News from the Theoretical Chemistry Subdivision

-- Reported by Ned Sibert, Subdivision Chair

The Executive Committee of the Theory Subdivision, which consists of current and past officers, met Sunday, April 7th, at the Orlando ACS meeting. Present were Anne Chaka, Casey Hynes, Martin Head-Gordon, Ken Jordan, Richard Stratt, and myself. Topics discussed at the meeting included the IBM graduate student computational chemistry awards, ideas for future symposia, and suggestions for the appointment of the nominating committee to choose the next Vice Chair of the Subdivision. We also considered how we might enhance ties between Computational Chemistry, particularly in regard to planning future symposia.

Following the advice of the Executive Committee, Jack Simons (Utah), and Charlie Brooks (Scripps) and I were selected to form a nominating committee to find the next Web Master and Vice Chair Elect. The nominating committee proposed that John Adams continue to serve as the Web Master and Sharon Hammes-Schiffer, Penn State University, was proposed for the position of Vice Chair. I am pleased to report that both have agreed to serve. They will begin their respective terms at the conclusion of the Fall ACS meeting. Sharon Hammes-Schiffer will succeed to Chair

Elect in 2003 and to the Chair of the Division in 2004.

Speaking of Web Masters, please visit the Subdivision web page at http://www.chem.missouri.edu/theory/. You will find links of interest to the theoretical chemistry community as well as postdoctoral announcements. Please send John Adams any comments you might have.

This year's competition for the IBM graduate Fellowships had many high quality applicants. The selection committee of Martin Head-Gordon, Jamie Coffin (of IBM), and myself had a difficult time selecting the two recipients from this talented pool. The two recipients are Collin Wick (University of Minnesota, working with Ilja Siepmann) and Feng Wang (University of Pittsburgh, working with Ken Jordan). Collin's proposal was entitled "Simulation Studies of Reversed-Phase Liquid Chromatography". Feng's proposal was entitled 'Drude Oscillator Models to Incorporate Dispersion Interactions into Model Potentials Describing the Interaction of Excess Electrons with Clusters of Polar Molecules".

Our congratulations go to Collin Wick and Feng Wang for winning the 2002 Graduate Student Awards in Computational Chemistry. Many thanks to Jamie Coffin and IBM for their continued support of these awards and to Don Truhlar and the Minnesota Supercomputing Center for making available grants of CPU time for the awardees. I urge you to encourage your students to apply next fall. Martin Head-Gordon mhg@bastille.cchem.berkeley.edu will be in charge of the competition.

Several excellent suggestions for symposia topics were raised over our lunch meeting, and I passed these along in my report at the Physical Chemistry Division Executive Committee meeting on Sunday evening. As always, we welcome suggestions for symposia for the national meetings. For past and planned meeting symposia visit the physical chemistry site at http://hackberry.chem.trinity.edu/PHYS/. Please send your suggestions along to me or Martin-Head Gordon, who will be rotating into the Chair position after the Fall meeting.

We would also like to remind faculty, who are members of the Subdivision, to encourage their students and postdoctoral fellows to join both the Theory Subdivision and the Physical Chemistry Division.

I look forward to seeing you all in Boston.

Ned

Theory Subdivision Webpage

Visit the new, redesigned Theory Subdivision website at **www.acstheory.org**! There are many new features. We hope that this web site will be a resource for Subdivision members and for those generally interested in the theoretical aspects of chemistry. Please let us know how we can make this site more useful to you by directing your comments to the Subdivision's Webmaster.

NEW: We are compiling a list of useful and interesting links to web sites for theoretical and computational chemists or for individuals wanting to learn more about theoretical/computational chemistry. If you have a recommendation for a site that might be of interest to the larger community, please send the URL and a brief description of the site to the webmaster, John Adams (AdamsJE@missouri.edu).

Theoretical Chemistry Postdoctoral Position Clearinghouse

The Subdivision continues to run a clearinghouse for people looking to hire postdocs and people looking for postdoc positions. Currently there is a list of those looking for a position and one for those looking to hire, both of which are available on the Subdivision web page. If you wish to be on either list, please send John e-mail or drop him a line. The address to contact him is:

Prof. John E. Adams
Department of Chemistry
University of Missouri
Columbia, MO 65211

email: AdamsJE@missouri.edu
voice: (573) 882-3245

Membership

The subdivision now has about 800 members. If you would like to join the Theory Subdivison:

If you are already a dues-paying member of the Division of Physical Chemistry ($7.00/year, $2.00 for students), just send a note to the Secretary of the Subdivision (National Institute of Standards and Technology, 100 Bureau Drive Stop 8380, Gaithersburg, MD 20899-8380, anne.chaka@nist.gov) indicating your wish to join. Please state that you are already a member of the Division.

If you are not already a member of the Division of Physical Chemistry but you do belong to the ACS, join the Division by sending a note to Professor Ken Jordan, Department of Chemistry, University of Pittsburgh, 219 Parkman Avenue. Pittsburgh PA, 15260, USA, enclosing a check for $7.00 ($2.00 for students) and stating your wish to join the Subdivision at the same time.

IBM Graduate Student Awards in Computational Chemistry

CALL FOR APPLICANTS FOR IBM 2002 AWARDS!
(Deadline is September 30, 2002)

There are two Awards in Computational Chemistry that are open to current graduate students. We are grateful to IBM and the Minnesota Supercomputing Institute for their support of these awards. Last year's winners are announced below.

Let me urge you to encourage your graduate students to apply. The competition is open to any graduate student (regardless of citizenship) who began graduate study after August 1, 1999 and who is an ACS member (or whose advisor is an ACS member). These awards are designed to encourage graduate work in computational chemistry, to recognize research accomplish-ments, and to stimulate interest in the Subdivision of Theoretical Chemistry and the Physical Chemistry Division of the ACS.

An Awards Committee will consider all the applicants. The awards applications should be sent to Professor Martin Head-Gordon at the University of California, Berkeley. Note that the deadline for applications is September 30, 2002.

These two awards, supported by IBM, will provide one-time cash stipends of $2500 and $1000 as supplements to normal financial aid to doctoral candidates in the research-dissertation stage in the 2002-2003 academic year. The Minnesota Supercomputing Institute will provide each awardee up to 2500 node-hours on an IBM SP2 cluster for the awardees to actually carry out a portion of the awarded research. The awardees will have access to the consulting services of the Institute normally available to all users. Awardee selection will be made on a competitive basis. Applicants should be working on new and innovative computational chemistry methods or applications in theoretical chemistry.

Applicants should prepare a written description of a computational chemistry research project that combines novel science with high performance parallel computing. The proposal should be concise, consisting of no more than 4 double-spaced pages. It should clearly explain both the significance of the project and the approach that will be followed in the research. This should include an estimate of the computing resources required in SP2 cpu-hours, and how applicants plan to use the grant funds. Two letters of recommendation, including one from the student's advisor, along with a vita and transcript, are required. In addition, a faculty person (typically the applicant's research advisor) responsible for the applicant's use of the Minnesota Supercomputing Institute resources must be identified.

Forward applications by September 30, 2002 to: Professor Martin Head-Gordon
          Department of Chemistry
          University of California
          Berkeley, CA 94720

The awardees will be announced in the Fall 2002 Subdivision newsletter.

THE 2001 IBM AWARDEES:

1st Prize: Collin Wick, Department of Chemistry and Biochemistry, University of Minnesota. Advisor: Professor Ilja Siepmann. Proposal: Simulation Studies of Reversed-Phase Liquid Chromatography

2nd Prize: Feng Wang, Department of Chemistry, University of Pittsburgh. Advisor: Professor Kenneth Jordan. Proposal: Drude Oscillator Models to Incorporate Dispersion Interactions into Model Potentials Describing the Interaction of Excess Electrons with Clusters of Polar Molecules.

NSF Rotator Positions

The National Science Foundation seeks scientists to serve in temporary (rotator) positions in Theoretical and Computational Chemistry. Interested individuals are encouraged to contact the Theoretical Chemistry Subdivision (Ned Sibert, elsibert@facstaff.wisc.edu, 608-262-0265).

The NSF augments its permanent staff of professional employees through the temporary (rotator) appointment of individuals on leave of absence from research and/or educational institutions. This arrangement provides the Foundation with visiting scientists, engineers, and educators who are current in academic, scientific, engineering, or managerial matters. In return, these individuals and their institutions gain knowledge of the philosophy and mechanisms of Federal support for research. The Foundation, the participant, and his/her home institution all benefit from this program.

A basic fact sheet about the NSF can be accessed at: http://www.nsf.gov/cgi-bin/getpub?nsf9763 while general information regarding rotator positions can be accessed at:
http://www.nsf.gov/home/chart/rotate.htm.

Most academic scientists become rotators under the Visiting Scientist program (http://www.nsf.gov/home/chart/visiting.htm) although some enter under the Intergovernmental Personnel Act (http://www.nsf.gov/home/chart/intergov.htm). Both of these sites contain information about salary, benefits, relocation allowances, and the Independent Research/Development program. This program permits a scientist temporarily performing service at NSF to maintain involvement with his/her research at his/her home institution.

Symposium Reports

The following are reports from the Spring 2002 national ACS meeting in Chicago. We thank the symposium organizers for taking the time to put these wonderful reports together for us.

RECENT ADVANCES IN ELECTRON CORRELATION METHODOLOGY. Reported by Angela K. Wilson (University of North Texas), Organizer.

This symposium focused upon recent developments in advanced *ab initio* and density functional methods, basis set approaches, high accuracy benchmark calculations, and hybrid methods. **Mark Gordon** opened the meeting by providing an overview of the symposium in addition to a brief discussion about scalable quantum chemistry.

Session I: Coupled Cluster and Configuration Interaction Methods

Marcel Nooijen discussed developments toward an internally contracted multireference coupled cluster theory which scales the same as closed shell CCSD (apart from the final "first-order" CI diagonalization), but for a different prefactor, reflecting the complexity of the scheme. Applications of the resulting coupled cluster and perturbation theory variants for sytems like p-, m-, and o-benzyne and the excitation spectra of ozone (including low-lying doubly excited states) were presented.

Daniel Crawford discussed the extension of the coupled cluster local correlation idea to electronically excited states for low-lying transitions, including diffuse Rydberg states. "Non-local" states involving charge-transfer in large molecules are more problematic, however, and require new orbital domain definitions beyond those applicable for ground states.

Piotr Piecuch presented a new approach to the many-electron correlation problem, termed the method of moment of coupled-cluster equations (MMCC), and the renormalized coupled-cluster methods that remove the failing of the standard coupled-cluster approximations, such as CCSD(T), at larger internuclear separations. He also discussed the extensions of the MMCC theory to excited states as well as the recently proposed active-space equation-of-motion and multi-reference coupled-cluster methods that can be used to study ground and excited-state potential energy surfaces.

John Stanton's talk focused upon coupled-cluster methods, which are especially well-suited to the study of adiabatic potential energy surfaces in the immediate vicinity of conical intersections. This work exploits that feature of the methods and applies them to the simulation of spectra in which vibronic effects play a major role.

Emily Carter and **Derek Walter** have developed a reduced scaling configuration interaction method which combines local correlation techniques and pseudospectral methods. The method they presented is over 7 times less costly than the non-local analytic CI method.

Session II: Advanced *Ab Initio* Methodology

Martin Head-Gordon discussed new enhancements to single reference coupled cluster methods designed to be more accurate for bond-breaking problems. These included the generalization of coupled cluster doubles to the quadratic coupled cluster doubles method, and the formulation of second order corrections for higher excitations to both QCCD and conventional CCSD.

A discussion about the Spin-Flip approach to bond-breaking problems and diradicals was presented by **Anna Krylov**. In the Spin-Flip method, both closed and open shell singlet states are described within a single reference formalism as spin-flipping, e.g., excitations from a triplet $(Ms=1)$ reference state for which both dynamical and non-dynamical correlation

effects are much smaller than for the corresponding singlet state.

Peter Gill's talk focused upon Wigner intracules. Wigner intracules contain important information about the probability of finding electrons at a given separation and moving with a given relative momentum. There are good reasons for believing that these intracules contain the key information required to estimate electron correlation energies and early numerical investigations support this.

Peter Pulay, **J. Baker**, **S. Saebo**, and **K. Wolinski** discussed parallel Linux implementation of canonical MP2 with local prescreening, allowing unprecedented calculations on an inexpensive Linux cluster. Examples of calculations included the dispersion interaction in supercoronene dimer, $C_{108}H_{36}$, C2h, 6-311G*, 2052 basis functions, and a representative calculation for the porphine dimer, $C_{40}H_{28}N_8$, 6-311G*, 948 functions, which takes 73 minutes on an 8-processor cluster. For large basis sets, dual-basis MP2 calculations, first suggested by Almlöf, are virtually identical with conventional; calculations and an order of magnitude faster.

Laimis Bytautus and **Klaus Ruedenberg** find that the use of localized molecular orbitals, i. e. orbitals that have been localized in SCF-HF occupied and SCF-HF virtual space, respectively can be of great aid in eliminating huge amounts of CI configurations that are insignificant, so-called "dead-wood". They showed that very few but physically well-motivated arguments based on the localized molecular orbitals can lead to a rather simple although remarkably efficient scheme for generating very compact yet very reliable CI-based wave-functions as confirmed by subsequent tests on a number of molecules.

Session III: Density Functional Theory

Katharine Hunt derived a new expression for the total electronic energy of a molecule in terms of the average electron charge density, the nonlocal charge-density susceptibility evaluated at imaginary frequencies, nuclear charges, and nuclear positions. The expression is exact within the non-relativistic Born-Oppenheimer approximation. Ref: J. Chem. Phys. 116, 5440 (2002).

A new, real-space density functional model of nondynamical correlation in molecular systems was presented by **Axel Becke**. Existing functionals do not explicitly represent the proper deepening of the exchange-correlation hole due to non-dynamical correlation. His new model remedies this.

Kieron Burke talked about the construction and meaning of energy densities in density functional theory, discussing the non-interacting kinetic energy, the exchange-correlation energy, and the total energy, for atoms and molecules.

Carlos Gonzalez examined the transferability of hybrid DFT functionals such as B3LYP in the treatment of different chemical problems. The need for generating exchange functionals that do not contain spurious correlation and that can treat correctly the self-interaction problem was stressed. A brief description of a new X-Alpha exchange functional with such characteristics and whose parameters are variationally obtained throughout the Kohn-Sham procedure was also discussed.

Stephan Kuemmel and **John Perdew** defined the exact Kohn-Sham potential for orbital dependent functionals, e.g., the exact exchange energy, as the solution of the "optimized

effective potential" integral equation. They showed that the exact potential can also be calculated iteratively from differential equations, thus avoiding the numerically very involved direct solution of an integral equation.

Sesison IV: Density Functional Theory

John Perdew - For general use in quantum chemistry and condensed matter physics, density functionals for the exchange-correlation energy are best constructed non-empirically. The local density and generalized gradient approximations have been so constructed, and there are good prospects for non-empirical or nearly non-empirical constructions of meta-generalized gradient approximations (which use the orbital kinetic energy density) and hyper-generalized gradient approximations (which use the exact exchange energy density).

Dennis Salahub gave an overview of Density Functional Theory for "difficult" applications involving hydrogen bonds, transition metals and transition states. Functionals incorporating the Laplacian of the density and the kinetic energy density are encouraging, but there is still much need for further work on new functionals.

Karel Piers presented a simple algorithm to extract the exchange-correlation potentials in density functional theory from high-level, correlated one-body densities as obtained by self-consistent Green's function calculations up to second order in the two-body interaction. The resulting potentials show the correct asymptotic behavior and can be used to provide an *ab initio* basis for exchange-correlation functionals by including these potentials in the fitting procedure of the functionals.

Nicholas Handy delivered a lecture on density functional theory. He explained a derivation of

accurate exchange-correlation functionals. He also argued in favor of the use of Slater-Type-Orbitals (rather than Gaussian-Type-Orbitals) in density func-tional calculations

J. Andzelm, K. Glassford, N. Govind, G.Fitzgerald, and **Klaus Stark** discussed several different aspects of accuracy and applicability of state-of-the-art density functional theory implementations in areas including structure and energetics of organic molecules, reactions using organometallic homogeneous catalysts, molecular crystals, and solid state structures and reactions on catalytic surfaces for research in heterogeneous catalysis.

Ivana Adamovic and **Mark Gordon** discussed the development of a density functional theory (DFT) based Effective Fragment Potential (EFP) approach for the treatment of solvent effects. The DFT based method has the same energy contributions as the HF based EFT: electrostatic, polarization, and exchange repulsion/charge transfer.

Session V: Basis Sets and CBS Limits

Jan Martin discussed new correlated basis sets for the alkali and alkali earth metals which he recently developed and validated. The importance of inner-shell correlation was assessed: its inclusion is absolutely essential for K and Ca, strongly advised for Na, and recommended for Li and Mg, but can be treated additively for Be.

George Petersson discussed linear $e^{-a\,n}$ extrapolation of SCF energies from balanced ntuple-z augmented polarized (nZaP) basis sets, $(l + 3/2)^{-5}$ extrapolation of MP2 aa-pair energies, $(l + 1)^{-3}$ extrapolation of MP2 ab-pair energies, and linear $(l + 1/2)^{-3}$ extrap-olation of

the 2Z and 3ZP1d triple excitation energies which leaves an RMS error of 1.4 mE_h. Comparable accuracy (0.8 mE_h) for the [CCSD MP2] component of energies still requires a nonlinear extrapolation, but they are getting very close to achieving a linear extrapolation to the CCSD(T)/CBS limit, and thus analytical derivatives giving CBS geometries and frequencies.

Kirk Peterson developed a new series of correlation consistent-like basis sets for the entire group 13-18 post-d elements in conjunction with new small-core relativistic pseudopotentials optimized by the Stuttgart/Bonn groups. Initial CCSD(T) calculations with these new basis sets show very close agreement with all-electron Douglas-Kroll results.

C. David Sherrill has implemented a new parallel algorithm for the explicitly correlated MP2-R12/A method and has used this method to obtain complete basis set estimates for benzene dimer, which features exceptionally large basis set effects. When corrected for higher-order correlation effects via CCSD(T), the T-shaped and parallel-displaced configurations are nearly isoenergetic.

Robert J. Harrison addressed multi-resolution approaches to quantum chemistry, highlighting the non-standard format of operators and functions used for multi-resolution analysis (MRA) and multi-wavelet bases. The promise of MRA in many-body methods is to provide a full numerical solution of the electron pair equation for general polyatomic systems, thereby eliminating the slow convergence of the correlation energy with respect to the (atom centered) basis set.

Shijun Zhong and **George Petersson** discussed CBS extrapolations of both the SCF energies and the correlation energies and how they have been improved by rebuilding or adjusting basis set sequences.

Session VI: High Accuracy Approaches

Thom Dunning, Jr. discussed quantifying accuracies of methods used to solve the electronic Schrödinger equation through the use of the correlation consistent basis sets. A detailed statistical analysis of the errors for a sample set of atoms and molecules showed that neither the singles and doubles configuration interaction method nor perturbation methods (MP2-4) yield reliable electron affinities whereas coupled cluster methods that included the effect of triple excitations and core-valence effects yielded electron affinities to better than chemical accuracy (1 kcal/mol).

W. Klopper and **C.C.M. Samson** reported on recent progress in the development of explicitly correlated methods for large molecules. They employed auxiliary basis sets for the closure approximation and Gaussian-damped interparticle distances in the trial wave function.

Krishnan Raghavachari discussed recent advances in quantum chemical models for accurate thermochemistry.

Poul Jorgensen emphasized that to establish the errors of electronic structure calculations of molecular properties as equilibrium geometries for the currently best electronic structure models it is important to have experimental data of uniform high accuracy.

Rodney Bartlett's presentation showed the new standards in the hierarchy of CC methods, adding CCSDTQP for single states and EOM-

CCSDT for excited states. He discussed ab initio DFT and showed that unlike the other DFT methods applied, the ab initio route gives the correct exchange and correlation potentials. He also introduced the 'transfer Hamiltonian' as a way to potentially retain the accuracy of CC forces in simulations of large molecules, illustrating the dramatic differences between such QM forces and those from classical potentials for a 109 atom silica system.

Session VII: Electronic Structure Advances and the Future

Keiji Morokuma and **Tom Vreven** discussed the recent development of the hybrid method ONIOM and its application to the determination of accurate bond dissociation energies of large molecules, in which the correlation energy is evaluated at different theoretical levels for different parts of the molecular system.

Don Truhlar presented joint work with **Benjamin Lynch** in which they have developed improved multi-coefficient correlation methods, which are electronic structure methods suitable for thermochemical applications and kinetics. A suite of four third generation methods was presented, and these

methods (MCG3/3, MC-QCISD/3, MCOPMP2/3, and SAC/3) were validated with a new database (Database/3) including energetic and kinetic data. Additional work was presented showing the very high accuracy achievable for transition state geometries with these methods and with MPW1K/6-31+G(d,p).

Anne Chaka provided an overview of current and future needs for improvement in electron correlation from an industrial perspective. Some of the needs mentioned included greater numerical accuracy for thermochemistry and kinetics, improved approaches for transition metals, faster multi-reference and post-Hartree Fock methods which can be extended to 100 atoms with large basis sets, accurate band gaps for materials, an ONION-type approach for fluids.

Henry F. Schaefer III overviewed the symposium, providing highlights and comments on past, current, and future direction. He discussed several areas of development including: (1) exceptionally efficient analytic second derivative techniques, (2) routine calculations on 100 atom systems with 2000 basis functions by the year 2006, (3) further improvements in computational scaling.

MODERN ASPECTS OF STRUCTURE FUNCTION CORRELATIONS OF BIOMOLECULES: PHOSPHORYL AND NUCLEOTIDYL TRANSFER REACTIONS
Reported by Arieh Warshel (University of Southern California). Arieh Warshel and Amnon Kohen (University of Iowa), Organizers.

In the first session of the meeting, **Nick Williams** and **Arieh Warshel** characterized the reactivity and mechanisms of the phosphate mono- and diester hydrolysis in aqueous solution from the experimental and theoretical points of view, respectively. **Alfred**

Wittinghofer and **Klaus Gerwert** highlighted recent advances in understanding the structural and mechanistic details of the GTPase reaction in rasp21 and related GTP-binding proteins. Several mechanisms for the regulation of the rate of the GTP hydrolysis, which is the key

switch in the cell signaling pathways, were discussed by **Alfred Wittinghofer**, **Stephen Sprang** and **Arieh Warshel**.

GTPases typically regulate the function of the next step in the signal transduction pathway, protein kinases, the task of which is to specifically phosphorylate their target proteins. The session on protein kinases was opened by **Michael Eck**. The focus of his talk was the catalytic activity of the tyrosine kinases Lck and Fyn, which play important role in the antigen-dependent activation the lymphocyte development. **Elizabeth Goldsmith** presented X-ray study of the structures of the MAP kinase p38 in complex with docking site peptides. **Joseph Adams** stressed the importance of solution studies in complementing X-ray structural data. He showed that both small and complex protein kinases undergo conformational changes that are associated with the product release. The viability of the thio-effects as probes of the mechanisms of enzymatic phosphoryl transfer reactions was critically examined by **Alvan Hengge**. The session was concluded by **Roger Goody**, who presented crystal structures of the thymidylate kinase with various inhibitors.

The second day of the meeting was devoted to the enzymes that catalyze nucleotide transfer reactions. The solution and crystallographic studies of the structure of the active site of the

group I and II ribozymes were presented by **Joseph Piccirilli** and **Jennifer Doudna**. **Ronald Raines** evaluated key factors responsible for the cytotoxicity of ribonucleases. **John Perona** presented crystallographic and mutational analysis of the catalytic function of the active-site residues in the EcoRV endonuclease. The quantum-chemical study of the catalytic mechanism in the DNA polymerase ? by **Stanley Burt** revealed that this polymerase is likely to use a substrate-assisted associative mechanism. The crystallographic, kinetic, and theoretical study of the replication fidelity of this enzyme was presented by **Samuel Wilson** and **Jan Florian**. Structural aspects of the loss of the fidelity in error-prone polymerases were analyzed by **Ming-Daw Tsai** and **Hong Ling**. Further insights into the intriguing source of the polymerase fidelity was provided by **Sylvie Doublie**, who examined the X-ray structure of a template-independent RNA polymerase.

The symposium was concluded with a short session about the DNA base excision and DNA repair (talks by **John Tainer** and **Monika Fuxreiter**). The enzymatic hydrolysis of phosphate triesters, which play significant role in the detoxification of organophosphate-based insecticides and chemical warfare agents, was the subject of the talk of **Hazel Holden**.

MODERN ASPECTS OF STRUCTURE FUNCTION CORRELATIONS OF BIOMOLECULES: ENZYME ACTION. Reported by A. Kohen (University of Iowa) and Arieh Warshel (University of Southern California), Organizers.

Introductory remarks were given by **Arieh Warshel**.

M.J. Osborne: *Dynamics and Catalytic Function of DHFR: Insights from NMR.* M. J.

Osborne, J. R. Schnell, D. J. McElheny, R. P. Venkitakrishnan, E. Zaborowski, P. E. Wright. NMR relaxation experiments were used to elucidate dynamic motion of DHFR at ns and μs

time scale. The role of loop Met20 and coupled motion was specifically illustrated.

S. Hammes-Schiffer: *Network of coupled promoting motions in enzyme catalysis: Evidence from mixed quantum/classical simulations.* MM/QM MD simulation of hydride transfer in the DHFR catalyzed reaction. Quantum effects (e..g, ZPE and tunneling) seem to have great effect on KIEs

J. Villà: *Do dynamical effects represent a major factor in enzyme catalysis?* J. Villà, A. Warshel. A similar contribution of dynamics to an enzymatic reaction and to a similar reaction in water from computer simulation suggested a small contribution of dynamics to catalysis.

C.K. Bagdassarian: *Dynamical tuning of enzymatic conformational fluctuations.* C. K. Bagdassarian, M. Singla, K. O. Alper, J. L. Stone. Theoretical studies of the contribution of dynamics to enzymatic reactions.

R. Wolfenden: *Benchmark reactions for assessing contributions to catalysis by the structural elements of enzymes and substrates.*
Methods for observing reaction rates at temperatures up to the critical point of water were described. Minor changes in structure of cytidine deaminase and OMP decarboxilase result in a most significant effect on catalysis.

C.J. Murray: *Mapping the transition state for general acid-base catalysis of a serine protease.* C. J. Murray, R. R. Bott, G. Chan, A. G. Day, G. Ganshaw, C. Y. Hsia, B. Domingo. Studies of the linear free energy relationship between Log k and pKa explained how enzymes may discriminate between GS and TS in serine protease catalyzed reactuions.

J. Hajdu: *Accelerator - base X-ray sources: new tools for new science.*

D. Ringe: *Protein flexibility, ligand recognition and catalytic activity.* Structural enzymology and low temperature X-ray crystallography studies of enzyme dynamics were presented. A functional dynamical phase transition was suggested at 220 K.

R. Subramanian: From Structure to Dynamics by X-ray crystallography. R. Subramanian, B. Plapp. Anisotropic B factors from X-ray crystallography reviled a possible role of dynamic motion at ps time scale. Studies with ADH were presented.

D.G. Truhlar: *Ensemble-averaged variational transition state theory with multidimensional tunneling.* D. G. Truhlar, J. Gao, M. Garcia-Viloca, T. Poulsen, J. Pu, C. Alhambra, J. C. Corchado, M. L. Sánchez. MM/QM methods where the QM is NDDO or hybrid DFT were presented. Applications in studies of enolase, ADH, methylamine dehydrogenase and other enzymes were demonstrated.

A. Kohen: *Studying the chemical step in enzyme catalysis.* A. Kohen, K. A. Markham, J. A. McCracken, M. S. Moore. Studies of hydride transfer with in complex kinetic cascade and the contribution of H-tunneling and coupled motion were described. Applications in the investigation of ADH and DHFR were discused.

A.S. Mildvan: *Solution structure and mechanism of the MutT pyrophospho-hydrolase.* A. S. Mildvan, V. Saraswat, M. A. Massiah. NMR studies of the enzyme MutT pyrophosphohydrolase confirmed tight binding

and slow exchange of 8-oxo-dGMP and other structure – mechanistic effecs.

W.W. Bachovchin *A catalytic tetrad and reaction-driven histidine ring flip mechanism for the serine proteases.* A catalytic tetrad, instead of the classic triad, and histidine ring flip, were suggested as alternative mechanism for serine proteases.

M.B. Hall: *Theoretical studies on the reaction mechanisms of the nickel-iron and iron-only hydrogenases.* M. B. Hall, H. Fan, Z. Cao, S. Li, S. Niu, L. M. Thomson. Studies of model compound for NiFe and Fe only hydrogenases by combination of DFT and experimental data were presented.

J.F. Kirsch: *Low barrier hydrogen bonds and directed evolution in enzymology.* J. F. Kirsch, C. Apicella, J. Stratton, T. Handel, J. Pelton, S. Rothman. Site-directed-mutagenesis studies of the PLP dependent aspartate aminotransferase (AATase) suggested no significant role of low barrier hydrogen bonds in catalysis. Directed evolution studies of this enzyme were also presented.

A. Shurki: *How important is the steric contribution (NAC) to enzyme catalysis?* A. Shurki, J. Villà, A. Warshel. Theoretical studies compared the reaction of haloalkane dehalogenase in the enzyme and in a water cage. The contribution of preorganizing the substrate in water to the enzymatic near-attack-conformation (NAC) was calculated to be only ~2 kcal/mole.

T.C. Bruice: *Ground states and transition states in enzyme reactions.* MD studies with several enzymes and their reaction in a water cage suggested a significant contribution (>8 kcal/mole) of NAC to catalysis.

A.J. Mulholland: *Relating enzyme structure and function through mechanistic modelling.* The development and applications of QM/MM methods was presented. Calculations of a flavoprotein were compared to experimental results and a new catalytic interaction was suggested.

W. Yang: *Developments and applications of a DFT QM/MM free energy method for simulation of chemical reactions in enzymes.* W. Yang, Y. Zhang, H. Liu. A density functional theory (DFT) MM./QM calculations were applied to enzymatic reactions.

M.H. Vos: *Ultrafast studies of ligand dynamics in oxidases.* The correlated motion of ligand and protein at ps and fs time scale was studied with the enzyme cytochrome C oxidase.

D.N. Silverman: *Kinetic and structural analysis of proton transfer through intervening water molecules in catalysis by carbonic anhdrase.* D. N. Silverman, C. Tu. A hydrogen bonds network was presented that can explain the rate limiting H-transfer in the carbonic anhydrase catalyzed reaction.

J.P. Guthrie: *Proceeding from equilibrium constants to rate constants for bioorganic reactions.* A theory that premits calculation of the free energies of activation given only the equilibrium constants in solution and the distortion energies was presented

D. Arad: *QCT - Quantum Core Technology - Rational Drug Design in the link between Structure and Mechanism.* A new approach to rational drag design was presented.

S.L. Springs: *Cytochrome b(562) variants: a library for examining redox potential evolution.* G. L. McLendon, S. L. Springs, S.

E. Bass. A library approach was presented that investigate the range of redox potential that occurs through random mutation in the region near the heme of cytochrome b562 (*E. coli*).

J. Gao: *Dynamics, Pathways, and Tunneling in Enzymatic Reactions: A Modern Perspective of Enzyme Action.* J. Gao, M. Garcia-Viloca, R. Rajamani, K. Byun, Y. Mo, L. D. Kesavan. MM/QM simulations of several enzymatic systems were presented.

A.D. Robertson: *Correlated motions in native proteins from MS analysis of NH exchange.* A. D. Robertson, D. M. Ferraro, C. B. Arrington. MS studies of amide exchange at the microsecond to second time scale near the EX1 kinetic limits were presented.

V.L. Schramm: *Reaction coordinate motion and transition state structure in N-ribosyltransferases.* V. L. Schramm, S. C. Almo, A. Fedorov, W. Shi. Mechanistic studies of transition state analogues suggest that enzymes simultaneously activate and immobilize attacking and leaving groups, causing electrophilic migration between nucleophiles.

R.L. Schowen: *Structure-function relationships for S-adenosylhomocysteine hydrolase.* R. L. Schowen, P. E. Elrod, X. Yang, D. Yin, J. Zhang, R. T. Borchardt. Ala scanning of catalytic residues and kinetic characterization of the mutants facilitate mechanistic studies of S-adenosylhomo-cysteine hydrolase.

K. Morokuma: *Free 5'-deoxyadenosyl radical: accessibility and stability of structure with 2'-OH...N3 hydrogen bond.* K. Morokuma, D. V. Khoroshun, K. Warncke, S. Ke, D. G. Musaev. Theoretical calculation of model compound at the gas phase were presented using B3LYP and MP2 methods.

Conference Announcements

Future ACS Meetings

Boston, MA, September 8-12, 2002

Program Chair: Professor John C. Hemminger, Department of Chemistry, University of California, Irvine, CA 92697, jchemmin@uci.edu

- Applications of Neutron Scattering in Structural Biology and Biophysics
- Biologically Relevant Molecules in the Gas Phase
- Classical and Quantum Statistical Mechanical Studies of Solvation
- Chemical Studies Important to Astrobiology
- Nonlinear Dynamics in Polymeric systems
- Mesoscale Phenomena in Fluid systems
- Ordered Molecular assemblies of Nanoparticles
- Frontiers in Atmospheric Chemistry
- New Developments in ForceFields for Molecular Modeling

New Orleans, LA, March 23-27, 2003

Program Chair: Professor James L. Skinner, Department of Chemistry, University of Wisconsin, Madison, WI 53706, skinner@chem.wisc.edu

New York City, NY, September 7-11, 2003

Program Chair: Professor James L. Skinner, Department of Chemistry, University of Wisconsin, Madison, WI 53706, skinner@chem.wisc.edu

EURESCO: Biophysics from First Principles: From the Electronic to the Mesoscale
September 7-12, 2002

Organizers: Anne Chaka, Flavio Seno
San Feliu du Guixols, Spain
http://www.esf.org/euresco/02/pc02182

AIChE Annual Meeting, Indianapolis, IN, November 3-8, 2002
Industrial Fluid Properties Challenge Symposium

"How well can molecular modeling and simulation predict fluid properties?" In November 2001 the AIChE Computational Molecular Science and Engineering Forum (CoMSEF) established an open competition for scientists and engineers to calculate results for the prediction of physical properties for industrially challenging fluids: http://www.cstl.nist.gov/FluidSimulationChallenge/. The results of the competition will be presented at a special symposium Sunday, November 3: http://www.aiche.org/conferences/techprogram/sessiondetail.asp?SessCode=21017&DSN=annual02

Sanibel Symposium February 23- March 1, 2003

The first half of the Symposium will be focused on Chemistry and Materials Physics, while the second half will be dedicated to Biology. The Organizers have extended the length of the Symposium for inclusion of a workshop.

Organizers: Quantum Theory Project, University of Florida

Ponce de Leon Resort, St. Augustine, Florida

http://www.qtp.ufl.edu/~sanibel/

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