadhyay and M.S. Gordon, "A Combined Discrete/Continuum Solvation Model: Application to Glycine", J. Chem. Phys., 113, 1104 (2000).

22. K. Yagi, T. Taketsugu, K. Hirao and M.S. Gordon, "Direct Vibrational Self-Consistent Field Method: Applications to H_2O and H_2CO", J. Chem. Phys., 113, 1005 (2000).

23. M. Pak and M.S. Gordon, "Full CI and CASSCF spin density in boron and carbon atoms", J. Chem. Phys., 113, 4238 (2000).

24. M.S. Gordon, J. Shoemaker and L.W. Burggraf, "Reply to 'Comment on "An *ab initio* cluster study of the structure of the Si(100) surface", [J. Chem. Phys., 112, 2994 (2000)]" ', J. Chem. Phys., 113, 9355 (2000).

25. M.S. Gordon, M.A. Freitag, P.Bandyopadhyay, V. Kairys, J.H. Jensen, and W.J. Stevens, "The Effective Fragment Potential Method: A QM-Based MM Approach to Modelling Environmental Effects in Chemistry", J. Phys. Chem. (Feature Article), A105, 293 (2001).

26. C.H. Choi, K. Ruedenberg and M.S. Gordon, "A new parallel optimal-parameter fast multipole method", J. Comp. Chem., 22, 1484 (2001).

28. S. Koseki, D.G. Fedorov, M.W. Schmidt and M.S. Gordon,"Spin-Orbit Splittings in the Third-Row Transition Elements: Comparison of Effective Nuclear Charge and Full Breit-Pauli Calculations", J. Phys. Chem., A105, 8262 (2001).

29. D.G. Fedorov and M.S. Gordon, "Speeding Up Spin-Orbit Calculations", ACS Symposium Series 828, Low-Lying Potential Energy Surfaces, M.R. Hoffmann and K.G. Dyall, Eds., Oxford Press, 2002.

30. G.D. Fletcher, M.S. Gordon and R.S. Bell, "Gradient of the ZAPT2 Energy", Theor. Chem. Accts., 107, 57 (2002).

31. T.I. Solling, D.M. Smith, L. Radom, M.A. Freitag, and M.S. Gordon, "Multi-reference equivalents of the G2 and G3 methods using reduced Moller-Plesset orders", J. Chem. Phys., 115, 8758 (2001).

32. Y. Alexeev, R.A. Kendall and M.S. Gordon, "The Distributed Data SCF", Computer Physics Commun., 143, 69 (2002).

33. M.V. Pak and M.S. Gordon, "Hyperfine coupling tensors for multi-configurational quasi-degenrate perturbation theory (MCQDPT)", J. Chem. Phys., 118, 40 (2003).

34. C. M. Aikens, S. P. Webb, R. Bell, G.D. Fletcher, M.W. Schmidt, and M.S. Gordon, "A derivation of the frozen-orbital unrestricted open shell and restricted closed shell MP2 analytic gradient expressions", Theor. Chem. Accts., 110, 233 (2003).

35. Z. Gan, Y. Alexeev, R.A. Kendall, and M.S. Gordon, "The Parallel Implementation of a Full CI Program", J. Chem. Phys., 119, 47 (2003).

36. D.G. Fedorov, S. Koseki, M.W. Schmidt and M.S. Gordon, "Spin-orbit coupling in Molecules: Chemistry beyond the adiabatic approximation", Int. Revs. Phys. Chem., 22, 551 (2003).

37. D. Fedorov, M.W. Schmidt, S. Koseki, and M.S. Gordon, "Spin-Orbit Coupling and Applications to Chemistry", "Recent Advances in Relativistic Molecular Theory", Vol. 5, K. Hirao and Y. Ishikawa, Eds., World Scientific, Singapore, pp. 107-136, 2004.

38. C.M. Aikens and M.S. Gordon, "Parallel Unrestricted MP2 Analytic Gradients using the Distributed Data Interface", J. Phys. Chem., 108, 3103 (2004).

39. H. Netzloff and M.S. Gordon, "Fast Fragments: The Development of a Parallel Effective Fragment Potential Method", J. Comp. Chem., 25, 1926 (2004).

40. M.S. Gordon and M.W. Schmidt, "Advances in Electronic Structure Theory: GAMESS a Decade Later", Theory and Applications of Computatinoal Chemistry, C. Dykstra, Ed., Elsevier, in press.

41. H.M. Netzloff, M.S. Gordon, and M.A. Collins, "Growing Multi-Configurational Potential Energy Surfaces with Applications to $X + H_2$ (X = C, N, O) Reactions", J. Chem. Phys., submitted.

7. Interactions/Transitions:

Participation/presentations at meetings, conferences, seminars, etc.

TALKS AT PROFESSIONAL MEETINGS

1. "Gridless Density Functional Theory", presented by K. Glaesemann, ", National

American Chemical Society Meeting, Dallas, TX, April 1998.

2. "Parallel MP2 Gradients", Mardi Gras Symposium on High Performance Compting, Baton Rouge, LA, February 1998 (INVITED), presented by G. Fletcher.

3. "Chemical Reaction Dynamics", AFOSR Molecular Dynamics Contractors' Meeting, Monterey, CA, May 1998.

4. "Effect of Solvents on Chemical Processes", Canadian Symposium on Theoretical Chemistry (INVITED), Vancouver, BC, August 1998.

5. "The Role of Theory in Chemical Vapor Deposition", Electrochemical Society Meeting (INVITED), Boston, November 1998

6. "The Mechanism of Formation of POSS Species", Symposium on High Temperature Materials (INVITED), Maui, HI, January 1999

7. "Effect of the Medium on Chemical Reactions", Morokuma Symposium, Atlanta, GA, May 1999 (INVITED)

8. "Enabling Calculations on Large Molecules Using Parallel Computers", AFOSR High Energy Density Materials Meeting, Cocoa Beach, FL, June 1999 (INVITED)

9. "Medium Effects on Chemical Reactions",, American Conference on Theoretical Chemistry, Boulder, CO, June 1999

10. "Restricted High-Spin Open Shell Theory: The Z Avreaged Perturbation Theory (ZAPT) Gradient", presented by Robert Bell, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

11. "Structure and Energetics of Silicon Carbide Clusters, Si_nC_m, n + m = 4", presented by Jamie Rintelman, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

12. "Improved Implementation of the Fast Multipole Method (FMM)", presented by Cheol Ho Choi, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

13. "Distributed Dtat MP2 on PC Clusters", presented by Mike Schmidt, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

14. "The Study of Water Solvation of Electrolytes by Using the Effective Fragment Potential Model", presented by Akihiko Yoshikawa, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

15. "A Theoretical Study of the Catalyzed Bis-Silylation Reaction", presented by Yuri

Alexeev, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

16. "Full CI and MCSCF Calculations of Spn Density Using Gaussian Basis Sets", presented by Michael Pak, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

17. "Investigation of the First Potential Surfaces of the Systems B + H_2 and B_2 + H_2 with Large Scale Ab Initio Calculations, presented by Vassiliki-Alexandra Glezakou, , American Conference on Theoretical Chemistry, Boulder, CO, June 1999

18. "QM/MM Methods for solvation and Surface Chemistry", National ACS Meeting, New Orleans, LA, August 1999. (INVITED)

19. "Cycloaddition reactions of 1,3-cyclohexadiene on Silicon (001) surfceusing SIMOMM", presented by Cheol Ho Choi, National ACS Meeting, New Orleans, LA, August 1999

20. "Direct recurrence relations for the rapid and stable determination of rotation matrices between complex spherical harmonics", presented by Cheol Ho Choi, National ACS Meeting, New Orleans, LA, August 1999

21. "A Cluster Approach to Solvation and Surface Chemistry", AFOSR Dynamics Contractors' meeeting, Boston, May 2000.

22. "Hydrogen Transfer in Materials and Biomolecules", National ACS Meeting, Washington, DC, August 2000 (INVITED)

23. Excited State Potential Energy Surfaces from Diatomics to Biomolecules, National ACS Meeting, San Diego, April 2001 (INVITED)

24. "Potential Energy Surfaces and Dynamics for Potential High Energy Species", AFOSR HEDM Contractors' Meeting, October 2000 (INVITED).

25. "The mechanism for formation of Al_2O_3 from Al and O_2" AFOSR HEDM Contractors' Meeting, October 2000, Michael Pak presenting.

26. "Effect of Solvation on Chemical Processes", Pacific Basin Chemical Societry Meeting, Honolulu, December 2000 (INVITED).

27. "A Cluster Approach to Surface Chemistry", Pacific Basin Chemical Societry Meeting, Honolulu, December 2000 (INVITED).

28. "A Cluster Approach to Surface Chemistry", Workshop on Computational Materials Science, Maui, December 2000 (INVITED).

29. "Cluster Approaches to Solvation and Surface Chemistry", New Frontiers in

Theoretical Chemistry, Tokyo, March 2001 (INVITED)

30. "The Use of Multi-Reference Wavefunctions in Surface Chemistry", National ACS Meeting, Chicago, August 2001.

31. "Cluster Approaches to Solvation and Surface Chemistry", National ACS Meeting, Chicago, August 2001.

32. "Cluster Approaches to Solvation and Surface Chemistry", Midwest Thoeretical Chemistry Conference, Minneapolis, MN, Oct. 2001.

33. "Recent Advances in Electron Correlation", National ACS Meeting, Orlando, April 2002.

34. "Tools for Exploring Potential Energy Surfaces", National ACS Meeting, Orlando, April 2002.

35. "An Overview of the Effective Fragment Potential Method" Workshop on Time-Dependent Density Functional Theory, Air Force Research Laboratory, May 2002.

36. "HPC Computational Chemistry on the MSRC Systems", HPC Users Forum, Princeton, NJ, September 2003.

37. "Enabling High Performance Electronic Structure Theory", Theoretical and Computational Chemistry Symposium, Gyeongju, S. Korea, Feb. 2004

38. "Scalable implementation of analytic gradients for for second order Z-averaged perturbation theory using the distributed data interface", National American Chemical Society Meeting, Philadelphia (INVITED), August 2004, Christine Aikens presenting.

39. "High Performance Electronic Structure Theory: Strategies and Applications", Seventh Congress of World Association of Theoretically Oriented Chemists", Capetown South Africa, Jan. 2005 (INVITED).

40. "Scalable Correlated Electronic Structure Methods: Straegies and Applications", Lise Meitner Symposium, June 2005, Jerusalem, Israel (INVITED)

41. "Scalable Correlated Electronic Structure Methods: Straegies and Applications", 1st Naregi Conference, June 2005, Nara, Japan

INVITED LECTURES

1. "Ubiquitous Water", Advanced Supercomputer Center, Wright-Patterson AFB, October 1997

2. "Ubiquitous Water", Coulson Lecture, University of Georgia, October 1997

3. "Ubiquitous Water", University of Utah, November 1997

4. "Ubiquitous Water", Australian National University, January 1998

5. "Ubiquitous Water", Melbourne University, February 1998

6. "Ubiquitous Water", Sydney University, February 1998

7. "Ubiquitous Water", Roseman Lecture, Johns Hopkins University, April 1998

8. "The Effect of Solvation on Chemical Processes", Air Force Research Laboratory, Edwards AFB, CA, September 1998

9. "Ubiquitous Water", University of Nebraska, September 1998

10. "The Role of Water in Chemical Processes", Grinnell University, February 1999

11. "Ubiquitous Water", Marquette University, February 1999

12. "The Effective Fragment Method", Pople Symposium, Amelia Island, FL, March 1999

13. "Ubiquitous Water", Long Island University, Brooklyn, NY, March 1999

14. "Water as a Catalyst", Union Carbide Corp., May 1999

15. "The Effect of the Medium on Chemical Reactions", Boston University, October 1999

16. "The Effect of the Medium on Chemical Reactions", University of Arizona, October 1999

17. "The Effect of the Medium on Chemical Reactions", University of Michigan, October 1999

18. "Quantum Chemistry at Iowa State University", University of Sydney, March 2000

19. "Effect of the Medium on Chemical Reactions", Kansas State University, April 2000

20. "Effect of the Medium on Chemical Reactions", Princton University, May 2000

21. "Cluster Approaches to Solvation and Surface Chemistry", Gustavus Adolphus College, March 2001

22. "Cluster Approaches to Solvation and Surface Chemistry", St. Mary's College, April 2001

23. "Cluster Approaches to Solvation and Surface Chemistry", University of Southern California, April 2001

24. "Cluster Approaches to Solvation and Surface Chemistry", University of California-Irvine, May 2001.

25. "Cluster Approaches to Solvation and Surface Chemistry", Penn Sate University, February, 2002

26. "Cluster Approaches to Solvation and Surface Chemistry", University of North Texas, May 2002

27. "Cluster Approaches to Solvation and Surface Chemistry", NASA-Ames Research Center, September 2002

28. "Cluster Approaches to Solvation and Surface Chemistry", Workshop on Time-Dependent Density Functional Theory, Wright-Patterson AFB, September 2002.

29. "Potential Energy Surfaces for Polynitrogen Compounds", Workshop on Energetic Materials, Lawrence Livermore National Laboratory, September 2002.

30. "A Cluster-based Approach to Solvation", University of Western Australia, March 2003

31. "A Cluster-based Approach to Solvation", University of Tasmania, April 2003

32. "A Cluster-based Approach to Solvation", University of Melbourne, April 2003

33. "A Cluster-based Approach to Solvation", Australian National University, April 2003

34. "A Cluster-based Approach to Solvation", Sydney University, May 2003

35. "A Cluster-based Approach to Solvation", North Dakota State University, September 2003

36. "A Cluster-based Approach to Solvation", University of Wisconsin, April 2004

37. "A Cluster-based Approach to Solvation", Texas Tech University, October 2004

38. "A Cluster-based Approach to Solvation", Australian National University, November 2004

39. "A Cluster-based Approach to Surface Science", University of Melbourne, December 2004

40. "Effective Fragment Potentials: Solvation and Beyond", The Hebrew University, June 2005

41. "Effective Fragment Potentials: Solvation and Beyond", The Weizmann Institute, June 2005

Consultative and advisory functions to other laboratories and agencies, especially Air Force and other DoD laboratories. Provide factual information about the subject matter, institutions, locations, dates, and name(s) of principal individuals involved.

- Served as co-advisor to Major James Shoemaker, who received his Ph.D. from the Department of Engineering Physics, Air Force Institute of Technology, October 1997. Several papers will result from this work; one is already in print [J. Phys. Chem. A, 103, 3245 (1999)], one is submitted to J. Chem. Phys, and a third is in preparation.

- Presented CHSSI workshop on GAMESS at the Army Research Laboratory, June 1998 and July 1999 (presented by Jerry Boatz).

- Colaborating with the Group of Dr. Ruth Pachter (AFRL) to develop new codes for molecular dynamics and Monte Carlo simulations (ongoing).

- Collaborating with Dr. Ruth Pachter to develop density-functional-based effective fragment potentials.

c. Transitions. Describe cases where knowledge resulting from your effort is used, or will be used, in a technology application. Transitions can be to entities in the DOD, other federal agencies, or industry. Briefly list the enabling research, the laboratory or company, and an individual in that organization who made use of your research.

Both GAMESS and MacMolPlt have an increasing number of users in universities, industry, and government laboratories. The latest version of parallel GAMESS is on-line at all DoD Major Shared Resource Centers.

8. New discoveries, inventions, or patent disclosures. (If none, report None.) **None**

9. Honors/Awards: List honors and awards received during the

grant/contract period. List lifetime achievement honors such as Nobel prize, honorary doctorates, and society fellowships prior to this effort.

- ¶ Coulson Lecturer, University of Georgia, October, 1997
- ¶ Roseman Lecturer, Johns Hopkins University, April, 1998
- ¶ Named Distinguished Professor of Chemistry, May, 1998
- ¶ Named to list of 100 most cited chemists, 1981-2000.
- ¶ Named Fellow, American Physical Society, 2000
- ¶ Named 2004 recipient of ACS Midwest Award
- ¶ Elected to International Academy of Quantum Molecular Science (2004)

10. Markings: In order to ensure prompt receipt and acceptance, mark the outside of the package clearly to indicate that it is a progress report.