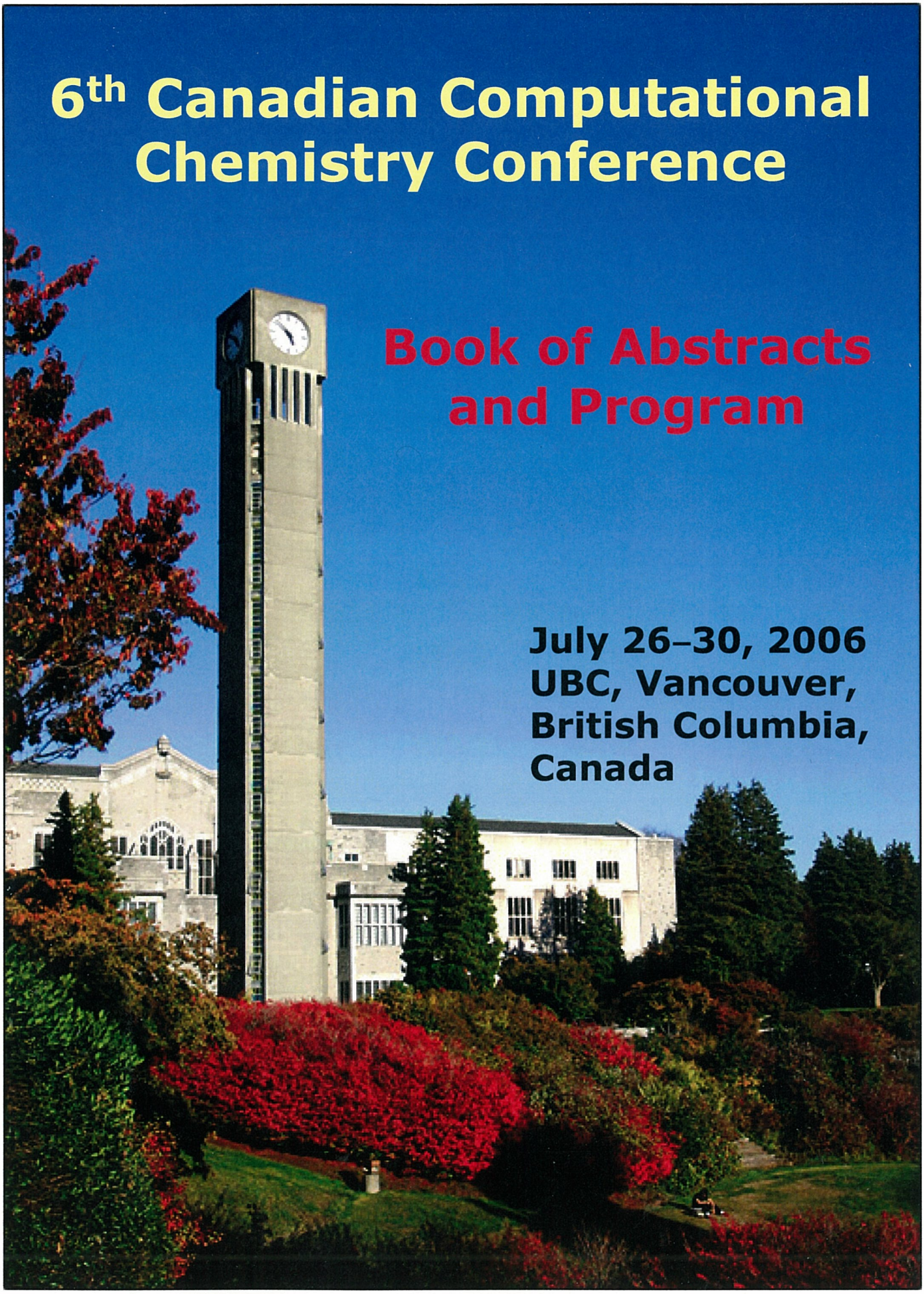
6th Canadian Computational Chemistry Conference



Book of Abstracts and Program

July 26–30, 2006
UBC, Vancouver,
British Columbia,
Canada

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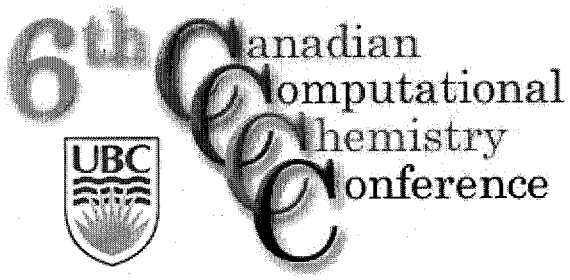

University of British Columbia
Vancouver, British Columbia, Canada
July 26-30, 2006

CRC Press Award for Excellence in Computational Chemistry

Taylor & Francis Books/CRC Press has generously sponsored a book award, the *CRC Press Award for Excellence in Computational Chemistry*, for posters presented by students and postdoctoral fellows at the CCCC6. Each awardee will receive one copy of the latest edition of the "CRC Handbook of Chemistry and Physics." During the lunch break on July 30, three recipients of this book award will be announced. Moreover, CRC Press has agreed to form a permanent partnership with the CCCCs to continually sponsor this book award in the future. We are grateful for the unwavering support from Taylor & Francis Books/CRC Press to our conference.

Welcome

It is our great pleasure to welcome you to the *6th Canadian Computational Chemistry Conference* (CCCC6) at the University of British Columbia, Vancouver, British Columbia, Canada.

Held every three years, the CCCC continues the tradition of celebrating the latest achievements and advances of computational chemistry in Canada and all over the world. It has been nearly ten years since the last CCCC was held in the western part of Canada. Below is the full list of all CCCCs:

- CCCC1-1992, Orford, Québec;
- CCCC2-1994, Kingston, Ontario;
- CCCC3-1997, Edmonton, Alberta;
- CCCC4-2000, Lennoxville, Québec;
- CCCC5-2003, Toronto, Ontario;
- CCCC6-2006, Vancouver, British Columbia.

The scope of the CCCC6 is devoted to all areas of Computational Chemistry, with special emphasis on novel method developments and state-of-the-art applications in life and materials sciences. We have assembled a star cast composed of 52 world-renowned computational scientists from academia and the biotech industry as our honored speakers. To our amazement, we have 177 participants from 21 countries and 85 poster presentations, which makes this conference the biggest CCCC ever.

Many members, especially Steven Hepperle, of the Wang Group at UBC have offered their assistance in organizing the CCCC6. We are particularly grateful to Lisa D'Alfonso and Sarah Johnston who have worked on all aspects of the local arrangements on the campus through the office of Conferences and Accommodation at UBC. We are also grateful to Bev Evans, Tricia Smurthwaite, Judy Wrinskelle, and Sheri Harbour of the Business Office of UBC Chemistry Department, who have helped us in a timely manner. Bev deserves our deepest appreciation for her highly efficient handling of the monetary affairs of the CCCC6: Bev has deposited all the donation and registration cheques!

We also thank the sponsors who have provided generous financial or material support for this meeting. Without a doubt, the contributions of the sponsors have enabled us to maintain the high-quality standard for the CCCC6. Especially, we would like to acknowledge Professor John W. Hepburn, UBC Vice President of Research, Professor Edward R. Grant, Head of UBC Chemistry Department, and Professor George A. Sawatzky, Director of the Advanced Materials and Process Engineering Laboratory (AMPEL) at UBC, who have genuinely supported and encouraged our organizing the CCCC6.

Finally, we hope that you will enjoy your stay at UBC and Vancouver during the CCCC6 from July 26 to 30, 2006. May the scientific aroma and inspiration be with you!

The CCCC6 Organizing Committee
Yan Alexander Wang (UBC), Conference Chair
Pierre-Nicholas Roy (Alberta), Conference Co-chair
Enrico O. Purisima (BRI, NRC), Conference Co-chair
Mark Thachuk (UBC), Conference Co-chair

List of Sponsors

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Daily Program

July 26 (Wednesday)		
08:30-18:30	Excursion #1: Whistler Mountain Trip (Pickup at 8:00 outside the Gage Towers)	
07:00-18:30	Excursion #2: Elfin Lakes Hiking Trip (Contact **Mark Thachuk** and/or **Gren Patey** for further details.)	
17:00-20:00	Registration in Fireplace Lounge at the Lobby of the Gage Towers (5959 Student Union Blvd.)	
22:00-22:30	HSBC Fireworks Competition (Team Italy) at English Bay	
July 27 (Thursday)		
08:30-08:40	**Alex Wang**	Welcoming Remarks
Session Chair: Alex Plyukhin		
08:40-09:20	**Grenfell Patey**	Structure and Interaction in Nematic Colloids
09:20-10:00	**David Manolopoulos**	Quantum Effects in Liquid Dynamics
10:00-10:30	**Richard Bowles**	Freezing in Small Clusters
10:30-10:45	Coffee Break (on-site)	
Session Chair: David Luckhaus		
10:45-11:25	**Piotr Piecuch**	Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems
11:25-11:55	**Marcel Nooijen**	New Developments in Single-Reference and Multi-Reference Electronic Structure Methods
11:55-12:35	**Tomasz Wesolowski**	Approximating the Kinetic Energy Differences as Explicit Density Functionals: Challenge for Theory and Possible Pay-offs in Large-Scale Computer Simulations
12:35-14:00	Lunch (on-site)	
Afternoon session sponsored by: Chemical Computing Group		
Session Chair: Lê H. Dao		
14:00-14:40	**Harold Scheraga**	The Two Aspects of the Protein Folding Problem
14:40-15:20	**Ruben Abagyan**	Modeling, Ligand Docking and Screening for Drug Discovery
15:20-15:50	**Nicolas Moitessier**	FITTED 1.0, Docking to Flexible and Solvated Macromolecules
15:50-16:20	**Jonathan Essex**	Recent Advances in the Calculation of Binding Affinities
16:20-16:35	Coffee Break (on-site)	
Session Chair: Aurora Clark		
16:35-17:15	**Michael Gilson**	Theory and Modeling of Molecular Recognition: Insights and Applications to Design
17:15-17:45	**Matthew Jacobson**	Protein Electrostatic Switches: Conformational Changes Induced by Post-Translational Phosphorylation and pH Changes
17:45-18:15	**Alexey Onufriev**	Analytical Approaches to Bio-molecular Electrostatics
18:15-18:35	**Sathesh Bhat**	Solvated Interaction Energy for Scoring Protein Ligand Binding Affinities: Exploring the Parameter Space and Application to Virtual Screening
18:35-20:00	Reception (on-site) Use your Reception Ticket for a free drink (wine, beer, juice, or pop)	
July 28 (Friday)		
Session Chair: Philip Hoggan		
08:30-09:10	**Rodney Bartlett**	Progress in *Ab Initio* DFT
09:10-09:50	**Emily Carter**	A New View of the Kondo Effect from an *Ab Initio* Embedding Theory

09:50-10:30	**Todd Martinez**	*Ab Initio* Molecular Dynamics Beyond the Born-Oppenheimer Approximation
10:30-10:45	Coffee Break (on-site)	
	Session Chair: T. Tung Nguyen-Dang	
10:45-11:15	**Radu Iftimie**	A Critical Assesment of the Importance of the k-Space Cutoff and the Fictitious Mass in Plane-Wave Based Car-Parrinello Calculations of Time-Correlation Functions
11:15-11:45	**Peter Kusalik**	Heterogeneous Crystal Growth: Insights from Molecular Simulations
11:45-12:15	**Matthias Ernzerhof**	Continuation of Density Functional Theory into the Complex Plane
12:15-12:45	**Baojing Zhou**	An Accurate Total Energy Density Functional
	Afternoon session sponsored by: AstraZeneca Canada, Inc.	
12:45-15:15	Lunch (on-site) Poster Session I with Coffee (end at 15:15)	
	Session Chair: James Gauld	
15:15-15:55	**Sergei Noskov**	Na^+/K^+ Selectivity in Biological Systems
15:55-16:35	**Andriy Kovalenko**	Molecular Theory of Solvation: A Novel Tool of Computational Chemistry
16:35-16:50	Coffee Break (on-site)	
	Session Chair: Lev Gelb	
16:50-17:20	**Andreas Klamt**	COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics
17:20-17:50	**Themis Lazaridis**	Modeling Peptide Binding to Membranes Using Implicit Solvation
17:50-18:20	**Gilles Peslherbe**	Recent Advances in Realistic Simulations of Excited-State Dynamics
	Dinner by yourself	
	July 29 (Saturday)	
	Session Chair: Mariusz Klobukowski	
08:30-09:10	**Axel Becke**	Post-Hartree-Fock Correlation Models
09:10-09:50	**Tom Ziegler**	The Application of TDDFT to Systems with a Spin or Space Degenerate Ground State
09:50-10:30	**Troy Van Voorhis**	Investigating Electronic Structure and Dynamics Via Constrained Density Functional Theory
10:30-10:45	Coffee Break (on-site)	
	Session Chair: Bernard Shizgal	
10:45-11:25	**Moshe Shapiro**	Entanglement and Coherent Control, and the Coordinate-Momentum Commutation Relations
11:25-11:55	**Alexander Brown**	Pulse Shaping for the Optimal Control of Molecular Processes
11:55-12:25	**Roman Krems**	Electric and Magnetic Field Control of Atomic and Molecular Dynamics at Low Temperatures
12:25-12:45	**Wei Quan Tian**	Efficiency Improvements on the Sum-Over-States Module for Hyperpolarizability Modeling and Applications to Fullerenes C_{60}, C_{70}, C_{180}, and C_{240}
12:45-15:15	Lunch (on-site) Poster Session II with Coffee (end at 15:15)	
	Session Chair: Sayyed Faramarz Tayyari	
15:15-15:55	**Jiali Gao**	Mechanism and Free Energies of Enzymatic Reactions
15:55-16:35	**Weitao Yang**	Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics
16:35-16:50	Coffee Break (on-site)	

	Session Chair: Delano Chong	
16:50-17:30	**Yuriko Aoki**	Elongation Method for Large Systems and Its Application to Nonlinear Optical Material Design
17:30-18:00	**Paul Ayers**	Interpreting Chemistry Using the Hard/Soft Acid/Base (HSAB) Paradigm
18:00-19:00	CCCC7 Meeting in the same lecture theater	
19:00-22:00	Banquet at Green College (6201 Cecil Green Park Road) Cash Bar starts at 19:00 in the Reception Room (first floor) Buffet Dinner starts at 19:30 in the Great Hall (second floor)	
22:00-22:30	HSBC Fireworks Competition (Team China) at English Bay	
	July 30 (Sunday)	
	Morning session sponsored by: Schrödinger, Inc.	
	Session Chair: Michael Eikerling	
08:30-09:10	**Anne McCoy**	Using Quantum Monte Carlo Approaches to Investigate the Spectroscopy and Dynamics of CH_5^+, $H_3O_2^-$ and $H_5O_2^+$
09:10-09:50	**Russell Boyd**	The Electron Density as an Interpretive Tool in Chemistry
09:50-10:30	**Dan McKay**	Rational Design of Phosphotyrosine Phosphatase 1B (PTP1B) Inhibitors
10:30-10:45	Coffee Break (on-site)	
	Session Chair: Franklin Chayette	
10:45-11:25	**Woody Sherman**	Structure-based Pharmacophores Derived from Fragment Docking
11:25-12:05	**Zsolt Zsoldos**	eHiTS: a Fast, Exhaustive Flexible Ligand Docking with Novel Scoring Function
12:05-12:45	**Ajay Jain**	Improvements in Docking: Ligand Energetics and Robust Search
12:45-14:00	Lunch (on-site)	
	CRC Press Award for Excellence in Computational Chemistry sponsored by Taylor & Francis Books/CRC Press	
	Session Chair: Arvi Rauk	
14:00-14:20	**Viktor Staroverov**	Effective Local Potentials for Orbital-Dependent Density Functionals
14:20-15:00	**Julian Gale**	Watching Crystals Assemble: Connecting Nanoscale Detail to Microscopic Observations
15:00-15:30	**Tom Woo**	The High Pressure World of Quantum Chemistry: Modeling the Chemistry of Materials under Extreme Pressure
15:30-15:50	**Ata Roudgar**	*Ab-Initio* Simulations at a Minimally Hydrated Array of Acid-Functionalized Surface Groups as a Model for Fuel Cell Membranes
15:50-16:05	Coffee Break (on-site)	
	Session Chair: Jolanta Lagowski	
16:05-16:45	**Jeremy Schofield**	Event-Driven Simulations
16:45-17:15	**Régis Pomès**	Distributed Replica Sampling
17:15-17:55	**Peter Tieleman**	Computer Simulations of Lipids
	End of the CCCC6 Meet at the CCCC7 in 2009	
	July 31 (Monday)	
07:30-20:20	Excursion #3: Victoria (Vancouver Island) Trip (Pickup at 7:00 outside the Gage Towers)	
09:00-17:30	Excursion #4: Vancouver City Local Tour (Pickup at 8:30 outside the Gage Towers)	

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Poster Schedule

Poster Session I, Friday afternoon, July 28

No.	*Presenter*	*Title*
P1-1	Zhu, Hongjuan	A Theoretical Study of the Original Shilov Reaction Involving Methane Activation by Platinum Tetrachloride ($PtCl_4^{2-}$) in an Acidic Aqueous Solution
P1-2	Abou-Rachid, Hakima	First-Principles Prediction of Heats of formation of Energetic Materials
P1-3	Abou-Rachid, Hakima	Atomistic Molecular Mechanics Simulation of Binder and Plasticizer Blends for Use in Plastic Bonded Explosives
P1-4	Baoukina, Svetlana	Molecular dynamics simulations of lipid monolayers
P1-5	Barnes, Brian	Meta-Optimization and Evaluation of Evolutionary Strategies for Empirical Potential Fitting
P1-6	Brown, Trevor	Computational Determination of Aqueous pK_a Values of Protonated Benzimidazoles
P1-7	Campagna-Slater, Valérie	Development of a "Quasi *ab initio*" Loop Modelling Algorithm
P1-8	Chen, Zhida	Geometric spin frustration for isolated plaquettes of the lattices: An extended irreducible tensor operator method
P1-9	Cheng, Chiao-Lun	Reorganization Energies from Molecular Dynamics with Constrained Density Functional Theory
P1-10	Chyatte, Franklin	Restricted Visceral Green Florescent Protein Expression Patterns in Transgene Mice
P1-11	Chyatte, Franklin	Utilizing Vertically Integrated Partnerships in Science Education to Develop Future Scientists
P1-12	Clark, Aurora	DFT and TDDFT Studies of the Conformational Dependence of the Optical Properties of Perylene Aggregates
P1-13	Cuervo, Javier	Path Integral Ground State Study of Finite Size Systems: Application to Small p-Hydrogen Clusters
P1-14	Difley, Seth	Charge-Transfer Excited State Energy Splittings by Constrained Density Functional Theory
P1-15	Plyukhin, Alex	Non-Markovian effects in Brownian motion
P1-16	Ernzerhof, Matthias	The method of generating potentials for the description of open systems
P1-17	Esquivel, Rodolfo O.	Electronic Structure and Physicochemical Properties of Selected Penicillins
P1-18	Evans, Jeremy	Calculation of Charge Transport Properties by Explicit One-Particle Density Matrix
P1-19	Fadda, Elisa	QM/MM Free Energy Study of Proton Transport in Protein Channels
P1-20	Firanescu, George	A combined molecular dynamics, exciton and harmonic analysis approach for the study of size effects in NH_3 nanoparticles
P1-21	Gajewski, Melissa	DFT AND MP2 calculations on the electronic structure and geometry of 18-crown-6, hexaaza-annulene and their complexes with Ba^{2+}, Ca^{2+}, Cd^{2+}, Hg^{2+}, K^+, Mg^{2+}, Na^+, Sr^{2+} and Zn^{2+} cations
P1-22	Galea, Natasha	Overcoming Hydrocarbon-based Performance Degradation (Coking) and Sulfur Poisoning on Solid Oxide Fuel Cell Anode Surfaces using Periodic DFT
P1-23	Gelb, Lev	*Ab Initio* Monte Carlo simulations of Fluid Phase Equilibria at Extreme Conditions
P1-24	Gilson, Michael	Novel Methods for Computer-Aided Drug Design

No.	***Presenter***	***Title***
P1-25	Grunwald, Robbie	Generalized Master Equation Analysis of Surface Hopping Dynamics
P1-26	Gusarov, Sergey	Self-Consistent Combination of the Three-Dimensional RISM Theory of Molecular Solvation with Analytical Gradients and the Amsterdam Density Functional Package
P1-27	Han, Heekyung	Distinguishability and Chiral Stability in Solution
P1-28	Hanna, Gabriel	Analysis of Kinetic Isotope Effects for Nonadiabatic Reactions
P1-29	Haras, Alicja	Copolymerization of polar and non-polar monomers by neutral asymmetric Pd(II) complexes: DFT study
P1-30	Mendez-Villuendas, Eduardo	Freezing of gold nanoparticles
P1-31	Hernandez de la Pena, Lisandro	Simulating Liquid Water with Discontinuous Molecular Dynamics
P1-32	Hoggan, Philip	Study of the optimised STO-nG expansion and its derivatives
P1-33	Hratchian, Hrant	Efficient modeling of silicon and silicon oxide surface chemistry with electronic structure theory using pseudo-atoms
P1-34	Huh, Yoonjung	Inclusion of symmetry in centroid molecular dynamics
P1-35	Iron, Mark A.	Tight Binding-Configuration Interaction (TBCI): A Novel Non-Iterative Method to Incorporate Charges into Tight Binding
P1-36	Issack, Bilkiss	Constrained Semiclassical Dynamics
P1-37	Kandt, Christian	Computer Modeling of the Vitamin B12 ABC Transporter BtuCD-F
P1-38	Kelly, Aaron	Nonadiabatic Dynamics in External Fields
P1-39	Lodriguito, Maricris	Externally Corrected Coupled-Cluster Methods Employing Method of Moments of Coupled-Cluster Equations and Multi-Reference Perturbation Theory
P1-40	Sinelnikov, Evgueni	Quantum chemical concepts and methods for intense field molecular dynamics: Tunnel ionization
P1-41	Peters, Michel	Quantum chemical concepts and methods for intense field molecular dynamics: Electron dynamics
P1-42	Jalili, Seifollah	Study of Xe and Kr Adsoption on Open-Single Walled Carbon Nanotubes using Molecular Dynamics Simulation
P1-43	Al Sunaidi, Abdullah	Mesoscale Simulation of Field-Induced Alignment in Rod-Like and Rod-Coil Copolymers
P1-44	Douali, Latifa	On The QSAR Studies of Non-Nucleoside Inhibitors of HIV Reverse Transcriptase: Hydrophobic and Steric Effects

Poster Session II, Saturday afternoon, July 29

No.	*Presenter*	*Title*
P2-1	Gubskaya, Anna	Prediction of Fibrinogen Adsorption onto Polymer Surfaces: 3D Case Study
P2-2	Johnson, Erin	Van der Waals Interactions from the Exchange Hole Dipole Moment
P2-3	Kelly, Evan	QM/MM and MD models of *Vinca* alkaloid interactions with Tubulin heterodimers
P2-4	Kong, Liguo	Unitary Coupled Cluster For Ground and Excited States
P2-5	Lagowski, Jolanta	Electronic Structure Properties of Phenylene and Thiophene Derivatives of Fluorene: TD-DFT Study
P2-6	Chen, Yakun	DFT Studies of Au_m and $PtAu_n$ Clusters and Their N_2 and O_2 Adsorption Complexes
P2-7	Lamoureux, Guillaume	Peptide Hydrolysis in Thermolysin: Reactant Structure and Reaction Mechanism Studied with Classical and QM/MM Molecular Dynamics
P2-8	Leon, Christopher	Similarity Transformations Applied to Vibronic Coupling Models
P2-9	Li, Hui	Improved Dissociation Energy and Potential Curve for BeH $X^2\Sigma^+$ from an Empirical and Ab Initio Study
P2-10	Zhang, Yu	Theoretical Studies on the Tautomers of Pyridinethiones
P2-11	Li, Rui Jiang	First-Principles Study of Electronic and Optical Properties of Nitrogen Doped Single-wall Carbon Nanotubes
P2-12	Li, Yvonne	A high-throughput computational approach to find new uses for old drugs
P2-13	Lo, John	DFT Investigation of The Fischer-Tropsch Synthesis on Fe Surface
P2-14	Lu, Aiyan	A New Hybrid Meta-GGA Density Functional
P2-15	Mahboob, Abdullah	Computational studies on a novel redox-active crown ether
P2-16	Mane, Jonathan	Quantum mechanical and hybrid quantum mechanical/molecular mechanical approach in the study of colchicine derivatives as potential anti-cancer drugs
P2-17	Yeung, Charles	Novel nanotube-coordinated platinum complexes
P2-18	Hemming, Christopher	Microheterogeneity in a Lattice Gas Model for Amphiphilic Solutes in Water
P2-19	Morales, Giovanni	Static Modeling of Ketene Dimerization Reaction in Gas and Liquid Phase
P2-20	Muchova, Eva	Conformationally Dependent Photodynamics of Glycine
P2-21	Tian, Wei Quan	AuPt binary clusters: structure and reactivity within density functional theory
P2-22	Narasimachary, Sudha	Molecular Modeling of Proton Dynamics in Fuel Cell Membranes
P2-23	Navidpour, Latifeh	Receptor docking studies of 1,5-diarylimidazole and 3,4-diaryltriazole derivatives possessing alkylthio substituent as a search for COX-2 selective enzyme inhibitors
P2-24	Tayyari, Sayyed Faramarz	Effect of O...O distance on the spectroscopic behaviors, structural parameters, and hydrogen bond strength in the enol form of beta-diketones
P2-25	Paul, Sandip	Why tert-Butyl Alcohol Associates in Aqueous Solution but Trimethylamine-N-oxide does not
P2-26	Pomogaev, Vladimir	Adaptation of the GIAO theory of NMR chemical shifts to periodic systems
P2-27	Rejnek, Jaroslav	On geometries and stabilization energies of H-bonded nucleic acid base pairs containing unusual base pairs tautomers: Complete Basis Set Calculations at the MP2 and CCSD(T) levels

No.	***Presenter***	***Title***
P2-28	Rickard, Gail	Calculated Cu(II)/Cu(I) Reduction Potentials of a Copper Bound His-His Dipeptide
P2-29	Rowley, Christopher	Generation of Initial Reactive Trajectories and Accelerated Sampling for Transition Path Sampling
P2-30	Sabaye Moghaddam, Maria	Effect of Pressure on Hydrophobic Interactions
P2-31	Zgid, Dominika	Orbital Optimalization with Density Matrix Renormalization Group Method in the Active Space
P2-32	Shadnia, Hooman	Quantitative Docking: Prediction Of Binding Affinities and Novel Estrogen Receptor Agonists
P2-33	Sokolovskii, Ruslan	Transition from molecular to hydrodynamic diffusion regimes: A molecular dynamics study
P2-34	Tomasi, Simone	Density Functional Theory Investigation into the Stereocontrol of the Syndiospecific Polymerization of Propylene Catalyzed by Cs-Symmetric Zirconocenes
P2-35	Trudeau, Travis	QSPR Approaches to Calculating the pKa Values of Protonated Aliphatic Amines
P2-36	Wanasundara, Surajith N.	Dissociation of Charged Protein Complexes in Gas Phase
P2-37	Williams, Sarah	Study of the Conformational Dynamics of HIV-1 Protease using Reversible Digitally Filtered Molecular Dynamics
P2-38	Zeng, Tao	Studies of APX_3 systems (A=O, S and X= Br and I)
P2-39	Klamt, Andreas	From Molecules to Properties: The Suite of Programs around COSMO-RS
P2-40	Sahnoun, Riadh	On the Design of Raney-Type Catalysts: A Density Functional Study
P2-41	Lamei Ramandi, Navid	Docking study of 3-(N,N-dimethylamino)-1,2-diphenyl-1-prpanone and other opioid analgesic

Lectures

Abstracts in presentation order

[O-1]

Structure and Interaction in Nematic Colloids

Gren Patey, T.G. Sokolovska and R.O. Sokolovskii

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Colloidal particles suspended in a liquid crystal induce nanoscale structure in the fluid media. Particularly in the nematic phase, the density and orientational distributions about the colloidal particles are highly directional, and lead to strong, highly directional interactions amongst the colloidal particles. The nature and physical origin of the colloid-nematic structure, and of the resulting forces will be discussed. Particular attention will be focussed on the influence of the the colloid-nematogen interactions, and on the strong effects of applied fields.

[O-2]

Quantum effects in liquid dynamics

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We have recently shown how the standard path integral molecular dynamics method, which has been used for the last twenty years to calculate the static equilibrium properties of quantum mechanical systems, can be generalized to calculate approximate real-time quantum correlation functions, and so applied to the study of chemical dynamics [1]. The resulting ring polymer molecular dynamics (RPMD) correlation functions are exact in several important limits, including the classical limit, the short-time limit, and the limit of a harmonic potential. They are also fully consistent with the exact quantum mechanical time-reversal and detailed-balance symmetries. So far, these correlation functions have been applied to the calculation of chemical reaction rates, to the diffusion in and the inelastic neutron scattering from a strongly quantum mechanical liquid (para-hydrogen), and to the translational and orientational diffusion in ambient liquid water, with encouraging results in all cases [2-6]. This talk will review these developments with an emphasis on the role of quantum mechanical fluctuations in liquid dynamics. These fluctuations are extremely important in liquid para-hydrogen, and they also play quite a significant role in the dynamics of room-temperature liquid water.

[1] I.R.Craig and D.E.Manolopoulos, J. Chem. Phys. 121, 3368 (2004).
[2] I.R.Craig and D.E.Manolopoulos, J. Chem. Phys. 122, 084106 (2005).
[3] T.F.Miller III and D.E.Manolopoulos, J. Chem. Phys. 122, 184503 (2005).
[4] I.R.Craig and D.E.Manolopoulos, J. Chem. Phys. 123, 034102 (2005).
[5] T.F.Miller III and D.E.Manolopoulos, J. Chem. Phys. 123, 154504 (2005).
[6] I.R.Craig and D.E.Manolopoulos, Chem. Phys. 322, 236 (2006).

[O-3]

Freezing in small clusters

Richard Bowles, Ivan Saika-Voivod, Eduardo Mendez-Villuendas
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110 Science Place
Saskatoon, SK S7N 5C9

Recent advances in Monte Carlo simulation techniques have revolutionized the molecular approach to nucleation. We combine parallel tempering with biased MC simulations to study freezing in small clusters with an emphasis on addressing the following two questions: 1. Is there a limit of stability of the liquid cluster with respect to its icosahedral phase and how can we use nucleation phenomena to find it? 2. What are the relative roles of surface and bulk ordering in the freezing of clusters?

[O-4]

Advances in electronic structure theory: single-reference coupled-cluster methods for multi-reference problems

Piotr Piecuch,[1,2] *Marta Wloch*[1], *Jeffrey R. Gour*[1], *and Armagan Kinal*[1]

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The key to successful description of molecular potential energy surfaces involving bond breaking, biradicals, and excited electronic states is an accurate and balanced description of dynamical and non-dynamical correlation effects. Conventional single-reference coupled-cluster methods, such as, for example, CCSD(T), provide an accurate description of dynamical correlation effects, which dominate electron correlations in the closed-shell regions of potential energy surfaces, but they fail when the bond breaking, biradicals, and other situations characterized by larger non-dynamical correlation effects are investigated. Traditionally, the adequate treatment of ground- and excited-state potential energy surfaces along bond breaking coordinates and biradicals has been the domain of expert multi-reference methods, but multi-reference methods have their limitations as well. For example, the low-order multi-reference perturbation theory methods may encounter serious difficulties with balancing dynamical and non-dynamical correlations in studies of reaction mechanisms, while the more robust multi-reference configuration interaction approaches are often prohibitively expensive. Practical single-reference procedures that could be applied to at least some of the most frequent multi-reference situations, such as single and double bond dissociations, biradicals, and excited states dominated by two-electron transitions, and that could provide a balanced description of dynamical and non-dynamical correlation effects with a more or less black-box effort would be an important step toward widespread progress. We will discuss our recent attempts to develop such procedures.

Specifically, we will focus on two ideas in electronic structure theory that have resulted in the development of renormalized and active-space coupled-cluster methods. The renormalized coupled-cluster methods, such as CR-CCSD(T), CR-CCSD(TQ), and CR-EOMCCSD(T), and, particularly, the recently developed rigorously size extensive formulation of CR-CCSD(T), termed CR-CC(2,3), which are all derived from the underlying method of moments of coupled-cluster equations (MMCC) and the asymmetric energy expressions that define all MMCC theories and are available in the GAMESS package, represent single-reference approaches that eliminate the failures of conventional coupled-cluster approximations, such as CCSD(T), CCSD(TQ), or EOMCCSD, whenever electronic quasi-degeneracies become more severe. At the same time, the CR-CC(2,3) approach is at least as accurate as CCSD(T) for closed-shell molecules near the equilibrium geometries. Formally, the active-space coupled-cluster methods and their extensions to excited states of radicals and other open-shell systems via the electron-attached and ionized variants of the equation-of-motion coupled-cluster theory represent the state-selective multi-reference coupled-cluster methods, but they largely preserve the simplicity of single-reference calculations. They use active orbitals only to select higher-than-double excitations of the otherwise single-reference coupled-cluster and equation-of-motion coupled-cluster methods. We will show that the relatively inexpensive renormalized and active-space coupled-cluster approaches provide an accurate and balanced description of reaction pathways involving bond breaking and biradicals, and excited states of radical and other molecular systems dominated by two-electron transitions.

[O-5]

New developments in single-reference and multi-reference electronic structure methods

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Transition-metal compounds, as occur for example in many industrial catalysts and in biological processes, pose severe challenges to both wave function and density functional based electronic structure methods. The systems are often large, when including the ligands in the calculation, while the 'magnetic part' of the system, consisting of the metal valence d and s electrons, requires consideration of configuration interaction in a large active space. Moreover, metal-ligand interactions are often highly correlated as a consequence of the fairly weak bonds involved. The satisfactory treatment of these systems using wave function based electronic structure methods that properly incorporate the spin and spatial symmetries, as well as a potential non-adiabatic treatment of nuclear reaction dynamics, lies in the future.

In our research group we are working on several aspects of the problem: local correlation techniques to reduce computational costs, coupled cluster type methods to treat the metal-ligand correlation problem, and efficient CI and DMRG approaches to treat the active space diagonalization are explored and combined to make the problem tractable. The focus of this talk will be an internally-contracted multi-reference coupled-cluster approach that shows significant promise. In addition, single-reference orbital-invariant CEPA type of approaches will be discussed that simplifies the non-linearity of coupled-cluster theory and might therefore be of significant advantage in local correlation approaches and parallel computation.

[O-6]

Approximating the kinetic energy differences as explicit density functionals: challenge for theory and possible pay-offs in large-scale computer simulations

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We will review our work dealing with approximating the bi-functional of the non-additive kinetic energy and its functional derivative by means of explicit functions of two electron densities. The approximated quantities are of key importance in possible computer simulations using the Cortona's formulation of density functional theory [1] or applying additional approximations concerning the electron density of a selected part of the investigated system [2] (orbital-free embedding) in multiscale-type of simulations. Examples of recent applications of the developed approximations in computer simulations based on orbital-free embedding formalism for systems embedded in various environments (liquids, enzymes, and solids for instance) will be given [3-6].

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[O-7]

An Accurate Total Energy Density Functional

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We propose a new density functional, *i.e.*, the Wang-Zhou (WZ) functional, for the evaluation of the total electronic energy. As guaranteed by the Roothaan inequality, it always produces a total energy lower than that from the Hohenberg-Kohn-Sham (HKS) functional, which is usually used in self-consistent Kohn-Sham (KS) density functional theory (DFT) calculations. Moreover, the WZ functional usually converges to the exact total energy from below, althouth whether it provides a lower bound remains to be investigated. Following the same spirit of the Zhou-Wang-λ (ZWλ) functional in the recently proposed orbital-corrected orbital-free (OO) DFT method [1], we linearly mix the WZ functional with the HKS functional to allow further systematic error cancellations. The resulting Wang-Zhou-λ (WZλ) functional is compared with the ZWλ functional in OO-DFT calculations for systems of different chemical environments. We found that the optimal value of λ for the former is more stable than that for the latter as the density gets closer to the exact density. This renders the direct evaluation of λ for the WZλ functional more plausible in the application of the linear-scaling OO-DFT method for large systems.

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[O-8]

The Two Aspects of the Protein Folding Problem

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There are actually two aspects of the theoretical approach to the protein folding problem. The first is to compute the thermodynamically stable native structure, and the second is to compute the folding pathways from the unfolded to the folded native form. I will discuss the evolution of computational methodology from an all-atom representation of the polypeptide chain to a united-residue representation of the chain. Blind tests in successive CASP exercises demonstrate increasing prediction success, in computing protein structure, from one CASP test to another. As for folding pathways, two different methods are used: (1) a stochastic difference equation procedure, and (2) Lagrangian dynamics with the united-residue force field. The results of all the computations, and the methods leading to them will be discussed.

[O-9]

Modeling, Ligand Docking and Screening for Drug Discovery

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Computational prediction of protein structure, protein function, and ligand binding is an area of critical importance considering the rapidly growing number of protein structures in Protein Data Bank. We focused on several related computational tasks:
(i) predicting druggable binding sites from a single structure;
(ii) predicting protein-protein interaction patches from a single structure
(iii) predicting conformations of protein loops in models by homology with high accuracy
(iv) accurate docking of flexible ligands to flexible protein pockets and virtual screening
(v) protein docking and refinement of flexible protein interfaces

We demonstrated that the small molecule binding pockets can be predicted with a certain transformation of the Lennard Jones potential [1]. This algorithm is useful in predicting new or allosteric binding sites or the feasibility of inhibiting protein-protein interaction with a small molecule. Predicting transient protein-protein interaction interfaces without known the partner was also proposed and validated on a large benchmark.

Including the receptor pocket flexibility into account in ligand docking remains a task highly specific to the nature of the receptor. We formulated a docking protocol that is relatively general and includes both the side-chain sampling and loop movements [3]. The ICM docking protocol led to discoveries of novel inhibitors against a number of biomedical targets, including de novo discovery of antagonists of RAR and thyroid hormone receptor ([4]), the discovery of inhibitors of alpha1-antityrpsin amyloid formation, and the discovery of new antimalarial agents.

The CAPRI protein docking experiment provides a good platform for evaluation of protein docking algorithms. While a fully reliable prediction of the association geometry given two uncomplexed structures remains unattainable, a considerable progress have been made of the last few years [5]. The difficulty of the problem is a function of the scale of the induced conformational changes upon association. We demonstrate that at least in some cases these changes can be correctly predicted. A new way of exchanging and browsing the chemical and structural data is also presented [6].

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[O-10]

FITTED 1.0, docking to flexible and solvated macromolecules.

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In response to the continual increase in the number of new potential therapeutic targets newly discovered targets, cost and time efficient designs and syntheses must be devised for active enzyme inhibitors, receptor antagonists/agonists, nucleic acid binders,.... The low hit rate observed with the expensive HTS of large combinatorial libraries has contributed proportionally less in the identification of novel leads compared with traditional rational or semi-rational design and synthesis.
The overview of the latest progress in the structure-based drug design field and the apparent weaknesses of the current molecular docking methods show that significant improvements must be achieved in order to develop a highly accurate molecular docking and virtual screening method, which may be used universally in the world of drug design. We have started an research program which investigates and proposes solutions to the docking of small molecules to flexible and solvated proteins and nucleic acids. Our efforts resulted in the development of FITTED 1.0 (Flexibility Induced Through Targeted Evolutionary Description) that comes with two additional modules ProCESS 1.0 (Protein Conformational Ensemble System Setup) and SMART (Small Molecules Atom typing and Rotatable Torsions assignment). This suite of programs docks flexible ligands to virtually flexible proteins while the modules sets up the protein files and ligand files for docking. In the mean time, we have developed a highly accurate force field-based scoring function now implemented in FITTED.

[O-11]

Recent Advances in the Calculation of Binding Affinities

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The calculation of binding affinties between a macromolecular host and a small guest molecule has been commonplace for at least the last 15 years. However, there are still significant difficulties with these methods relating to the level of approximation used in the actual binding free energy calculation itself. In addition, the force fields used to model the critical intermolecular interactions are still deficient, and the extent of sampling observed in these simulations makes the simulation of very different ligands a significant challenge. In this presentation I will describe some of the work we have been doing to address these issues, principally through the development of more efficient free energy calculation algorithms, the adoption of simplified solvent models, and developments to improve simulation sampling and efficiency.

[O-12]

Theory and Modeling of Molecular Recognition: Insights and Applications to Design

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We have developed a method for computing binding affinities, the second-generation Mining Minima algorithm, or M2, which gives encouragingly accurate agreement with measures affinities for a range of model systems. The talk will present applications to protein-ligand binding and to the analysis and computational design of synthetic receptors, as well as surprising results regarding the magnitude and character of changes in rotational, translational, and conformational entropy upon binding.

[O-13]

Protein Electrostatic Switches: Conformational Changes Induced by Post-Translational Phosphorylation and pH Changes

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Post-translational phosphorylation and the modulation of intracellular pH are very different biological mechanisms for regulating protein activity that share a common physico-chemical basis: site-specific modification of the charge on protein side chains. Kinases catalyze the covalent addition of phosphate, which predominantly carries a -2 charge at physiological pH, to specific amino acids. Cellular pH can vary between intracellular compartments and can be modulated in the cytoplasm by membrane ion channels. We have undertaken computational investigations of how phosphorylation and pH-driven changes in protonation states perturb the energy landscapes of proteins, which can drive changes in conformation and dynamics. With respect to phosphorylation, I will focus on activation loop phosphorylation in protein kinases, and demonstrate that it is possible to predict the structures of phosphorylated proteins starting from the structures of the unphosphorylated proteins, using loop and side chain sampling algorithms we have developed. CDK2 provides a case study where we analyze how and why the effects of phosphorylation differ depending on whether the kinase domain is unbound or bound to cyclin A or its phosphatase, KAP. I will also present some more recent results where we have begun to understand how certain proteins are engineered to respond to small changes in pH (less than one unit).

[O-14]

Analytical approaches to bio-molecular electrostatics

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The implicit solvent model has become popular in many bio-molecular applications due to its computational efficiency. Accurate representation of electrostatic interactions is key, but is often an unbalanced trade off between accuracy and speed. Traditionally, the popular generalized Born (GB) model has been used in this context, especially in computationally intense applications such as protein folding. We have recently proposed an approximate analytical approach to solving the (linearized) Poisson-Boltzmann (PB) equation that goes beyond the GB model. The new approach (ALPB) is rigorously derived, does not have fitting parameters and, unlike the GB model, permits definition of electrostatic potential everywhere in space. Some key physics missing from the GB formalism is recovered within the ALPB: as a result, the new approach is more accurate. Surprisingly, there is no additional computational overhead. The foundation and applications of the new model will be discussed.

[O-15]

Solvated Interaction Energy for Scoring Protein Ligand Binding Affinities: Exploring the Parameter Space and Application to Virtual Screening

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We present a binding free energy function that consists of force field terms supplemented by solvation terms (SIE or solvated interaction energy). The function was used to calibrate the solvation model along with the binding interaction terms in a self-consistent manner. In developing the function, we systematically explored different solute dielectrics constants, different methods of protein preparation as well as scaling of atomic radii, intermolecular van der Waals interaction energy and non-polar solvation terms. The resulting SIE function, coupled with Openeye's FRED docking program, was then applied in a virtual screening validation study using 16 pharmaceutically relevant targets. Our protocol gave good enrichment values for the majority of targets. In particular, it produced enrichment values for two targets (thymidine kinase and estrogen receptor), which were equal to or better than the majority of currently available virtual screening protocols.

[O-16]

Progress in Ab Initio DFT

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In our efforts to construct a seamless connection between wavefunction theory and density functional theory, we have recently generalized the ab initio dft approach to apply to open-shells and excited states. This enables us to address how the correct potential changes when a system is ionized or an electron is added. In particular, the issue of charge-transfer excited states has been addressed.

[O-17]

A New View of the Kondo Effect from an Ab Initio Embedding Theory

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Over the past decade, we have been developing an ab initio theory to describe localized correlated many-electron states in condensed matter. This theory embeds a correlated quantum chemistry description into surroundings described by periodic density functional theory (DFT). Recent technical advances in the theory include: (i) implementation of ultrasoft pseudopotentials (USPPs) in a consistent manner across all levels of theory (periodic DFT, CASSCF, and CI), (ii) self-consistent updates of the density of the total system, thereby allowing a fully-self-consistent embedding operator, and (iii) a multi-reference singles and double excitation CI (MRSDCI) treatment of electron correlation in the embedded region. Our current embedded configuration interaction (ECI) theory is now more efficient (via USPPs), less approximate (by use of self-consistent embedding potentials), as well as more accurate (via MRSDCI) than earlier versions that were based either on many-body perturbation theory or valence CI/CASSCF wavefunctions. The current version is now being used to study a variety of systems/phenomena where DFT is known to fail, due to either neglect of many-body effects or self-interaction artifacts. Time permitting, more than one example will be given of how the embedding theory is able to give a qualitatively (as well as quantitatively) different view of these systems/phenomena. We will focus on the Kondo effect, a long standing problem in condensed matter physics, which has not had a first principles solution until now. The Kondo effect refers to the observation of an anomalous resistivity minimum at low temperatures for materials containing magnetic transition metal impurities in nonmagnetic host metals. We will show that the ECI theory is able to capture the physics and offer a new view of this phenomenon, while periodic DFT and finite cluster quantum chemistry calculations do not.

This work was done in collaboration with Dr. Patrick Huang, Michele Pavone, and Sahar Sharifzadeh. It was funded by the U.S. National Science Foundation and the U.S. Department of Energy, Basic Energy Sciences.

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[O-18]

Ab Initio Molecular Dynamics Beyond the Born-Oppenheimer Approximation

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The ab initio multiple spawning (AIMS) method has been developed to model molecular dynamics including quantum mechanical effects such as nonadiabatic transitions and tunneling. The electronic and nuclear Schrodinger equations are solved simultaneously, i.e. "on-the-fly". We begin with a discussion of some recent developments in the multiple spawning method and some benchmarks on large-dimensional model systems. A pseudospectral method for evaluation of the required integrals which uses information from all basis functions is presented and evaluated. New methods of adaptively expanding and contracting the nuclear basis set are discussed. After discussing the spawning method for dynamics, we present recent results of AIMS simulations for photoinduced isomerization, excited state proton transfer, and electronic relaxation in DNA and RNA bases. We find a conical intersection between three electronic states simultaneously to be important in excited state intramolecular proton transfer and we discuss the extent to which dynamics around a three-state intersection might differ from that around two-state intersections. Simulation results are compared with recent ultrafast experiments where these are available.

[O-19]

A Critical Assesment of the Importance of the k-Space Cutoff and the Fictitious Mass in Plane-Wave based Car-Parrinello Calculations of Time-Correlation Functions

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We will investigate the conditions in which plane-wave based Car-Parrinello simulations can be employed to estimate time-dependent linear response properties of aqueous systems with good accuracy. The properties we will be focusing on include the diffusion constant, the molecular reorientation time and the infrared spectrum.

The role of the k-space cutoff in plane-wave based methods will be carefully analyzed. We will see that larger cutoffs must be employed for accurate determination of time-correlation fucntions than for statical ones. The effect of the fictitious mass in Car-Parrinello simulations of time-dependent properties will also be investigated, leading to quantitative predictions of infrared spectra.

We will conclude by commenting on the influence of other factors that limit the accuracy in Car-Parrinello simulations, such as the exchange-correlation functional, the neglect of nuclear quantum effects and quasi-ergodicity sampling problems.

[O-20]

Heterogeneous Crystal Growth: Insights from Molecular Simulations

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While the molecular behaviour within liquids and solids has been extensively studied, one important aspect of these systems that has remained poorly understood at the molecular level is the first order phase transition between them. Since very few experiments are able to probe directly the microscopic environment of the interface of a growing crystal, molecular simulation affords us an excellent opportunity to investigate liquid/solid interfaces and mechanisms of crystal growth at a molecular level. In this paper I will briefly review some previous approaches and the results obtained. I will then describe a new approach we have developed for the simulation of heterogeneous crystal growth and will demonstrate its success with simple atomic systems. I will report specific results for the ice-water interface and the growth of ice (I) crystals, where I will clearly demonstrate that the process of crystal growth is characterized by a collective phenomenon involving many molecules (rather than the "sticking" of individual molecules). I will present data from work with gas hydrates, where the properties of the interface are key to an understanding of the systems. Finally, very preliminary results for studies of crystal grow from solution for simple model LJ systems, from which we are already been able to extract some important insights, will be discussed.

[O-21]

Continuation of density functional theory into the complex plane

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We present an extension of Hohenberg-Kohn-Sham density functional theory to the domain of complex local potentials and complex electron densities. The formalism provides a DFT applicable to resonance (Siegert) states and other scattering and transport problems that can be described by a bound state of a Hamiltonian containing a complex local potential. The theory is illustrated for systems that are homogeneous or close to homogeneous.

[O-22]

The time-dependent quantum wave packet approach to the electronically nonadiabatic processes in chemical reactions

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The time-dependent quantum wave packet approach has been improved and formulated to treat the multiple surface problems and thus provided a new simple but clear quantum picture for interpreting the reaction mechanism underlying the nonadiabatic dynamical processes. The method keeps the salient feature of the original quantum wave packet theory developed for single surface problems, i.e., the introduction of the absorbing potential and the grid basis including the discrete variable representation and the fast Fourier transformation, which made the present methodology a very efficient implement for nonadiabatic quantum scattering calculations. Here we review the theoretical basis of this approach and its applications to fundamental triatomic chemical reactions, the latter include the nonadiabatic dynamics calculations on the F+H2, F+HD, F+D2, O(1D)+N2, O(3P, 1D)+H2, D++H2 and H++D2 reactions. We also present a thorough historical overview of the theoretically nonadiabatic dynamical investigations particularly on triatomic systems, and show how the time-dependent wave packet approach complements to the time-independent quantum scattering theory.

[O-23]

Na+/K+ Selectivity in Biological Systems

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One of the main physiological functions of biological channels and transporters is efficient and often very selective transport of certain ions through the membrane to the cell. However, molecular origin of the observed ability to discriminate between very similar ions such as Na+/K+ selectivity is unclear. To elucidate how channels achieve high selectivity for K+ over Na+ and molecular dynamics (MD) simulations free energy perturbation (FEP) were performed on the basis of the crystallographic structure of the KcsA, NaK and LeuT pores embedded in a fully solvated phospholipid membranes. The results show that KcsA or NaK channels does not select for K+ or Na+ ions by providing a binding site of an appropriate (fixed) cavity size. Rather, selectivity for K+ depends on the intrinsic local physical properties of ligands coordinating the cation in the binding site, and is a robust feature of a pore symmetrically lined by backbone carbonyl groups. Difference in water accessibility to different binding sites modulates observed magnitude of the Na+/K+ selectivity from highest at the site S2(KcsA), where ion is fully dehydrated to modest or even opposite sign selectivity for other sites in the KcsA and NaK channels.

Further analysis reveals that it is the interplay between the attractive ion-ligand (favoring smaller cation) and repulsive ligand-ligand interactions (favoring larger cations) that is the basic element governing Na+/K+ selectivity in flexible protein binding sites. Because the number and the type of ligands coordinating an ion directly modulate such local interactions, this provides a potent molecular mechanism to achieve and maintain a high selectivity in protein binding sites despite a significant conformational flexibility. Precise role of the surrounding water in the determination of the ion selectivity was illustrated by the detailed analysis of ion permeation through NaK channel and QM/MM MD simulations of the ion hydration in the cavity of KcsA.

Main conclusions about Na+ binding sites organization and energetics were drawn from the analysis of MD and FEP simulations of LeuT. It was shown that still there is no need in overall structural rigidity, however the actual selectivity can be achieved through two very different mechanisms.

[O-24]

Molecular Theory of Solvation: A Novel Tool of Computational Chemistry

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Prediction of the electronic properties of molecules in solution has been a crucial and challenging problem of modern quantum chemistry. A description entirely from the first principles is provided by the Car-Parrinello method which performs molecular dynamics (MD) coupled with the Kohn-Sham density functional theory (KS-DFT) applied to each molecule of the liquid. However, this approach gets prohibitively slow even for relatively small systems with thousands solvent molecules. This severe limitation is overcome in a multiscale approach with quantum mechanics (QM) applied to a solute molecule or cluster with several solvent molecules in the self-consistent field of classical solvent. Coupled with MD for solvent, it becomes a powerful first-principle approach to electronic and classical solvation structure of macromolecules in solution. Unfortunately, MD is extremely time-consuming, if feasible at all, for realistic systems with complex species forming hydrogen bonding networks and hierarchic supramolecular nanostructures. Two examples are organic nanotubes in aqueous electrolyte solution and organic solvents, and sorption of electrolyte solutions in nanoporous electrodes. Furthermore, dynamics of such systems and processes can be very slow, far beyond the reach of MD simulations.

A popular alternative has been the models of continuous medium effectively representing the solvent reaction field. While being very simple, affordable, and therefore attractive for routine computations, such models are not transferable and thus do not have predictive capability. Every new solvent or solvent mixture requires another parameterization for the shapes and sizes of a cavity encapsulating a solute molecule, based on the results of a first-principle approach. Moreover, continuum models do not provide an adequate physical picture of solvation, neither for the structure of solvation shells nor for the solvation thermodynamics, including the impossibility of getting the solvation entropy. For instance, they could never distinguish between the tetrahedral and zigzag hydrogen bonding of water and alcohol, not speaking of such complex microheterogeneities as micromicelles in their mixtures.

A principally advantageous approach provided by statistical physics is integral equation theory of molecular liquids, or molecular theory of solvation. Given a force field for solution species, it yields the solvation structure and thermodynamics from the first principles by solving the integral equations for the correlation functions and then getting the free energy and its derivatives in a close analytical form in terms of the correlations. A great advantage compared to molecular simulations is that the theory works at an ensemble of system realizations in the entire phase space, and thus gives access to processes occurring on large space and time scales. The three-dimensional reference interaction site model (3D-RISM) integral equation theory [1] predicts in three-dimensional detail the solvation structure of macromolecular species in a given molecular solvent, and properly accounts for the effect of their geometry and chemical specificities such as excluded volume features and hydrogen bonding. It yields the solvation free energy and its thermodynamic derivatives such as entropy, partial molar volume, compressibility, etc; and the potentials of mean force between solute and solvent molecules in solution.

A self-consistent field combination of the 3D-RISM theory of molecular solvation with the KS-DFT for electronic structure was recently introduced [1,2], and has been implemented in the Amsterdam Density Functional (ADF) quantum chemistry software package [3]. (The 3D-RISM method can be similarly coupled in a self-consistent field combination with any multireference electronic structure theory, such as the CASSCF/3D-RISM approach [4].) This self-consistent multiscale method gives from the first principles electronic and classical structure in solution, including the analytical gradients which determine

the energy surface driving chemical reactions. With reasonable computational efforts, it allows one to predict the chemistry of complex macromolecules in a given solvent, which renders it an attractive alternative to QM/MD and a superior replacement to continuum solvation schemes in theoretical chemistry.

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[O-25]

COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics

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Due to the rapid developments of methods and computers, reliable quantum chemical calculations on molecules of up to 50 - 100 atoms can nowadays be performed within the time-scale of a day on cheap computer hardware. Thus quantum chemistry, and here especially the density functional theory (DFT), has become an efficient source of information for molecular properties. Nevertheless, the traditional quantum chemistry is restricted to the calculation of single molecules in vacuum or to small clusters. Hence it cannot be directly used for the calculation of properties of molecules in liquids or even for fluid phase equilibrium properties.

In this situation, dielectric continuum solvation methods as PCM or COSMO have become quite popular. In this talk I will specially focus on the extension of COSMO by a combination with statistical thermodynamics, COSMO-RS. This provides an efficient link between quantum chemistry and fluid phase thermodynamics. COSMO-RS starts from a quantum chemical DFT/COSMO calculation for each chemical species under consideration, i.e. for solutes and solvent molecules, in which each molecule is treated as if embedded in a perfect conductor. This state of ideal electrostatic screening is used as reference point for the consideration of molecules in the liquid phase. All energies are expressed relative to this state, and interaction energies of molecules in solution are described as contact interactions of ideally screened molecular surface pieces. All interactions are quantified by the screening charge densities on the adjacent surface pieces. Combined with an extremely efficient and nevertheless exact statistical thermodynamics algorithm of pair-wise interacting surfaces, this description of molecular interactions in solution enables the calculation of the chemical potentials, i.e. the activity coefficients, of almost arbitrary solutes in almost arbitrary solvents, even in multi-component mixtures. Finally this enables the calculation of phase diagrams of liquid systems, i.e. of activity coefficients, vapor pressures, excess free energies and enthalpies. COSMO-RS can be applied not only to neutral systems, but as well to charged species, i.e. to electrolyte systems, pKa-calculation, and even to complex systems as ionic liquids, micelles and bio-membranes.

COSMO-RS opens a wide area of applications in all areas of computational chemistry, i.e. in general physical chemistry, drug design, and in chemical engineering. Examples from different areas will be given.

[O-26]

Modeling peptide binding to membranes using implicit solvation

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Implicit solvation models have generated a lot of interest thanks to their convenience and speed. With minimal effort these models can be extended to lipid membranes with even greater payoffs. We recently extended the EEF1 function for soluble proteins to an implicit membrane model (IMM1) by making the solvation parameters and the dielectric screening dependent on the vertical coordinate. The membrane surface charge is modeled by use of the Gouy-Chapman theory. The transmembrane voltage is also straightforward to incorporate. Using this model we have studied the interaction of a number of membrane-active peptides with membranes. The influenza hemagglutinin fusion peptide prefers a shallow, slightly tilted orientation at the membrane interface, but trimerization facilitates membrane insertion. Alamethicin exhibits two different orientations of similar energy, with voltage favoring deeper insertion. We have also developed a formalism for calculating absolute, pH-dependent membrane binding free energies and applied it to the membrane targeting domain of phosphocholine cytidylyltransferase.

[O-27]

Recent Advances in Realistic Simulations of Excited-State Dynamics

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Computer simulations of the real time-evolution of complex chemical systems in their electronically excited states, resulting for example from photoexcitation, represent many challenges for modern computational chemistry. One such challenge lies in the proper description of the electronic structure of the system of interest in various electronic states and along different trajectories. In this contribution, we will discuss two approaches to address this challenge, which will be illustrated by realistic simulations of the excited-state dynamics of ions and salt ion pairs clustered with a number of solvent molecules.

One of the fascinating features of ionic clusters such as iodide-solvent clusters lies in the possibility of photochemical transfer of an electron from the ion to the solvent, giving rise to so-called charge-transfer-to-solvent (CTTS) excited states, which eventually leads to precursor states of the solvated electron. We will show how multi-level first-principles dynamics techniques can be employed to simulate the relaxation of photoexcited iodide-solvent clusters, producing simulation results amenable to connection with recent femtosecond photoelectron spectroscopy experimental data.

The second topic discussed deals with the photochemistry of sodium iodide salts in aqueous clusters. Sodium iodide has long been a paradigm for ultrafast nonadiabatic dynamics and our interest focuses on the influence of solvation on this process. In this context, we will discuss Quantum Mechanics / Molecular Mechanics (QM/MM) nonadiabatic simulations of photoexcited $NaI(H_2O)_n$ clusters, in which the electronic structure of sodium iodide is described by semiempirical valence-bond theory and the water molecules are represented by model potentials. The importance of employing polarizable model potentials and force fields to describe the ground-state structure and energetics of chemical and biochemical systems is now well recognized. We will show how a proper account of solvent polarization is also essential in performing realistic excited-state simulations of $NaI(H_2O)_n$ relaxation, the results of which can then be used to interpret experimental results.

[O-28]

Post-Hartree-Fock Correlation Models

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We have developed post-Hartree-Fock correlation models for all types of correlation of importance in chemistry: dynamical, nondynamical, and dispersion. All of these are based on real-space modelling of the correlation hole. The latest developments will be reported, as well as a new and very simple approximation for the effective potential of the exact exchange part.

[O-29]

The application of TDDFT to systems with a spin or space degenerate ground state

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Ordinary time-dependent density functional theory (TDDFT) is not able to treat single excitations involving spin-flips and can thus not treat systems with spin generate ground state. We introduce in the first part of our talk a formulation of TDDFT based on a non-collinear representation of the XC potential. Within the non-collinear representation, we are able to apply TDDFT to atoms and molecules with a spin-degenerate ground state and thus study spin-multiplet splittings. The second part of the talk deals with spatially degenerate ground states using time-dependent density functional theory (TDDFT). We propose here a new "Transformed reference via an intermediate configuration Kohn-Sham TDDFT (TRICKS-TDDFT) method. This method avoids the complications caused by the multi-reference nature of spatially degenerate ground state by taking a non-degenerate excited state with desirable properties as the reference for the TDDFT calculation. The scope and practical application of the method is discussed.

[O-30]

Investigating Electronic Structure and Dynamics Via Constrained Density Functional Theory

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We show that the well-known shortcomings of approximate density functionals for treating electron transfer (ET) can be overcome by applying physically motivated constraints to the electron density. We summarize our implementation of this constrained density functional theory (CDFT) and present several illustrative applications that demonstrate the strengths of the new formalism: 1) CDFT allows charge transfer excitations to be treated accurately within a ground state formalism, including the long range -1/r interaction between the electron and the hole 2) One directly obtains diabatic states, which can be unambiguously associated with Marcus theory parameters 3) Charge recombination can be studied in real time by releasing an initially constrained state and monitoring the ensuing time evolution. Applications of CDFT to ground state electronic structure problems – such as the prediction of exchange couplings and reaction barrier heights – will also be touched on as time permits.

[O-31]

Entanglement and coherent control, and the coordinate-momentum commutation relations.

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We first discuss the role of entanglement in the measurement process and show that the familiar diagonalized form of the density matrix upon measurement is a direct result of entanglement induced by the system-apparatus scattering process and our incomplete knowledge of the apparatus. We then show that coherent control can be viewed as a disentanglement transformation.

In the second part of the talk we give a derivation of the coordinate-momentum commutation relations that invokes only the mathematical structure of the Hilbert space underlying quantum mechanics, classical mechanics, and the 1:1 correspondence between classical-observables and the linear operators of quantum mechanics.

[O-32]

Pulse shaping for the optimal control of molecular processes

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The use of tailored laser pulses to control chemical processes has received much attention recently, in part due to the rapid development of experimental pulse shaping techniques. With respect to controlling quantum dynamics, optimal control theory (OCT) has been utilized as an effective tool for determining the shaped laser field that will induce a desired quantum process. The optimal control of a laser driven system can be viewed as an inverse problem: rather than knowing the laser field and determining the final molecular states populated after the interaction of the field, a desired final state is `known' and the laser field that takes the system to this state must be found. The goals of optimal control are two-fold: first, to achieve a desired quantum process utilizing shaped laser pulses, and second, to detect the properties of the system by analysing the optimized pulse.

In this talk, the use of optimal control theory to find laser fields for controlling quantum dynamics will be reviewed. In particular, a new method that we have proposed to design optimized control fields with desired temporal and/or spectral properties will be outlined. Restriction of laser parameters such as frequency and amplitude is required in order to propose experimentally realistic shaped laser fields. The method will be illustrated by examining the optimal control of vibrational excitation of the Cl-O bond with both temporally and spectrally restricted pulses.

[O-33]

Electric and Magnetic Field Control of Atomic and Molecular Dynamics at Low Temperatures

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The development of experimental techniques for the production of ultracold (nano-Kelvin temperature) atoms has generated a resurgence in atomic collision physics. New fields of research such as coherent control of atomic and molecular processes, quantum information and matter wave interferometry make extensive use of ultracold atoms. A major thrust of the research is now to create ultracold molecules. The creation and trapping of ultracold molecules will be a revolution in molecular physics and physical chemistry. Spectroscopic measurements of unprecedented precision, manipulation of chemical reactions, and molecular Bose-Einstein condensation may become possible, leading to new fundamental discoveries.

I will review our work on quantum simulations of molecular collisions at very low temperatures in the presence of external electric and magnetic fields. The kinetic energy of atoms and molecules at subKelvin temperatures is smaller than perturbations due to interactions with external electric or magnetic fields available in the laboratory. External fields may therefore be used to induce dissociation of weakly bound molecules [1], stimulate forbidden electronic transitions and control dynamics of cold atoms and molecules in a variety of ways [2]. I will present our recent work on mechanisms of manipulating and controlling dynamics of cold atoms and molecules with external electromagnetic fields. In particular, I will discuss the possibility of using electric fields to induce novel three-channel Feshbach resonances [3] and to manipulate spin degrees of freedom of cold molecules. I will discuss the differential scattering of ultracold atoms and show that moderate electric fields (~100 kV/cm) can be used to manipulate the angular dependence of the scattering cross sections at ultracold temperatures. I will show that electric fields may also be used to induce or suppress collisional spin decoherence in diatomic molecules. The mechanism of electric-field control of spin-flipping is based on the interplay of the molecule - field interaction and intramolecular spin-rotation couplings. Finally, I will discuss the possibility of controlling molecular collision processes by rotating superimposed magnetic and electric fields relative to to one another.

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[O-34]

Efficiency improvements on the sum-over-states module for hyperpolarizability modeling and applications to fullerenes C_{60}, C_{70}, C_{180}, and C_{240}

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The original sum-over-states (SOS) module within time-dependent perturbation theory in hyperpolarizabilities modeling has unfavorable scaling factor ($\sim n^{m+1}$, n is the number of states for electronic excitations and m is the order of hyperpolarizability) in term of CPU time. Three-stage strategies are proposed in our work to improve the computational efficiency of the SOS module. Test cases will be presented for the second order hyperpolarizability (γ) studies on fullerenes C_{60}, C_{70}, C_{180}, and C_{240}.

[O-35]

Mechanism and Free Energies of Enzymatic Reactions

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Protein dynamics encompasses a wide range of time and length scales that are essential to biological processes including ligand binding, energy transfer, and catalysis. However, the relationship of protein dynamics and enzyme catalysis is still poorly understood. In this talk, I will describe molecular dynamics simulation studies of the dynamic effects on enzymatic reactions, including the nucleophilic substitution reaction of dichloroethane by a carboxylate group in haloalkane dehalogenase and the amino acid racemization reaction by alanine racemase. In addition, I will present studies of vibrational energy relaxation of small ligand molecules in the enzyme active site.

We employ a combined QM/MM potential to model the chemical process. We found that protein dynamics accelerates the reaction rate by a factor of 2 over the uncatalyzed reaction. Compared to the thermodynamic effect in barrier reduction, protein dynamic contribution is relatively small. However, analyses of the friction kernel reveal that the origins of the reaction dynamics in water and in the enzyme are different. In aqueous solution, there is significant electrostatic solvation effect, which is reflected by the slow reorganization relaxation of the solvent. On the other hand, there is no strong electrostatic coupling in the enzyme and the major effect on reaction coordinate motion is intramolecular energy relaxation. Some of the misconceptions derived from empirical use of an effective state valence bond model will also be addressed.

I will also describe a study of the vibrational frequency shift and energy relaxation of an azide ligand in the active site of carbonic anhydrase as compared to an azide ion in aqueous solution. In this work the oscillator and the enzyme active site is treated explicitly by quantum mechanics. Thus, the dynamical change of the potential energy surface of the oscillator can be adequately represented. We found that although the average geometry of the azide ion is symmetric in aqueous solution, the instantaneous solute-solvent interactions induce localization of the resonance structures having triple bond characters, leading to a blue shift in the observed antisymmetric vibrational frequency in polar solvents. The best estimate of frequency shift of azide ion from water to the active site of carbonic anhydrase II is 56 cm-1, in good accord with the experimental value of 51 cm-1. Analyses of the computational results demonstrate that the origin of the protein-induced blue shift is due to a combination of ligand binding to the zinc metal ion and protein dynamical interactions. The former makes the dominant contribution by stabilizing the N∫N1+-N2- ionic state through ligand-metal coordination, whereas the latter attenuates the ligand-metal bonding, recovering some of the N1-=N1+=N1- valence bond character. Furthermore, the vibrational energy relaxation time has been determined both in water and in the enzyme. Intramolecular vibrational redistribution provides the main doorway for energy relaxation of the azide antisymmetric stretch in the enzyme, which is similar to that obtained previously for an azide ion in water by Morita and Kato. Following this mechanism coupled with the quantum correction factor suggested by Skinner and Park, we obtained vibrational relaxation times of about 2 ps in water and 6 ps in carbonic anhydrase, consistent with experiments. Importantly, the change in relaxation time by a factor of 2.5 from water to the enzyme active site is correctly reproduced.

[O-36]

Simulations of Complex Biological Systems with Quantum Mechanics and Statistical Mechanics

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The development of linear-scale and multi-scale methodologies and their applications to biological systems will be presented. These methods extend the realm of quantum mechanical theory to complex systems, which are otherwise beyond the reach of conventional approaches. Simulations of the complex mechanics of polymers in single-molecule atomic force microscopy experiments (AFM) and simulations of chemical reactions in enzymes will be featured. Recent development in the efficient determination of reaction paths, the development of reaction path potential and chemical reaction dynamics calculations will be described. Applications and comparison with experimental studies will be presented.

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[O-37]

Quantum mechanical methods for protein study

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An efficient MFCC (molecular fractionation with conjugate caps) approach for ab initio computation of proteins or other large biological molecules is presented. Newc development and implementation for ab initio computation of total electron density and energy of protein are discussed and various numerical examples are provided. Two specific approaches for protein energy calculations are discussed. One is based on constructing total electron density matrix of the system based on the MFCC ansatz, and the other employs direct MFCC energy calculation coupled with molecular mechanics for long range fragment interactions.

[O-38]

Elongation method for large systems and its application to NLO material design

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Since we proposed an elongation method in 1991[1], we developed this method to be applicable for large systems with high accuracy at the Hartree-Fock and Density Functional Methods[2, 3]. In this treatment, after we obtain the electronic structure of the starting cluster, we localize the canonical molecular orbitals into regional localized molecular orbitals[4] so that any polymer chain can be built up by adding a monomer unit to this starting cluster step by step. By this fashion, any random polymer can be theoretically synthesized by the elongation method.

The elongation method is implemented to GAMESS and applied to the determine electron density as well as the total energy with excellent accuracy(~10- 9 a.u./atom in total energy errors) [5-8] and the nonlinear optical properties of periodic and non-periodic polymers. The finite-field elongation approach is employed for test calculations of the electric (hyper)polarizabilities for some model systems at HF and DFT levels[9-11]. The most important advantage of this approach is the large compute time saving in the SCF stage since the dimension of the HFR equations remains the same regardless of the increasing number of the atoms in the system. Another advantage is that this approach can be used to treat non-periodic polymers by building up polymer chains with arbitrary sequence of monomers.

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[O-39]

Interpreting Chemistry Using the Hard/Soft Acid/Base (HSAB) Paradigm

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Reactions where a hard (or soft) acid (or base) replaces a soft (or hard) acid (or base) to form the product predicted by the hard/soft acid/base (HSAB) principle are examined. When electron transfer effects dominate the reactivity and other effects are negligible, the HSAB principle is driven by the surpassing stability of the soft acid/soft base product. Electrostatic effects are also treated, focusing on the tendency for hard reagents to be small and possess charged reactive sites. When electrostatic effects dominate the reactivity and other effects are negligible, the HSAB principle is driven by the surpassing stability of the hard acid/hard base product. Because electron-transfer and electrostatic considerations separately favor the HSAB principle, the overall picture of reactivity (which includes both effects) provides strong support for the HSAB principle. Computational methods for classifying whether a reagent's reactivity is dominated by electron-transfer or electrostatic effects can be based on these insights

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[O-40]

Using Quantum Monte Carlo approaches to investigate the spectroscopy and dynamics of CH_5^+, $H_3O_2^-$ and $H_5O_2^+$

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In this talk, I will discuss some recent work in our group that has been focused on identifying spectral signatures of large amplitude motions. In particular, the vibrational spectra of all of the systems, mentioned in the title, contain features that cannot be understood by the usual harmonic description of molecular vibrations that we learn in physical chemistry classes. This provides a hint that something interesting is going on.

In the case of CH_5^+, zero-point energy provides sufficient energy to allow the ion to sample all 120 (5!) equivalent minima with substantial amplitude at all of the transition states that connect the minima. This leads to complicated spectra at high resolution which simplify considerably when they are convoluted to resolutions of roughly 10 cm^{-1} FWHM.[1] The implications of this large amplitude motions on the spectra will be discussed. In the case of the complexes of water with halide ions, OH^- and H_3O^+, the vibrational spectra that have been measured exhibit unexpected intensity patterns.

For these studies, we use a combination of Diffusion Monte Carlo calculations on ab initio potential surfaces[2] with reduced dimensional treatments to try to unravel the physical origins of the observed behaviors.

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[O-41]

The Electron Density as an Interpretive Tool in Chemistry

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I will review some recent applications of the topological properties of the electron density to a variety of topics in chemistry. The examples will be taken from our recent studies on a variety of organic and biochemical systems. The list of topics will include fluorine-fluorine bonding interactions in aromatic compounds, extended weak interactions in DNA, weak interactions in host-guest inclusion complexes, the first example of a cage critical point in a single ring, and an analysis of the halogen resonance effect.

[O-42]

Rational design of Phosphotyrosine Phosphatase 1B (PTP1B) inhibitors

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PTP1B is thought to be a major negative regulator of insulin signaling and is hence considered a target for the treatment of type 2 diabetes. Using a number of in-house X-ray structures as a starting point, a number of novel scaffolds for reversible inhibitors have been designed. Novel replacements were found for all phosphate groups in the lead compounds. The designs were developed with a production level molecular dynamics environment using explicit solvent and periodic boundary conditions. These ligands were synthesized and found to be potent inhibitors of PTP1B. The dependency between the density of the system and hydrophobic binding was explored in the course of this work. In addition, MM/PBSA has been evaluated as a quantitative tool to assess the binding of 145 PTP1B inhibitors with IC50's that range over 4 orders of magnitude.

[O-43]

Structure-based Pharmacophores Derived from Fragment Docking

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With virtual screening, there is a trade-off between the faster speed of ligand-based approaches and the generally higher accuracy of structure-based techniques. We have developed a novel workflow that couples the best qualities of structure-based docking with ligand-based pharmacophore hypothesis generation and database searching. The methodology relies on the ability of the docking algorithm to accurately dock fragments and rank them based on their ability to interact favorably with the target. We show that Glide XP is able to perform this task well due to its special motif recognition terms in the energy function. Based on the most favorably docked fragments, a pharmacophore hypothesis is constructed and used to search a database for novel compounds. While the docking component of this workflow relies on highly accurate sampling and scoring, it is fast because of the small number of rotatable bonds in the members of the fragment library. The pharmacophore screening approach is approximately two orders of magnitude faster than the fastest docking algorithms and is able to detect novel compounds that may have been missed by traditional ligand-based screens.

[O-44]

eHiTS: a fast, exhaustive flexible ligand docking with novel scoring function

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The flexible ligand docking problem is divided into two subproblems: pose/conformation search and scoring function. For successful virtual screening the search algorithm must be fast and able to find the optimal binding pose and conformation of the ligand, while the scoring function must be able to distinguish the binding pose of the active ligands from other poses and other ligands.

The presentation will give a brief overview of the fast, exhaustive docking algorithm of eHiTS. Special features of the software will be described, such as its ability to handle all possible protonations states of the receptor and the ligand in a single run saving hours of preparation and processing time compared to other docking protocols.

A new statistically derived empirical scoring function is employed by the latest version of the eHiTS software. The scoring function will be described in detail, including the use of temperature factors from the PDB files to consider the true statistical distribution of the interaction geometries that occur in binding sites.

The unique algorithms and data structures employed in eHiTS make it possible to achieve exhaustive, systematic coverage of the solution space in minutes. The ability of the eHiTS software to produce highly accurate docking results will be demonstrated on a very large and diverse validation set.

The ability of the scoring function to correctly separate active ligands from inactive ones will be demonstrated on a practical example. A series of compounds have been docked to the CDK5 receptor by eHiTS and the results are compared to experimental binding data showing good correlation with the eHiTS prediction.

For more information, visit http://www.simbiosys.ca/

[O-45]

Improvements in Docking: Ligand Energetics and Robust Search

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Flexible molecular docking seeks to combine a scoring or energy function with a method of search. The former addresses the free energy change involving protein and ligand association from separate solvated states, and the latter seeks to find the extremum of the former by varying the alignment and conformation of the ligand. In many treatments, ligand strain energy is modeled only in a heuristic sense by avoiding obviously bad conformations. This presentation will address the benefits to be gained by explicit modeling of ligand energetics, yielding a method for general and effective ring search and all-atom optimization of ligands in the course of docking. The effects of these refinements in scoring and search on both docking accuracy and screening utility will be discussed.

[O-46]

Effective local potentials for orbital-dependent density functionals

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Practicality of the Kohn-Sham scheme for orbital-dependent functionals hinges on the availability of an efficient procedure for constructing local exchange-correlation potentials in finite basis sets. We have shown recently that the optimized effective potential (OEP) method, commonly used for this purpose, is ill-posed. We propose a robust alternative to OEPs, termed effective local potentials (ELPs), based on minimizing a certain measure of nonlocality of the exchange-correlation potential. The ELP method is applied to the exact-exchange-only problem and shown promising for overcoming the shortcomings of OEPs.

[O-47]

Watching crystals assemble: connecting nanoscale detail to microscopic observations

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The process of crystal growth is fundamental to the preparation of materials in chemistry. A full understanding of how this occurs would allow the creation of crystals of improved purity and size, or the suppression of growth where formation is undesirable. To simulate how crystals form is a considerable computational challenge since the length scale and time scale involved typically precludes explicit atomistic simulation. In this talk a method will be demonstrated where the rates of growth processes can be determined from dynamical simulations and then used in kinetic Monte Carlo to observe the growth of a nucleus on a scale comparable to the experimental observations. This approach offers insight as to the origin of surface features observed through atomic force microscopy. Finally, results from a new approach to exploring the phase space of nanoparticles will be presented to demonstrate how the structure of growth units may be explored.

[O-48]

The High Pressure World Of Quantum Chemistry: Modeling the Chemistry of Materials Under Extreme Pressure

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At conditions of extreme pressure, in the order of millions of atmospheres, materials can undergo unique chemical transformations. Quantum chemical simulations of such extreme conditions has developed into a powerful tool to investigate these processes that are often difficult to probe experimentally. We have applied ab initio molecular dynamics (AIMD) simulations to study the chemistry of materials under extreme pressure conditions. First, a study of how anti-wear engine oil additives function at the molecular level in automobile engines will be provided. We recently used AIMD simulations to unravel how zinc dialkyldithiophosphate (ZDDP) additives that are added to all automobile engine oils form and function at the molecular level. (Science, 2005, 307, 1612) Although ZDDPs have been used for over sixty years, the origin of their anti-wear functionality has remained a mystery. Our simulations show that high pressures induce cross-linking in the pads, increasing the hardness of the film and its ability to accommodate applied loads. Second, a study of how nitrogen under extremely high pressure can polymerize to form a meta-stable solid that can be used for energy storage will be given. Recently, a non-molecular, polymeric form of nitrogen composed solely of single bonds, in analogy to carbon in diamond, has been synthesized (Nature Mat. 2004, 3, 558) by compressing molecular nitrogen to over 110 GPa and heating it to over 2000 K. Three single-bonded phases of polymeric nitrogen have been proposed to exist, two based known structures of nitrogen's group 15 congeners and a new so-called cubic gauche structure not seen in any other element. We have performed an in silico search for new polymeric phases of nitrogen, using a combination of AIMD simulations, a new systematic approach, and genetic algorithms.

[O-49]

Ab-Initio Simulations at a Minimally Hydrated Array of Acid-Functionalized Surface Groups as a Model for Fuel Cell Membranes

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Theoretical relationships between chemical architecture, phase separation at the mesoscale, random morphology at the macroscale morphology and transport properties are crucial for the design of advanced Polymer Electrolyte Membranes (PEMs). In our work we explore mechanisms of proton transport along a layer of hydrated acidic surface groups that are tethered to the hydrophobic skeleton of the membrane. We consider a two-dimensional hexagonal array of flexible surface groups with fixed endpoints and one water molecule per group as a model for performing ab-initio quantum mechanical calculations. We study structural conformations and cooperative phenomena in this layer. At small surface group separations (~6 Ĺ), the array is found in a highly correlated conformation with full dissocation of surface groups. At larger separations (> 7 Ĺ), we observe the transition to a tilted conformation which exhibits clustering of surface groups and only retains short-range correlations. At separations > 9 Ĺ, surface groups are independent and non-dissociated. At short separation, an extra water molecule interacts only weakly with the minimally hydrated layer ($\approx$ 0.1eV), while the energy needed to remove one water molecule exceeds > 1 eV. The minimally hydrated systems are, thus, very stable and will persist at T > 400 K. Frequency spectra obtained from ab-initio molecular dynamics calculations were analyzed in view of the concerted dynamics of the hydrated array. We expect enhanced fluctuations in positions of sidechains and protons at the transition regions between different structural conformations. Overall, the model could provide valuable insight into proton transport mechanisms in PEMs at elevated temperature and minimal hydration.

[O-50]

Event-Driven Simulations

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Motivated by recent interest in the glassy behavior of structureless liquids of infinitely thin crosses, we develop a general scheme for performing molecular dynamics studies of semi-flexible and rigid bodies interacting via discontinuous potentials. Two different approaches will be presented. In the first, the dynamics and collision rules are derived from Lagrangian mechanics in the presence of constraints. This approach is most suitable when the body is composed of relatively few point masses or is semi-flexible. In the second method, the equations of rigid bodies are used to calculate the free evolution of rigid molecules and to construct a simple scheme for computing collision rules suitable for continuous and complicated rigid bodies. Explicit analytical expressions for computing free body motion and collision rules for arbitrary rigid bodies are obtained. Efficient algorithms for the collision events search are designed in this context, and the handling of missed collisions will be discussed. The methods will be illustrated by carrying out event-driven simulations on several rigid body systems. The feasability of extending the size or time scale of simulations using such methods will be discussed.

[O-51]

Distributed Replica Sampling

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Distributed replica sampling [Rodinger et al., *J. Chem. Theory Comput.* 2:725-731 (2006)] is a simple and general scheme for efficient Boltzmann sampling of conformational space by computer simulation. Multiple replicas of the system differing in temperature T or reaction coordinate λ are simulated independently. In addition, occasional stochastic moves of individual replicas in T or λ space are considered one at a time based on a generalized Hamiltonian containing an extra potential energy term or bias that depends on the distribution of all replicas. This extra energy term enforces the desired sampling distribution along the coordinate or parameter of interest. Contrary to replica exchange, in which pairwise reciprocal moves are considered, efficient implementation of the algorithm does not require synchronicity of the individual replica simulations. The method is therefore inherently suited for shared or heterogeneous computing platforms such as a distributed network. Large-scale applications of the approach to biomolecular studies, including the molecular mechanism of permeation in membrane channels and the calculation of enzyme/ligand binding free energies, will be presented and discussed.

[O-52]

Computer simulations of lipids

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A realistic description of interactions between lipids and other biomolecules is required to study a range of phenomena by atomistic computer simulation, including membrane protein function, membrane-active peptides and drug transport. Simulations are reaching time scales that are adequate for equilibration of lipids and for free energy calculations, enabling more accurate tests of parameters. We have calculated detailed thermodynamic information for the interactions between lipid bilayers and small molecules, including a potential of mean force for a range of molecules, and enthalpy, entropy, and heat capacity profiles for hexane in a lipid bilayer. We are also studying several experimentally well-characterized peptides in an effort to link experimental data to the computational predictions, and to improve the computational models.

Posters

Abstracts in presentation order

[P1-1]

A Theoretical Study of the Original Shilov Reaction Involving Methane Activation by Platinum Tetrachloride ($PtCl_4^{2-}$) in an Acidic Aqueous Solution

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Density functional theory (DFT) has been employed to investigate the rate-determining step for the Shilov reaction in which $PtCl_4^{2-}$ can catalyze H-D exchange of alkanes in acidic aqueous solution. C-H activation and methane uptake are the two possible candidates. Associative and dissociative pathways are both considered in the methane uptake step. It was not possible to determine whether methane uptake followed an associative or dissociative mechanism due to uncertainties in the calculated contributions to the free energy of activation from entropy and solvation. The active species in the Shilov reaction are $PtCl_4^{2-}$, $PtCl_3H_2O^-$ and $PtCl_2(H_2O)_2$. We have shown that $PtCl_2(H_2O)_2$ is the most active catalyst for H/D exchange. Rate expressions for the Shilov reaction have been derived for different reaction conditions.

[P1-2]

First-Principles Prediction of Heats of formation of Energetic Materials

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In this poster, we present first-principles calculations on the prediction of heats of formation of energetic materials using density functional theory with numerical pseudo-atomic orbitals. In comparison with conventional quantum chemistry calculations, our approach is tremendously less computationally demanding, but with reasonable accuracy using the Politzer description for macroscopic condensed phase properties, based on a statistical analysis of molecular surface electrostatic potential. As applications, we calculated the heats of sublimation on energetic molecules CL-20, HMX, RDX, TNT, FOX-7, TATB and LLM-105, using electrostatic potential surface mapping onto electron densities and fitted Politzer's parameters within a set of 8 aromatic molecules.

[P1-3]

Atomistic Molecular Mechanics Simulation of Binder and Plasticizer Blends for Use in Plastic Bonded Explosives

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Choosing the proper binder and plasticizer for use in formulating new plastic bonded explosives (PBX) materials is a very time-consuming and empirical process. The modeling of such systems by molecular mechanics and the evaluation of their properties by molecular dynamics could allow considerable time savings. Atomistic molecular mechanics simulations were performed using Materials Studio (Accelrys Inc.) and the COMPASS[1] forcefield, which allows accurate prediction of the condensed-phase properties of a broad range of materials. The amorphous phases of the blends were simulated according to the method first proposed by Theodorou[2]. Thus, several binder/plasticizer systems were created with hydroxy-terminated polybutadiene as the binder. Cohesive energy densities and pair correlation functions were calculated for all systems after equilibration using molecular dynamics. It was shown that the cohesive energy density correlated well with the observed miscibility of the systems and will therefore be useful for future formulation development.

[1] Sun, H. "COMPASS: An ab Initio Forcefield Optimized for Condensed-Phase Applications - Overview with Details on Alkane and Benzene Compounds", J. Phys. Chem. B., 102, 7338 (1998).
[2] Theodorou, D.N. PhD Thesis, Massachusetts Institute of Technology: Cambridge, MA, USA (June 1985).

[P1-4]

Molecular dynamics simulations of lipid monolayers

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Lipid monolayers are surfactant monomolecular films formed at hydrophobic-hydrophilic interfaces. Their structure and phase behavior depend on the lateral pressure. The properties of monolayers and their mechanic response to pressure are important in air-water and oil-water interfaces in general, and in particular for understanding the physiological function of lung surfactant. Lung surfactant is a complex mixture of lipids and surfactant-associated proteins forming a monolayer at the internal surface of the alveoli; its main function is the reduction of the surface tension at the air-liquid interface.
We have used molecular dynamics simulations with coarse-grained molecular models to study thermodynamic, dynamic and mechanical properties of lipid monolayers. In a coarse-grained model, several atoms are grouped into larger particles and short-range pseudo-potentials are used, which makes simulations of coarse-grained models 2-3 orders of magnitude faster than corresponding atomistic simulations. Thus it becomes possible to simulate surfactant monolayers on mesoscopic length and time scales. We have simulated simple mixtures of lipids and peptides that reproduce experimentally the function of lung surfactant. Our goal is to understand the mechanism of function and the role of the different components of lung surfactant. We first characterized the behavior of lipid monolayers in our coarse-grained model, by simulating the self-assembly process and calculating pressure-area isotherms. We studied the monolayer properties under different degrees of lateral compression, e.g. monolayer ordering, viscosity, and mechanical stability as a function of the area per lipid molecule. Based on simulations of model lung surfactant mixtures, we propose a possible mechanism of folding of the compressed monolayers involved in lung function.

[P1-5]

Meta-Optimization and Evaluation of Evolutionary Strategies for Empirical Potential Fitting

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We investigated the efficiency of Evolutionary Strategies for the purpose of fitting two- and three-body empirical potentials against a ``training set'' of configurational energies. As a trial problem, we optimized a simple water and silica potential. For comparison, we also include simulated annealing optimization results. Evolutionary strategies are similar to genetic algorithms in that they use parameter crossover and mutation in many simultaneous trial solutions with a competitive, generation-based search. Evolutionary strategies are more flexible and more efficiently parallelized than simulated annealing algorithms. The optimization was run with two types of training set. The first type is generated with an empirical potential, such that the algorithm may recover the original parameters; this is useful for testing the evolutionary optimization. The second type is *ab initio* surfaces generated from Density Functional Theory calculations, in which case the training set cannot be exactly fit by simple functional forms. Effects of crossover types, mutation rates, mutation size, and selection method in the evolutionary strategy are discussed. Inclusion of force data in the training set is examined. The techniques employed are general, and may be used to optimize new potentials of virtually any form.

[P1-6]

Computational Determination of Aqueous pK_a Values of Protonated Benzimidazoles

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Our aim is to develop an effective computational procedure for predicting the aqueous acid equilibrium constants of protonated benzimidazoles at 298.15 K. Acid equilibrium constants (K_a, pK_a=-log K_a) are an important property of organic compounds, and aqueous pK_a values are especially useful for environmental and pharmacological applications. Benzimidazoles have found applications in pharmacology as bactericides, antihistamines, analgesics, antiviral compounds and antiulcer agents. Benzimidazoles offer a number of challenges to the determination of their aqueous pK_a values, because of their low water solubility and because some derivatives are involved in tautomeric equilibria which increase the complexity of the theoretical pK_a determinations. A methodology for the accurate theoretical prediction of aqueous pK_a values of protonated benzimidazoles is developed. Different reaction schemes are considered to approximate the acid dissociation equilibrium, two distinct equations are used for the calculation of pK_a values, and a number of levels of theory are applied in the process of working towards this aim. Additionally a quantitative structure-property relationships (QSPR) is explored between the experimental aqueous pK_a values of a group of fifteen benzimidazoles and descriptors calculated at the B3LYP/6-31+G(d,p) level of theory, applying the PCM solvation model through both single-point energy calculations (PCM(sp)), and in the geometry optimizations and frequency calculations (PCM(opt)). The best correlations between the experimental and calculated data were obtained at the B3LYP/6-31+G (d,p)-PCM(opt) level of theory for both the direct calculations and the QSPR.

[P1-7]

Development of a "Quasi *ab initio*" Loop Modelling Algorithm

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Loop modelling remains one of the most challenging steps in homology and comparative modelling. Current methods for loop modelling can be classified in one of three groups: (1) knowledge-based, (2) ab initio, and (3) combined approaches. Our algorithm uses trivariate gaussian distribution functions developed by Cheng *et al.* [1] to preferentially search favourable areas of conformational space, and as such can be classified as a combined approach since it is not purely *ab initio*. This algorithm uses a Monte Carlo refinement step to ensure rapid closure of loop candidates. Next, we improved upon the initial algorithm by adding an intermediate scoring function based primarily on steric interactions of the loop backbone with the protein environment to weed out emerging bad solutions caused by unfavourable steric clashes. Validation of these algorithms on the 4 and 8 residue long loops from the Fiser test sets [2] will be presented.

[1] B. Cheng, A. Nayeem, and H.A. Scheraga, *J. Comp. Chem.* 17(12), 1453-1480 (1996).
[2] A. Fiser, R.K.G. Do, and A. Sali, *Protein Science*, 9, 1753-1773 (2000).

[P1-8]

Geometric spin frustration for isolated plaquettes of the lattices: An extended irreducible tensor operator method

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Spin frustration is related with the phenomenon of the spin glass behavior, and has recently been utilized in the molecular magnetism community. The geometric spin frustration (GSF) is often discussed in the simplest site-sharing frustrated systems, such as plaquettes of usually triangular, Kagome and pyrochlore lattices. Actually, the GSF concept has been evolved to describe the Spin frustration is related with the phenomenon of the spin glass behavior, and has recently been utilized in the molecular magnetism community. The geometric spin frustration (GSF) is often discussed in the simplest site-sharing frustrated systems, such as plaquettes of usually triangular, Kagome and pyrochlore lattices. Actually, the GSF concept has been evolved to describe the magnetic behavior of other more complicated systems with competing spin interactions. It is important to provide a quantum-mechanical description of the spin distribution in the plaquettes. In general, it is difficult to probe the eigenvalue spectrum of a spin system by the analytical means. The number of the spin basis function necessary to describe a spin system of the n spin sites is $(2s+1)^2$, so that the dimension of the associated spin Hamiltonian matrix becomes $(2s+1)^2 \times (2s+1)^2$. As a consequence, the diagonalization of the spin Hamiltonian matrix quickly becomes impossible with increasing values of s and n in order to get the analytical eigenvalue spectrum of the spin system.

In the recent work we suggest a new strategy to search for the good quantum numbers in order to reduce the calculation demand based on the irreducible tensor operator method, and within MATLAB we have coded a program of the extended irreducible tensor operator method with automatically searching for the good quantum numbers. As representative examples, the analytical energy spectra of the low lying spin states and matrix elements of the spin projections Sz, Sx and Sy at the sites for the spin pentamer of the tetrahedron with a centered spin site and the spin heptamer of three corner-sharing equilateral-triangle were examined in order to confirm efficiency and validity of the new strategy.

[P1-9]

Reorganization Energies from Molecular Dynamics with Constrained Density Functional Theory

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Diabatic states are constructed using Constrained Density Functional Theory. Nuclear distributions sampled from MD trajectories on the diabatic surface are used to construct the Charge Transfer Reorganization Energy of the Creutz-Taube ion in solution.

[P1-10]

Restricted Visceral Green Florescent Protein Expression Patterns in Transgene Mice

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The study's objective was to determine the Green Florescent Protein (GFP) marker expression patterns in sample tissues from Chimeric Mouse models. The reliability of GFP transgene markers to track metabolic processes is well known. GFP folds and the resulting three dimensional cylindrical structure protects the internal fluorophores. Mutations in the amino acid sequence in adjacent side chains can affect spectral properties. Cytomeglia Virus is considered to be a universal immediate early promoter of transgene expression in vitro. Quantitative analysis was completed with brain, parotid, liver, skin, bone, cardiac muscle, pancreas and skeletal muscle samples using transillumination and ultra violet exposure. Results indicate that GFP has various expression patterns in sample tissues with highest consistent expression in the pancreas. This study's conclusion is that the CMV promoter is restricted to specific tissues in vivo. Further studies must be done to determine if upstream CMV promoters have variant transgene expression due to site of integration and/or different coding lengths.

[P1-11]

Utilizing Vertically Integrated Partnerships in Science Education to Develop Future Scientists

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The project's objective is to determine the benefits of Vertically Integrated Partnerships focusing on Science Inquiry Methods of teaching in high school and college science programs. Statistical analysis was used to evaluate the efficacy of scaffolding inquiry methods for content retention. Results indicate improved comprehension and critical thinking skill development. This study's conclusions reflect that educational strata partnerships foster student and peer to peer centered learning. By closing the gap between prediction and observation these methods build confidence in students' own analytical judgment. Further studies must be done to determine future results for students continuing in science career paths.

Integrating Teaching and Research: A New Model for Graduate Education? by N.M. Trautmann and M.E. Krasny. 2006. BioScience 56(2): 159-165.

Beyond the Binary: Approaches to Integrating University Outreach with Research and Teaching, by A.S. Bartel, M. Krasny, & E.Z. Harrison. Journal of Higher Education Outreach and Engagement, 8(2), 89-104.

[P1-12]

DFT and TDDFT Studies of the Conformational Dependence of the Optical Properties of Perylene Aggregates

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Perylenes are robust chromophores that have been used extensively to study energy and electron transfer. Their thin films share properties with both conventional semiconductors and insulator-like molecular crystals, making them ideal to examine the two broad classes of materials. Within the realm of perylene aggregates (dimers, trimers, etc.), the exciton model has been used to describe the interactions of chromophores based upon the position of the lowest energy electronic transition and splittings of electronic excitations. This model is dependent upon the assumption that electron overlap between each perylene unit is negligible.

Here we use density functional theory (DFT) and time-dependendt DFT (TDDFT) to investigate the optical properties of different conformations of gas phase 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) aggregates and compare these results with those predicted by exciton theory. The observed vibrational progression within the lowest energy transition of PTCDI monomer has been simulated by calculating the Franck-Condon factors. These indicate that transitions within multiple modes (and their combination bands) contribute to the structure of the absorption. Experimentally, a distinct increase in the intensities of higher energy bands within the lowest electronic transition is observed. We have investigated the utility of several mechanisms (diplaced harmonic oscillator, Herzberg-Teller coupling, etc) to describe this experimental result.

[P1-13]

Path Integral Ground State Study of Finite Size Systems: Application to Small p-Hydrogen Clusters

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We use the path integral ground state method (PIGS) to study the energetic and structural properties of small p-hydrogen clusters of size ranging from two to ten molecules. A fourth order formula is used to approximate the short imaginary-time propagator. Our results are compared with exact quantum mechanical calculations and other quantum Monte Carlo methods. We find that for all studied clusters our results show lower ground state energy than literature values obtained by diffusion Monte Carlo (DMC) and variational Monte Carlo (VMC). In particular, our dimer and trimer ground state energies are in good agreement with the exact results obtained by discrete variable representation (DVR). We explore the use of Pekeris coordinates to examine trimer's structure and wave function as well as the structure of trimers within clusters of larger size. We also comment on the effect of different trial wave functions on the accuracy and efficiency of the results. Future work on dynamics from PIGS calculation will be outlined.

[P1-14]

Charge-Transfer Excited State Energy Splittings by Constrained Density Functional Theory

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Constrained density functional theory (DFT) is an inexpensive method for computing accurate charge-transfer (CT) energies. We demonstrate the utility of this method by computing singlet-triplet CT state energy splittings in tris(8-hydroxyquinoline) aluminum (Alq_3) and find that the singlet CT state lies as much as 70 meV below the triplet CT state. This suggests that kinetic exchange makes a larger contribution to the Alq_3 CT states than does direct exchange. Structural optimization of Alq_3 with constrained DFT allows CT reorganizational energies to be directly obtained. In an effort to predict whether singlet or triplet CT states will lie lower in energy for a general system, we investigate the geometry dependence of the CT singlet-triplet energy splitting. We find that the ordering of the singlet and triplet CT states can depend strongly on geometry and suggest that this is due to degree of overlap between the donor HOMO and acceptor LUMO.

[P1-15]

Non-Markovian effects in Brownian motion

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Conventional schemes of elimination of fast variables of a many-body system usually result in Langevin type equations which in general are non-local in time. For Brownian motion the memory effects may be important even when the coupling with slow collective modes in the surrounding bath is negligible. It is found that a perturbation analysis of an exact non-Markovian equation for a heavy Brownian particle yields a stationary solution which is inconsistent with Boltzmann-Gibbs statistics. The results of relevant numerical simulations will be presented.

[P1-16]

The method of generating potentials for the description of open systems

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We present a non-Hermitian Hamiltonian for the description of open systems that exchange current density with the surrounding. Our theory can be applied to molecular electronic devices in whose description the infinite contacts are replaced by complex (generating) potentials. The boundary conditions for the open system are also build into the generating potentials. The method is rigorous, i.e., we recover the exact solution.

To illustrate our approach, we consider certain prototypical molecular conductors and we show that there exist isolated molecular states in the continuum of contact states. We show that simple molecular orbital theory suffices to explain and to predict the existence of these localized molecular states.

[P1-17]

Electronic Structure and Physicochemical Properties of Selected Penicillins

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Traditionally, penicillins have been used as antibacterial agents due to its characteristics and wide spread applications with few collateral effects, which have motivated several theoretical and experimental studies. Despite the latter, their mechanism of biological action has not been completely elucidated. Herein, we present a theoretical study at the Hartree-Fock and Density Functional Theory levels of theory of a selected group of penicillins such as the penicillin-G, amoxicillin, ampicillin, dicloxacillin and the carbenicillin molecules, to systematically determine the electron structure of full β-Lactam antibiotics. Our results allow us to analyse the electronic properties of the pharmacophore group, the aminoacyl side chain, and the influence of the substituents (R and X) attached to the aminoacyl side chain at 6' (in contrast with previous studies focused at the 3' substituents), and to corroborate the results of previous studies performed at the semiempirical level, solely on the β-Lactam ring of penicillins. Besides, several density descriptors are determined with the purpose of analyzing their link to the antibacterial activity of these penicillin compounds. Our results for the atomic charges (fitted to the electrostatic potential), the bond orders, and several global reactivity descriptors such as the dipole moments, ionization potential, hardness, and the electrophilicity index, led us to characterize: the active sites, the effect of the electron attracting substituent properties and their physicochemical features, which altogether, might be important to understand the biological activity of these type of molecules.

[P1-18]

Calculation of Charge Transport Properties by Explicit One-Particle Density Matrix Propagation

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Real time one-particle density matrix propagation allows examination of time dependent quantities in systems undergoing charge transport. Of foremost concern is calculation of current as a function of applied potential bias. Additionally, because we are able to calculate a time dependent density matrix, we can calculate the time dependence of any single-particle operator. Thus, calculations of interesting properties such as emission spectra resulting from charge transport are possible. We demonstrate the utility of real time propagation methods using the Pariser–Parr–Pople (PPP) model applied to a conjugated carbon wire connecting two large gold wires acting as electron reservoirs. Additionally, parameter free time propagation calculations of realistic systems such as polyacetylene and benzene-1,4-dithiolate (BDT) connected to gold atom clusters are performed using density functional theory.

[P1-19]

QM/MM Free Energy Study of Proton Transport in Protein Channels.

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Proton transport across cell membrane is a fundamental subject in both biochemistry and biophysics. The lipid bilayer constituting the cell membrane is an extremely low dielectric medium, hence impermeable to charged species. Protons flow through water-filled transmembrane channels either by diffusion, following the direction of an electrochemical gradient, or propelled by pumping molecules against their concentration gradient. Independently from the driving force, proton translocation through water filled narrow pores takes place through a "HOP-AND-TURN" or Grotthuss relay mechanism1, involving the chemical exchange of hydrogen nuclei along extended chains hydrogen-bonded water molecules2. Here we will show the results of a new QM/MM free energy scheme applied to the study of proton translocation in transmembrane protein channels.

References and Notes

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[P1-20]

A combined molecular dynamics, exciton and harmonic analysis approach for the study of size effects in NH_3 nanoparticles

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Our previous investigations [1,2] have shown that the infrared spectra of molecular ice particles, with sizes between 10 – 100 nm are dominated by resonant transition dipole-transition dipole coupling. For particles with sizes below 10 nm additional spectral features appear, which are no longer based only on this type of intermolecular interactions. In this size range structural changes and surface effects are suspected to play a crucial role in the infrared spectra. These aspects are investigated here on the example of ammonia particles [3] with the help of a combined molecular dynamics, exciton and harmonic analysis approach. The exciton model can be extended to describe particles with non crystalline structure using an explicit intra- and intermolecular potential. Results indicate the particles to be composed of a crystalline core and an amorphous surface.

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[P1-21]

DFT AND MP2 calculations on the electronic structure and geometry of 18-crown-6, hexaaza-annulene and their complexes with Ba^{2+}, Ca^{2+}, Cd^{2+}, Hg^{2+}, K^{+}, Mg^{2+}, Na^{+}, Sr^{2+} and Zn^{2+} cations

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Crown ethers and annulenes have been studied both physically and computationally for many years. However, their hexaaza analogs have not been studied in great detail. While the calculations on the electronic and geometrical structures of 18-crown-6, annulene and their corresponding complexes with various cations have been performed, [1-4], little research on the hexaaza analogs of [18]-annulene and corresponding complexes was done. These systems should show a stronger binding affinity for cations due to the placement of the donor pair of the nitrogen atoms in hexaaza [18]-annulene, compared to the position of the donor pairs of the oxygen in 18-crown-6. We performed calculations on $M@C_{12}H_{12}N_6$, as well as M@18-crown-6, where M = Ba^{2+}, Ca^{2+}, Cd^{2+}, Hg^{2+}, K^{+}, Mg^{2+}, Na^{+}, Sr^{2+} and Zn^{2+}. Future work will focus on magnetic species with M being Fe^{3+} and Gd^{3+}.

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[P1-22]

Overcoming Hydrocarbon-based Performance Degradation (Coking) and Sulfur Poisoning on Solid Oxide Fuel Cell Anode Surfaces using Periodic DFT

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The Solid Oxide Fuel Cell (SOFC) is a high temperature electrochemical device (800-1000 °C) that generates O^{2-} ions from oxygen adsorption at the cathode (reduction) and migrates these ions via the electrolyte to the anode, where oxidation of an adsorbed hydrocarbon fuel source occurs. One of the most commonly used SOFC anode materials is porous nickel yttria-stabilized-zirconia (Ni-YSZ). Despite the fact that nickel is a good steam-reforming catalyst, the anode composite does have some disadvantages. Nickel catalyzes the formation of graphitic carbon (coking), from hydrocarbon anode fuels, and is intolerant to sulfur poisoning. Sulfur is found as an impurity in most hydrocarbon fuels and its removal requires costly pre-purification methods. Graphitic carbon (which cannot be oxidized) and sulfur strongly adsorb onto the anode surface, blocking adsorption sites, terminating further fuel adsorption and rendering the anode inoperable. Utilizing plane-wave gradient corrected periodic DFT calculations, using the Projector-Augmented-Wave (PAW) method, our research considers the adsorption and dissociation of the anode fuel (e.g. methane) and a typical sulfur species (e.g. hydrogen sulfide) on numerous metal / alloy surfaces. By studying the mechanistic processes involved during these reactions, we hope to understand and ultimately overcome the disadvantages currently associated with SOFC anode materials.

[P1-23]

Ab Initio Monte Carlo simulations of Fluid Phase Equilibria at Extreme Conditions

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We present a simulation framework in which a combination of modern Monte Carlo sampling methods are used in concert with standard electronic structure codes (CPMD and NWChem) to perform liquid-vapor and liquid-liquid coexistence calculations from first principles. The use of an approximate pre-sampling potential to generate large moves with a high probability of acceptance is critical to the method, and our implementation includes on-the-fly refinement of the approximate sampling potential for improved performance. Issues of efficiency, correctness and load-balancing arising from the use of iterative density functional theory potentials are addressed both directly and through analysis of model systems. The method is applied to phase coexistence and (P,V,T) data in simple metals including lithium and sodium, as well as to other systems. The prospects for extension of this technique to more complex systems and solid-liquid phase coexistence is also discussed.

[P1-24]

Novel Methods for Computer-Aided Drug Design

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Predicting protein-ligand binding affinities is a central challenge in structure-based drug-discovery, especially during lead-compound optimization. We present implementation of and promising early results from the M2 algorithm for protein-ligand modeling. Additional tools for generating accurate partial charges, conformational search, conformational filtering, etc., are also described.

[P1-25]

Generalized Master Equation Analysis of Surface Hopping Dynamics

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The study of nonadiabatic processes in the condensed phase has traditionally been treated using phenomenological techniques. The success of these approaches lies in the computational simplicity in modeling complex nonadiabatic processes. These approaches however improperly treat important properties such as coherence. Furthermore, these techniques are constructed using ad hoc phenomenological arguments. A rigorous approach to this type of dynamics will be presented. The dynamics can be represented exactly in the form of a generalized master equation which is desirable as it alludes to the type of dynamics prescribed by surface hopping approaches. By making physically sensible approximations to the memory kernel, we obtain dynamics that resemble these existing phenomenological methods thus providing us with a set of validity conditions for the existing methods. Furthermore, analysis of the unapproximated memory kernel provides us with insight into the role of coherence in dynamical processes.

[P1-26]

Self-Consistent Combination of the Three-Dimensional RISM Theory of Molecular Solvation with Analytical Gradients and the Amsterdam Density Functional Package

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Nowadays, the self-consistent filed combination of KS-DFT electronic structure methods and statistical-mechanical 3D-RISM theory of molecular liquids [1] represents one of the most efficient ways, in terms of accuracy and computational cost, for predictive description of solvent effects on structure and functions of solutes. This method supplemented by calculation of analytical gradients [2] allows one to calculate the properties, optimize geometries, search for transition states and reaction coordinates. In this work we present a deatiled evaluation of the new self-consistent field KS-DFT/3D-RISM method which has been implemented in the ADF package. We performed several characteristic tasks of computational chemistry: the free energies, energies of taumetrization for a number of organic compounds; water distribution inside the carbon nanotubes; the activation parameters and coordinates of SN2 reactions in aqueous solvent; and those of SN2 reactions in the inner part of a carbon nanotube. The results are similar to those obtained by continuum solvation approaches, and moreover, are at the level of ab-initio QM/MD methods [3]. We also discuss the timings in comparison to the COSMO method.

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[P1-27]

Distinguishability and Chiral Stability in Solution:

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We examine the effect of decoherence and intermolecular interactions (chiral discrimination energies) on the chiral stability and the distinguishability of initially pure versus mixed states. Under a two-level approximation for the system, intermolecular interactions are introduced by a mean-field theory, and interaction between a system and an environment is modeled by a continuous measurement of a population difference between the two chiral states. The resultant equations are explored for various parameters, with emphasis on the combined effects of the initial condition of the system, the chiral discrimination energies, and the decoherence in determining the distinguishability measured by population differences between the initially pure and mixed states, and the decoherence process and the chiral stability measured by the purity decay, and the stationary state of the system.

[P1-28]

Analysis of Kinetic Isotope Effects for Nonadiabatic Reactions

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Factors influencing the rates of quantum mechanical particle transfer reactions in many-body systems are discussed. The investigations are carried out on a simple model for a proton transfer reaction that captures generic features seen in more realistic models of condensed phase systems. The model involves a bistable quantum oscillator coupled to a one-dimensional double-well reaction coordinate which is in turn coupled to a bath of harmonic oscillators. Reactive-flux correlation functions that involve quantum-classical Liouville dynamics for chemical species operators and quantum equilibrium sampling are used to estimate the reaction rates. Approximate analytical expressions for the quantum equilibrium structure are derived and used to obtain the simulation results. Reaction rates are shown to be influenced significantly by both the quantum equilibrium structure and nonadiabatic dynamics. Nonadiabatic dynamical effects are found to play the major role in determining the magnitude of the kinetic isotope effect for the model transfer reaction.

[P1-29]

Copolymerization of polar and non-polar monomers by neutral asymmetric Pd(II) complexes: DFT study

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Herein we discuss results from our computational studies on copolymerization of polar and non-polar monomers in the presence of neutral palladium (II) complexes bearing anionic P^O ligands proposed by Drent et al. [Chem. Commun. 2002, 9, 964]. When applied to the copolymerization of ethylene with carbon monoxide, the catalytic systems afford non-alternating ethylene/CO polymers with microstructure of the growing chain containing multiple ethylene units, whereas any other transition metal system known up to date results in the strictly alternating sequence of both co-monomers. When ethylene is copolymerized with acrylates, the Pd(II) catalysts are able to incorporate similar amount of polar monomers as the classical Brookhart Pd(II) system, however, the topology of the formed copolymer is different. Our theoretical studies on processes that may compete during the chain growth rationalize the experimentally observed findings and allow us to suggest some modifications of the studied complexes aimed at increasing their activity.

[P1-30]

Freezing of gold nanoparticles

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Constrained Monte Carlo simulations, combined with parallel tempering, are used to calculate the free energy barriers to freezing in gold nano-clusters as a function of temperature. We are able to identify a kinetic spinodal temperature where the nucleation barrier goes to zero and find that the critical cluster size remains finite at the limit of stability of the fluid phase. Molecular dynamics simulations are used to examine the dynamics of freezing around the kinetic spinodal temperature.

[P1-31]

Simulating Liquid Water with Discontinuous Molecular Dynamics

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Due its important role in biological and chemical processes, the study of water and aqueous systems remains an active field of research. The development of new theoretical methods continuously stimulates the search for more accurate and/or economic theoretical models of water. In this contribution, the simulation of liquid water at ambient conditions via discontinuous molecular dynamics is presented. Several water models with different levels of complexity are designed. Their equilibrium and dynamical properties are computed and compared with the standard TIP4P model at the same density and temperature. The computational efficiency of the several models is also analyzed.

[P1-32]

Study of the optimised STO-nG expansion and its derivatives.

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For many years, it has been considered opportune to expand Slater Type Orbitals (STOs) as a sum of Gaussians. The aim of this procedure is to closely mimic the STO, although, clearly Kato's onditions (nuclear cusp and exponential decay at long range) are not satisfied. The advantage is that Gaussians have a simple product theorem.

In this work, the difference between an STO and its Gaussian expansion, globally optimised for exponents and coefficients is found to converge rapidly with n to a universal curve. Furthermore, the absolute error may be reduced to the nano-hartree for n=10-12 and pico-hartee for n=20. Expansions have been tested to n=30. The zeros of the universal curve may be used to extend the expansion from n to n+2 since each curve has 2n zeros.

This method of comparing Slater integals and integrals over STO-nG is discussed in conclusion, with emphasis on the physical properties which require analytical Slater functions, because of oscillations in the derivatives of STO-nG (tested by evaluating {grad (ρ) /(ρ)}) or by cusp and decay dependence.

[P1-33]

Efficient modeling of silicon and silicon oxide surface chemistry with electronic structure theory using pseudo-atoms.

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A first principles treatment of reactions at surfaces continues to be a significant challenge facing the theoretical and computational chemistry communities due primarily to the sheer size of the systems being studied. Despite algorithmic and technological advancements, practitioners are often limited to using so-called cluster models where dangling bonds are generally terminated with hydrogen atoms. However, hydrogen terminated clusters often suffer from a poor description of the electronic structure at the cluster boundary, an effect also observed in many QM/MM schemes where hydrogen termination is commonly used. We are developing pseudo-atoms for termination in silicon and silicon oxide clusters that can more appropriately model surface chemistry. In contrast to other developments in this area, our pseudo-atoms are capable of occupying divalent termination sites and saturating polar bonds, both of which are essential properties for accurate applications. Moreover, the presented pseudo-atoms can be directly employed in any electronic structure package equipped with code for including effective core potentials. We will describe our development approach and present results from initial applications to ongoing studies of silicon and silicon oxide surface chemistries.

[P1-34]

Inclusion of symmetry in centroid molecular dynamics

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Centroid molecular dynamics (CMD) is emerging as an important tool for the inclusion of quantum mechanical effects in molecular dynamics simulations. A formulation of CMD for problems possessing inversion symmetry is, however, still lacking. We show how one can include inversion symmetry in CMD via the use of the so-called symmetry-adapted quasi-density operator, as defined in [J. Chem. Phys. 115, 7822 (2001).]. We test this approach on two symmetric problems: the quartic oscillator and the double-well reaction profile. We assess the accuracy of the approach from time-correlation functions. We show that it is possible to improve upon the conventional CMD method by properly combining trajectories obtained from separate symmetries. Such a combination yields trajectories that are non-local in character and, in turn, allows one to recover some of the coherence that is absent in the conventional CMD approximation.

[P1-35]

Tight Binding-Configuration Interaction (TBCI): A Novel Non-Iterative Method to Incorporate Charges into Tight Binding

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The study of reactions and other processes in large molecules, clusters, solids and other condensed-phase materials, especially those including metal atoms, poses many unique quandaries. As one considers larger and more complex systems, the systems become too large to model with Density Functional Theory (DFT) or other reliable quantum chemical methods. Therefore, a different approach is required. We have developed a number of analytical potential energy functions that are very effective in modelling aluminium nanoclusters,[1] but systems that display atypical behaviour or undergo bond breaking and/or bond formation pose a challenge to these methods.

One approach that is gaining popularity in recent years is to apply the semi-empirical *Tight Binding* (TB) method. We have developed a series of TB methods to study aluminium nanoparticles.[2] One disadvantage of these TB methods is that they do not take charges into consideration. One consequence of this is that they do not predict, in contrast to experiment, neutral dissociations of aluminium clusters. Herein, a novel form of TB, coined *Configuration Interaction-Tight Binding* (TBCI), will be presented. This method blends the concepts of TB with the accurate *Configuration Interaction* (CI) method. In contrast to other schemes used to incorporate charges, such as the self-consistent charge (SCC) model,[3] this method is non-iterative. This method will be presented along with the results obtained for aluminium and aluminium-hydrogen nanoclusters.

[1]Jasper, A. W.; Schultz, N. E.; Truhlar, D. G., *J. Phys. Chem. B* **2005**, *109*, 3915-3920; Jasper, A. W.; Staszewski, P.; Staszewska, G.; Schultz, N. E.; Truhlar, D. G., *J. Phys. Chem. B* **2004**, *108*, 9886-9010.
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[P1-36]

Constrained Semiclassical Dynamics

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The Semiclassical Initial Value Representation (SC-IVR) offers an effective means of incorporating quantum effects in classical Molecular Dynamics. We have developed a method, based on the SC-IVR theory to study quantum dynamics in constrained molecular systems. An important and practical feature of our approach is its generality: the calculations are carried out in Cartesian coordinates thus making the method directly applicable to a variety of molecular systems.The method allows the computation of energy levels from the Fourier transform of the auto-correlation function. The auto-correlation function, in general, is built by evaluating an oscillatory integrand. As a result, the convergence of the calculations becomes increasingly demanding with the increasing complexity of systems. We are particularly interested in studying constrained systems where the integrands are conveniently less oscillatory. Consequently, the treatment of quantum effects becomes possible for larger systems. We test our method by calculating the vibrational energy levels of a series of 'constrained' weakly bound clusters. We will present recent findings and show that the method is able to accurately describe quantum dynamics.

[P1-37]

Computer Modeling of the Vitamin B12 ABC Transporter BtuCD-F

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The compartmentalization of cells from their environment is a fundamental property of life, and controlling the import and export of various substances is one of the most crucial processes for a cell. This task is carried out by channels and transporter proteins, among which ABC transporters form a particularly large class that is found in all forms of life. Their main function is to transfer a broad variety of substrates across biological membranes in an ATP-hydrolysis dependent manner. ABC transporters are involved in multidrug-resistance in bacteria and cancer cells, and in a number of human genetic diseases. The BtuCD-F system is the vitamin B12 importer for E. coli, and X-ray structures have been solved for both the transporter (BtuCD) and its periplasmic binding protein (BtuF). The latter belongs to a group of specialized substrate binding proteins that bind substrates with high affinity and deliver them to transporters in the inner membrane. We employ MD simulations to investigate how BtuCD transports vitamin B12 across the bacterial inner membrane. We have created possible docking complexes between BtuCD and BtuF, and performed simulations of both the periplasmic binding protein BtuF and the full BtuCD-F complex in a realistic lipid-water environment.

[P1-38]

Nonadiabatic Dynamics in External Fields

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The theory of mixed quantum-classical dynamics, as formulated by Kapral and Ciccotti[1], is a particularly appealing approximate method of solving the quantum Liouville-von Neumann equation. A selection of methods that aim to describe the influence of a time-dependent external force on an open quantum subsystem within the framework of MQCD will be discussed.

[1] R. Kapral and G. Ciccotti, "Mixed Quantum-Classical Dynamics", J. Chem. Phys., 110, 8919-29 (1999).

[P1-39]

Externally Corrected Coupled-Cluster Methods Employing Method of Moments of Coupled-Cluster Equations and Multi-Reference Perturbation Theory

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A new class of non-iterative coupled cluster (CC) methods, which improve the results of standard CC and equation-of-motion (EOM) CC calculations for ground and excited-state potential energy surfaces along bond breaking coordinates and for excited states dominated by two-electron transitions, is explored. The proposed approaches combine the method of moments of coupled-cluster equations (MMCC), in which the *a posteriori* corrections due to higher-order correlations are added to standard CC/EOMCC energies, with the multi-reference many-body perturbation theory (MRMBPT), which provides information about the most essential non-dynamic and dynamic correlation effects that are relevant to electronic quasi-degeneracies. The performance of the basic MRMBPT-corrected MMCC (MMCC/PT) approximations, in which inexpensive corrections due to triples (MMCC(2,3)/PT) or triples and quadruples (MMCC(2,4)/PT) are added to ground- and excited-state energies obtained with the CC/EOMCC singles and doubles approach, is illustrated by the results of a few test calculations, including bond breaking in HF, H_2O, and F_2, and excited states of CH^+.

[P1-40]

Quantum chemical concepts and methods for intense field molecular dynamics: Tunnel ionization.

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A major challenge in studying the dynamics of multielectron systems in intense fields is to calculate the dynamical electronic structure, including various multielectron ionization processes while accounting for electron correlation. We present and discuss here the methodology for the calculations and analysis of resonance orbitals and states corresponding to the tunnel ionization of H_2^+ and H_2, using a standard ab-initio method with an extended L^2 basis set.

[P1-41]

Quantum chemical concepts and methods for intense field molecular dynamics: Electron dynamics.

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A major challenge in studying the dynamics of multielectron systems in intense fields is to calculate the dynamical electronic structure, including various multielectron ionization processes and electron recollision while accounting for electron correlation. Ongoing work conducted in our laboratory explore the possibility of extending existing optimized quantum chemical codes to include strong field effects. We present here efforts made towards the development of a time-dependent Multi-Configuration Self-Consistent Field (TDMCSCF) which allows one to carry out direct time-resolved multielectron dynamics simulation within the existing quantum chemical codes, after proper adaptations have been made. Our final formulation of the TDMCSF method amounts to a split-operator algorithm involving the non-commutative one and two electron parts of the hamiltonian. We illustrate the procedure on the bound-electron dynamics of the two-electron H2 molecule in an intense laser field.

[P1-42]

Study of Xe and Kr Adsoption on Open-Single Walled Carbon Nanotubes using Molecular Dynamics Simulation

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We have used molecular dynamics simulation to study the adsorption isotherms of noble gases, Xe and Kr, on open single-walled carbon nanotubes. Adsorption isotherms of xenon at several temperatures between 95 and 130 K, and krypton between 75 and 95 K on (10,10) tubes have been investigated. The adsorption coverage and isosteric heat were calculated. It was found that the gas molecules prefer interior of the open ended single-walled carbon nanotubes. The interior coverage of 0.06 Xe-C and 0.08 Kr-C and exterior coverage of 0.23 Xe-C and 0.25 Kr-C were reported at saturation conditions. Our results are in reasonable agreement with experimental observations.

[P1-43]

Mesoscale Simulation of Field-Induced Alignment in Rod-Like and Rod-Coil Copolymers

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We investigated the effect of external electric fields on the liquid crystalline phases of rod-like and rod-coil copolymers using the dissipative particle dynamics (DPD) simulation method. With no electric field applied, rod-like particles exhibit crystalline, smectic-A, and nematic phases [1]. The isotropic-nematic transition is weakly first order. Applying the electric field has the effect of shifting the isotropic-nematic point to higher temperatures and the softening of the transition. Upon switching the filed off, the system relaxes to the zero-field case. The rod-coil copolymers showing istropic-smectic transitions with no applied field now show also a nematic phase under the influence of the external field. We will also present the effect of the field on cylindrical and spherical-forming rod-coil copolymers.

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[P1-44]

On The QSAR Studies of Non-Nucleoside Inhibitors of HIV Reverse Transcriptase: Hydrophobic and Steric Effects

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Non-nucleoside reverse transcriptase inhibitors (NNRTIs) are promising compounds in the search for potent and selective drugs for the treatment of AIDS. Several QSAR studies have been devoted to these compounds. Biological phenomena are complicated to be described by linear models Thanks to their ability to perform non-linear mapping of the physicochemical descriptors to the corresponding biological activity, neural networks (NN) proved to be a powerful QSAR modelling technique for this series of inhibitors [1,2].
One of the purposes of QSAR analyses is to use molecular information to provide key rules governing the activity of a particular class of compounds and to assist drug design. The present work rationalises in depth the relationship between the hydrophobic and the steric characters of NNRTIs and their anti-HIV activity. The variation of anti-HIV activity with respect to hydrophobic and steric parameters is performed by means of NN, and its non-linear aspect is discussed.

[1] L. Douali, D. Villemin, D. Cherqaoui; Comparative QSAR Based on Neural Networks for the Anti-HIV Activity of HEPT Derivatives, Curr. Pharm. Des. 2003, 9(22) 1817 – 1826
[2] L. Douali, D. Villemin, D. Cherqaoui; Exploring QSAR of TIBO Derivatives by Neural Networks, 9th Electronic Computational Chemistry Conference (ECCC9), http://eccc9.acooper.edu

[P2-1]

Prediction of Fibrinogen Adsorption onto Polymer Surfaces: 3D Case Study

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Computer modeling plays a critical role in prediction of bioresponse for combinatorial libraries of biodegradable polymers. The Surrogate Modeling approach recently proposed by Smith et al. [1] where connectivity-based 2D molecular descriptors were calculated for a set of selected biopolymers and then linked to the experimentally determined biological response (properties), allows good quantitative prediction of these properties for the whole combinatorial library. In the present work we combine Molecular Dynamics (MD) simulations and Surrogate Modeling with the aim to improve the accuracy of the Surrogate Model by using descriptors based upon 3D structure of the polymer obtained from MD simulations, rather than the simple "as drawn" 2D representation.

MD simulations were performed for a library of 45 structurally related biopolymers (polyarylates) for which experimental fibrinogen adsorption (FA) data were previously obtained. Next, 3D descriptors were calculated for molecular structures obtained from (a) preliminary (local) energy minimization, (b) MD simulations in vacuo and (c) MD simulations in implicit water. Then the Monte Carlo Decision-Tree methodology [2] was utilized to rank the descriptors in order of their correlation to FA, and an Artificial Neural Network [1,2] was used to model FA.

The computational protocol for MD simulations was established to obtain the lowest energy realistic conformations for the polymers of interest. It was found that globular-like packing pattern is typical for all investigated models within which specific intramolecular alignments due to the different flexibility of diphenol and diacid components of polyarylates were observed. Some of these features can be indicative of potential liquid crystalline behavior found in several representatives of these compounds [3]. Detailed investigation of the correlation "chemical structure-conformation-adsorption of fibrinogen" was carried out using 12 model sets of 45 polymers each. These sets were created to account for the influence of chirality related to the presence of two chiral centers in some polyarylates, effect of solvent, and a level of 3D organization (e.g. minimized structures vs those obtained from MD simulations). The quality of predictions of FA obtained for 2D and 3D case is compared and future directions are discussed.

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[P2-2]

Van der Waals Interactions from the Exchange Hole Dipole Moment

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Despite its importance in chemistry, the dispersion or van der Waals interaction is difficult to model accurately. Standard Density Functional Theory (DFT) methods, very popular in computational chemistry today, do not include the necessary physics. This often leads to qualitatively incorrect predictions when DFT is applied to dispersion-bound systems. The dispersion interaction between molecules arises when an instantaneous dipole moment in one molecule induces a dipole moment in another. What, however, is the source of these instantaneous dipoles? We have proposed a novel post-Hartree-Fock dispersion model in which the source is the position-dependent dipole moment of the exchange hole. This model is very economical to implement and yields remarkably accurate C_6, C_8, and C_{10} dispersion coefficients, separations, and binding energies of intermolecular complexes.

[P2-3]

QM/MM and MD models of *Vinca* alkaloid interactions with Tubulin heterodimers

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Cellular microtubules are the building blocks of the cytoskeleton and play an integral role in many important cellular processes, including mitosis. Tubulin is the protein that microtubules are comprised of. Cancer drugs that interfere with microtubule dynamics have proven successful in the past and are a promising target for future development. The *Vinca* alkaloids, with lead compound Vinblastine, are an example of a successful class of microtubule disrupting chemotherapeutic drugs. Force field molecular dynamics (MD) have been performed on several Tubulin structures. Also, hybrid quantum mechanical (QM/MM) models have been developed to study the interaction between Vinblastine and Tubulin with both energy minimizations and molecular dynamics simulations. Future work will use this model developed to study the differing interactions between different *Vinca* alkaloid drugs and different Tubulin isotypes, which may allow for the tuning of drugs to specific types of cancer, the reduction of drug resistance, and the reduction of harmful side-effects of chemotherapy.

[P2-4]

Unitary Coupled Cluster For Ground and Excited States

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Conventional coupled cluster methods for excited states, e.g. EOMCC/STEOMCC, use diagonalization of non-Hermitian Hamiltonian. Sometimes it leads to complex eigenvalues, in particular if states are nearly degenerate. We will consider a unitary version of STEOM that avoids this problem. In addition, the description of the ground state in the singles and doubles using this theory includes implicitly connected higher excitations. This possibly improves the description of the ground state. In this poster, we (plan to) report some results of this new methodology.

[P2-5]

Electronic Structure Properties of Phenylene and Thiophene Derivatives of Fluorene: TD-DFT Study

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Fluorene-phenylene (FP) and fluorene-thiophene (FT) based oligomers and polymers and their derivatives are good candidates for organic blue-light emitting diodes. In this work, the intrinsic properties of the ground and excited states of FP and FT monomers and their derivatives are studied. The ground state optimized structures and energies are obtained using the molecular orbital theory and the density functional theory (DFT). The ground state potential energy curves or surfaces of FP and FT and their derivatives are also obtained. The character and energy of the first 20 singlet-singlet electronic transitions are investigated by applying the time-dependent DFT approximations to the correspondingly optimized ground state geometries. The lowest singlet state is studied with the configuration interaction (singles) approach (CIS). When available, a comparison is made with experimental results.

[P2-6]

DFT Studies of Au_m and $PtAu_n$ Clusters and Their N_2 and O_2 Adsorption Complexes

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The small pure gold and Pt-Au bimetallic clusters were studied within density functional theory. The gold clusters have similar delocalized highest occupied molecular orbitals (HOMOs), while the bimetallic ones have more localized HOMOs on the Pt atoms specifically. This makes the bimetallic clusters more preferred over the pure gold clusters in regioselective electrophilic reactions. Adsorptions of N_2 and O_2 on these metal clusters were also studied. In the N_2 adsorption complexes, the metal clusters donate their electrons to the anti-bonding σ orbitals of N_2, resulting in an end-on conformation. In the O_2 adsorption complexes, more complicate interactions between the cluster and the π orbitals of O_2 favor a lateral-on conformation. The trend of the gaps between the HOMO and the lowest unoccupied molecular orbitals of these adsorption complexes is consistent with the prediction from the maximum hardness principle.

[P2-7]

Peptide Hydrolysis in Thermolysin: Reactant Structure and Reaction Mechanism Studied with Classical and QM/MM Molecular Dynamics

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Thermolysin is a monozinc enzyme that has a well-characterized endopeptidase function, but whose reaction mechanism is incompletely understood. We have assessed the reactivity of various structures of the peptide-enzyme complex using short QM/MM molecular dynamics simulations. The structures were obtained using a substrate-docking procedure allowing for peptide flexibility and for insertion of water molecules into the active site, and were refined using classical molecular dynamics on a force field corrected for charge-transfer effects. These studies show that additional water molecules are enhancing the reactivity of the structure by stabilizing the substrate into a conformation prone to a nucleophilic attack. The free energy profile of the complete hydrolysis reaction (nucleophilic attack and peptide bond dissociation) is obtained from constrained QM/MM simulations. The stabilization of the transition state in the enzymatic pocket which leads to rate enhancement of several orders of magnitude is discussed and analyzed by comparing to a model hydrolysis reaction in aqueous solution.

[P2-8]

Similarity Transformations Applied to Vibronic Coupling Models

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Non-adiabatic effects in molecules which arise from the interaction between electronic and nuclear degrees of freedom can be modelled with a vibronic Hamiltonian. The matrix representation of multistate-multimode vibronic coupling models scales exponentially with the number of vibrational quanta in each mode. This renders the problem computationally expensive even for small molecules. To circumvent this problem, an indirect approach involving second quantization and similarity transformations is used. Some preliminary results are discussed.

[P2-9]

Improved Dissociation Energy and Potential Curve for BeH $X^2\Sigma^+$ from an Empirical and Ab Initio Study

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A comprehensive ab initio study and a detailed empirical analysis of all available spectroscopic data for the $X^2\Sigma^+$ ground electronic state of BeH has yielded an improved dissociation energy of D_e= 17710(50 $cm)^{-1}$and analytic potential energy function whose eigenvalue spacings reproduce all experimental data (on average)within the experimental uncertainties. The resulting potential has the correct theoretically known limiting long-range D-C_6/r^6 behaviour, and the combined-isotopologue direct-potential-fit analysis yields improved estimates of effective Born-Oppenheimer breakdown radial strength functions for this system. This work definitively disproves a longstanding speculation regarding whether this state has a small potential barrier protruding above the potential asymptote.

[P2-10]

Theoretical Studies on the Tautomers of Pyridinethiones

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Pyridinethiones can be used as ligand precursors for some Ga(III), In(III), V(IV,III) complexes with important diagnostic and therapeutic applications, but their tautomerisms in solution have not been clearly understood. We have employed ab initio and DFT methods (plus solvation effect corrections) to study their spectroscopic properties, including NMR, UV-vis and IR data. We compared our theoretical results with the existing experimental data and identified the structures of Pyridinethiones in solution. Some disagreements between the calculated results and the experimental assignments should be resolved in the future.

[P2-11]

First-Principles Study of Electronic and Optical Properties of Nitrogen Doped Single-wall Carbon Nanotubes

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There has been much interest in the mechanical, electronic and structural properties of carbon nanotubes (CNTs) since their discovery in 1991[1], due to their great potential for various applications such as nanoelectronics, biosensors, gas storage, and optical communications[2, 3]. Besides the pure carbon nanotubes, other compound nanotubes such as Nitrogen doped carbon nanotubes have also been the focus of intensive theoretical and experimental strudies, due to their specific properties[4].

First-principles calculations based on the density functional theory (DFT) and the generalized gradient approximation (GGA) were carried out to systematically investigate the electronic and optical properties of N-doped CNTs. CNTs with different diameters, various content of nitrogen and different structure configurations were studied. The comparison of their density of states (DOS) showed that the metallicity of nanotubes were enhanced by increasing the content of nitrogen. It could also be concluded that the content of nitrogen and defection in structures of CNTs had significant effect on their optical properties such as constructivity, absorption, and dielectric function etc..

Keywords: Carbon Nanotubes, N-doped CNTs, DFT, Optical properties

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[P2-12]

A high-throughput computational approach to find new uses for old drugs

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Drug discovery today focuses on screening chemical databases to find 'magic bullet' drugs of specific protein targets. Several recent studies on drugs thought to target single proteins have shown that the drugs are not nearly as specific as previously thought. Understanding the potential off-target interactions of these chemicals is of major interest to pharmaceutical research, particularly for discovering novel therapeutic uses of drugs. Existing drugs represent an efficient approach to drug discovery, as they already have a clinical history and thus require much less time and money to develop into a drug specific for the new disease.

Molecular docking is a computational approach that predicts the binding conformation and affinity of a ligand with a protein, and is typically used to find potential inhibitors for specific protein targets. The inverse scenario, the use of docking to find potential protein targets of specific ligands, is well suited for finding off-target protein interactions of a given drug, but is little studied. We have developed a high-throughput inverse docking pipeline and applied it to the inverse docking of an extensive set of approved and experimental small molecule drugs against an extensive set of protein target structures. These protein targets are implicated in human diseases, so novel protein-drug interactions discovered may represent novel leads for a disease. Our preliminary results highlight the promising nature of the inverse docking method for identifying potential novel uses for candidate drugs.

[P2-13]

DFT Investigation of The Fischer-Tropsch Synthesis on Fe Surface

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The Fischer-Tropsch synthesis (FTS) is nowadays a widely employed process in the industrial production of valuable long-chain hydrocarbons and derivatives from cheap CO and H_2. Despite a highly-promising option for generating clean-burning fuels, this process suffers from a number of limitations such as the limited selectivity of products, high cost, and less than optimal thermal efficiency.

This presentation will demonstrate the results obtained in our recent computational studies of FTS on Fe surface. In particular, the C-H bond activation of various hydrocarbon fragments (e.g. CH, CH_2, CH_3 and CH_4) and the C-C bond coupling between them on the reactive Fe(100) surface were investigated utilizing the slab model and periodic plane-wave DFT method. Electronic structure and reaction kinetic analyses of FTS were also performed where appropriate.

[P2-14]

A New Hybrid Meta-GGA Density Functional

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We propose a new hybrid density functional, which incorporates (a high percentage of) exact exchange, Meta-GGA exchange correlation, and correlation from second order perturbation theory. We investigate the success and shortcomings of this functional by applying it to calculations of atomization energies of the G2 set, binding energies of van der Waals complexes, and reaction barrier heights. We present the performance of this functional by comparing our results to those of other well established GGA, meta-GGA, and hybrid functionals.

[P2-15]

Computational studies on a novel redox-active crown ether

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The geometrical as well as the redox properties of the novel redox-active crown ether, dibiphenyltetramide-six-crown, are discussed herein. Through the use of a combination of semiempirical and DFT calculations, insight into the binding cavity, as well as the reversible redox process which acts as a switch mechanism for binding is gained. Geometries of the neutral and the radical anion of the crown ether were obtained at the semiempirical level (PDDG/PM3 and PM3). Solvent corrections to energy were introduced as single point calculations using DFT level of theory. Measurements of the binding cavity and the binding preference of the crown ether to several metal ions and organic compounds are presented.

[P2-16]

Quantum mechanical and hybrid quantum mechanical/molecular mechanical approach in the study of colchicine derivatives as potential anti-cancer drugs

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Colchicine is an antimitotic agent in cancer research. It suppresses cell division by inhibiting division of the cell's nucleus. What colchicine does is it binds to the tubulin heterodimer and prevents them from polymerization to form microtubules. However, colchicine has a fairly narrow range of effectiveness as a chemotherapy agent. It would have to be administered in large doses to be effective in killing cancer cells. In doing so, however, not only the cancer cells would die, but also the patient. The purpose of the study is to find analogs and derivatives of colchicine as potential anti-cancer drug candidates, which can be administered with minimal side effects on the patient, through computational approach. The computational modeling involves evaluating the stabilities of colchicine analogs and derivatives first in the gas phase using quantum mechanical(QM) approach. Then, the interactions between the resulting stable colchicine analogs and derivatives with the α,β-tubulin heterodimer are studied using hybrid quantum mechanical/molecular mechanical (QM/MM) technique.

[P2-17]

Novel nanotube-coordinated platinum complexes

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The structure and electronic properties of Pt-doped (5,5) single-walled carbon nanotubes (SWCNTs) have been studied within density functional theory. A model system consisting of a single Pt center in a symmetrical nanotube segment with capping H atoms is employed for this investigation. The adsorption of carbon monoxide on the Pt atom is an exothermic process, yielding a new nanotube-coordinated organometallic complex. This new species bears some resemblance to classical alkylplatinum complexes, except that three coordination sites of the Pt center on the nanotube are essentially rigid. The HOMO-LUMO gap of the nanotube-adsorbate complexes is widened upon adsorption of multiple molecules of carbon monoxide. Our study illustrates that localized Pt atoms fixed on the sidewall of a nanotube can indeed display interesting properties that will be of importance to materials science and fundamental inorganic and organometallic chemistry alike and may lead to novel chemical reactivities.

[P2-18]

Microheterogeneity in a Lattice Gas Model for Amphiphilic Solutes in Water

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A lattice gas model for aqueous solutions of amphiphilic solutes such as 1-propanol is presented and studied by Monte Carlo simulations. The model exhibits mesoscale clustering without phase separation, as do 1-propanol/water solutions. It consists of a two-site "solute" and a one site "solvent" with nearest-neighbour interactions. The solvent possesses multiple internal states, one of which interacts favorably with the solute, reflecting the entropic penalty involved with ordering the water molecules solvating a hydrophobic solute. The two-site solute comprises a hydrophobic "body" and a hydrophilic "head".

[P2-19]

Static Modeling of Ketene Dimerization Raction in Gas and Liquid Phase

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We present the first static study of the ketene dimerization reaction in liquid phase. A previous calculation (DFT-mPW1K functional) on the dimerization reaction in gas phase was in excellent agreement with experimental values of the energy barrier and heat of reaction for diketene product. However, the free energy barrier obtained in this calculation was almost 20 kcal/mol greater than the experimental free energy barrier in acetone. This suggests that either solvent plays a major role in this reaction or an unknown catalyst is facilitating this reaction. To see the effect of the solvent, another calculation was performed with the COSMO model: dielectric constant of 20.56 and Radii of C=2.2 A, O=1.3 A and H=1.16 A. The results in this liquid phase calculation demonstrated the same behavior as in gas phase: reactions are concerted with asynchronous transition states. The liquid phase calculation also had a free energy barrier that differed only 1.0 kcal/mol to the experimental value. This shows that the solvent plays a major role in the stabilization of the transition state and also suggests that there is no catalyst facilitating the reaction.

[P2-20]

Conformationally Dependent Photodynamics of Glycine

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The conformational variety of aminoacids play crutial role in determining 3D structures of peptides and proteins. In the ground state at room temperature the barriers separating the minima on potential energy surfaces are relatively low; therefore, the molecules can form all possible structures. However, in the excited state (as was revealed recently Ref. 1), the system does not have to rapidly loose memory and the photodynamics can be conformationally dependent. The objective of our study was to theoretically explore the phodynamics of the smallest aminoacid - glycine. Glycine molecule in the ground state forms various conformers possesing different hydrogen-bonding patterns which was found to be crutial for dynamics in the excited state. The photodynamics was studied by employing the *ab initio* molecular dynamics - Full Multiple Spawning Method developed by T. Martinez et al. and described in Ref. 2.

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[P2-21]

AuPt binary clusters: structure and reactivity within density functional theory

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Within density functional theory with the general gradient approximation for the exchange and correlation, the bimetallic clusters AuPt, Pt_6Au, and Au_6Pt have been studied for their structure and reactivity. The bond strength of AuPt lies between those of Au_2 and Pt_2 and it is closer to that of Au_2. The Pt atom is the reactive center in both AuPt and $AuPt^+$ according to electronic structure analysis. $AuPt^+$ is more stable than AuPt.

Pt_6Au, in general, prefers 3-dimensional geometry and high spin electronic state with multireference character. The most stable conformation for Pt_6Au is a sextet with edge and face capped triangonal bipyramid, in which the Au atom caps an edge of the triangonal bipyramid. The electronic impact of the doping of Au in Pt clusters on the overall chemical activity of the doped bimetallic cluster is not significant as that of the doping of Pt in Au clusters, however, the doping of Au lowers the chemical activity, thus enhancing the chemo-selectivity in gas phase, of PtAu bimetallic clusters.

On the other hand, Au_6Pt prefers electronic states with low multiplicity. The most stable conformation of Au_6Pt is a singlet and has quasi-planar hexagonal frame with Pt lying at the hexagonal center. The doping of Pt in Au cluster enhances the chemical regioselectivity of the Au cluster. The Pt atom essentially serves as electron donor and the Au atoms bonded to the Pt atom acts as electron acceptor in Au_6Pt.

O_2 prefers to adsorb on Au and CO prefers to adsorb on Pt. O_2 and CO have stronger adsorption on AuPt than they do on Au_6Pt. CO has much stronger adsorption on AuPt bimetallic cluster than O_2 does. The adsorption of CO on Pt modifies the geometry of AuPt bimetallic clusters.

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W. Q. Tian, M. Ge, F. Gu, T. Yamada, and Y. Aoki, J. Phys. Chem. A 2006, 110, in press.

[P2-22]

Molecular Modeling of Proton Dynamics in Fuel Cell Membranes

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The overall performance of a Polymer Electrolyte Fuel Cell is largely determined by the transport properties of the Polymer Electrolyte Membrane (PEM). Proton conductivity of a PEM is strongly dependent on its morphology and its state of hydration. Theoretical relationships between morphology, water content and effective properties such as proton conductivity are, thus, crucial in view of the design of new, highly-performing membranes, preferably such that could operate at elevated temperature and under conditions of minimal hydration. A large number of theoretical models utilize full quantum mechanical calculations for small clusters of acidic functional groups and water molecules or they exploit continuum dielectric approaches. However, such approaches usually ignore the role of long range correlations between charged sidechains in assisting proton dissociation and conduction. For exploring these effects, we consider a basic model system that consists of a 2D hexagonal array of acidic surface groups in its minimum hydration state, i.e. with one water molecule added per surface group. We use the Vienna Ab-initio Simulation Package (VASP) to perform geometry optimization calculations based on DFT. A unit cell of the model system contains three surface groups of the type CH3SO3H and three water molecules. We varied the separation of surface groups from 5 Å to 12 Å. From 5 Å - 6.2 Å, the minimum energy conformation corresponds to an an "upright" dissociated structure. At ~ 6.2 Å we found a transition to a "tilted" minimum energy conformation. Upon increasing the surface group separation in the "tilted" conformation, we observed a transition from a highly correlated fully dissociated state (< 7.5 Å) with three H3O+ per unit cell to a cluster-like, partially dissociated state with one H2O and two H3O+ per unit cell (7.5 Å – 9 Å). When the surface group separation exceeds 9 Å a fully non-dissociated state (3CH3SO3H + 3H2O per unit cell) was found. The stability of these structures at different side chain separations is explained in terms of the number of hydrogen bonds per unit cell. Unlike CF3SO3H, for CH3SO3H we found that water molecules interact with CH3 groups as well, due to the lower hydrophobicity of CH3 as compared to CF3. Calculations for arrays with increased surface group lengths (i.e. CF3CF2SO3H, CH3CH2SO3H) reveal similar structures and transitions

[P2-23]

Receptor docking studies of 1,5-diarylimidazole and 3,4-diaryltriazole derivatives possessing alkylthio substituent as a search for COX-2 selective enzyme inhibitors

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The inducible form of cyclooxygenase, prostaglandin G/H synthase-2 (PGHS-2, COX-2), is inhibited by new non-steroidal anti-inflammatory drugs (NSAIDs) such as the diarylheterocycles celecoxib and rofecoxib. Inhibition occurs by blocking access to the cyclooxygenase active site where arachidonate is convereted to prostaglandin G2 in the biosynthesis of prostaglandins. The diarylheterocycle NSAIDs achieve reversible binding in the entry channel, followed by a stronger binding within the active site. The inhibition is nearly irreversible and time-dependent. The receptor docking studies of a group of heteroaryl modified 1,5-diarylimidazole and 3,4-diaryltriazole possessing an alkylthio group on the heterocycle were performed to investigate the binding mode (favorable binding configuration) of each compound by using MOE 2003.02. Searching is conducted within a specified 3D docking box, using simulated annealing based on Monte Carlo method and MMFF94 molecular mechanics force field. These compounds exploit the extra space of a side-pocket in the active site of COX-2 that is not found in COX-1. In view of these findings, some of them were chosen to be prepared and evaluated as selective COX-2 inhibitors.

[P2-24]

Effect of O...O distance on the spectroscopic behaviors, structural parameters, and hydrogen bond strength in the enol form of beta-diketones

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It has been shown that the vibrational behaviors, pi-electron delocalization and NMR chemical shifts of the enol form of beta-diketones are dependent on the hydrogen bond length of the system. To show these relations quantitatively the O...O distance of the enol form of malonaldehyde, as a simple model, was changed from 2.6 Ĺ to 2.2 Ĺ in steps of 0.02 Ĺ and the rest of the structural parameters were fully optimized by means of density functional theory (DFT) methods. Gaussian 03 program was used for all quantum chemistry calculations. The changes of all vibrational normal modes vs. the O...O distance were plotted and the results were compared with the experimental data for the real systems with known O...O distances.

Furthermore, the correlations between the calculated O...O distance with the calculated and observed 1H NMR chemical shift were also studied.

By mean of natural orbital theory (NBO), using the NBO 5.0 program, the relation between the extent of pi-electron delocalization and the hydrogen bond strength is also studied.

The results of our calculations indicate that in this system the symmetric single minimum potential energy surface is not possible at the O...O distances longer than 2.3 Ĺ. Therefore, it is concluded that in this intramolecular hydrogen bonded systems the potential energy for proton movement always has a double minimum well shape, which in extreme of the H bond strength the potential function approaches to a symmetric flat-bottom shape.

[P2-25]

Why tert-Butyl Alcohol Associates in Aqueous Solution but Trimethylamine-N-oxide does not

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In dilute aqueous solution, *tert*-butyl alcohol (TBA) tends to aggregate but trimethylamine-N-oxide (TMAO) does not. Given that both molecules have very similar geometry with hydrophobic and hydrophilic groups, it is interesting to ask why they behave so differently in aqueous solution. To explore this question, we use molecular dynamics simulations to study two models representing TBA and TMAO, that differ essentially only in their electrostatic properties. It is shown that this difference is sufficient to give the different solution behavior. Furthermore, the principal difference identified is that the hydrophilic group of TMAO (the oxygen) interacts on average much more strongly with water than the corresponding group (the hydroxyl) of TBA. A hydrogen bond analysis shows that water-TBA and water-TMAO hydrogen bonds are similar in number, but that the hydrogen-bond energy is much more negative for water-TMAO. In all likelihood, this accounts for the different behavior in dilute aqueous solution.

[P2-26]

Adaptation of the GIAO theory of NMR chemical shifts to periodic systems

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R3T 2N2

The calculation of NMR chemical shifts and other 2nd order properties has been quite successful for isolated molecular systems in the gas phase. There are also several promising attempts at calculating these properties for periodic systems, however, most of them use plane waves.

We are developing an alternative approach that is based on atomic orital (AO) basis functions. This enables us to use the GIAO approach for solving the gauge problem of magnetic properties. Because of the short-range nature of the magnetic interactions, a 'one-site' approximation was taken into consideration were only one or a few unit cells are used to calculate the second order property. The size of this cluster must coincide with a cut-off distance where the interaction that is being considered vanishes. With this approach, the molecular theory can be applied directly for a periodic system if the Bloch functions are formulated in terms GIAOs.

[P2-27]

On geometries and stabilization energies of H-bonded nucleic acid base pairs containing unusual base pairs tautomers: Complete Basis Set Calculations at the MP2 and CCSD(T) levels

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Unusual tautomeric forms of nucleic acid bases are very popular system for calculation. They are not very large system but the main reason is to discover whether or not they occur in hydrogen bonding patterns in nucleic acids. Many calculation were performed in the gas phase, microhydrated environment and bulk water environment only to compare the stability of single base with its canonical form.[1] These studies revealed a possibility of the presence of unusual base pairs in nucleic acids. Thorough and accurate study of stability and geometry properties of base pairs with unusual base tautomers is still missing.

In this study we present comparison of hydrogen-bonded base pairs interaction energies between selected base pairs containing unusual tautomers. We provide complete basis set calculations at the MP2 and CCSD(T) levels.

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[P2-28]

Calculated Cu(II)/Cu(I) Reduction Potentials of a Copper Bound His-His Dipeptide

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The chemistry of the Cu(II) complex of the amyloid-beta (A-beta) peptide of Alzheimer's disease prompted this investigation of the Cu(II)/Cu(I) redox couple. The potential redox activity of the Cu(II)/A-beta complex has been implicated in the production of reactive oxygen species (ROS) and subsequent neurotoxicity via pathways that involve the reduction of Cu(II). The copper center in both the oxidized and reduced forms of the Cu/A-beta complex is unlikely to be rigidly held in a particular geometry as A-beta is a relatively short peptide (40-42 residues) without defined secondary structure in aqueous solution. As such reduction of Cu(II) in the Cu(II)/A-beta complex may be accompanied by release of ligand/s due to the preference of Cu(I) for lower coordination numbers than Cu(II). The reduction has been investigated using ab initio calculations on model systems of copper bound to A-beta. A model His-His dipeptide has been used to represent the His13-His14 residues of A-beta bound to copper, with additional ligands (e.g. 4-methyl-imidazole) used to fulfill the coordination requirements of the copper. The effect of the coordination environment, release of ligands, and backbone reorganization on the Cu (II)/Cu(I) reduction potential has been examined.

[P2-29]

Generation of Initial Reactive Trajectories and Accelerated Sampling for Transition Path Sampling

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Transition path sampling is an innovative method for focusing a molecular dynamics simulation on a reactive event. It has the potential to overcome the timescale limitations of ab initio molecular dynamics in the study of chemical reactions. Although transition path sampling methods can generate an ensemble of reactive trajectories, an initial reactive trajectory must be generated by some other means. We have developed and evaluated three methods for generating initial reactive trajectories for transition path sampling with ab initio molecular dynamics. The first is to initiate trajectories from the potential energy transition state found using static calculations and atomic velocities found using normal mode analysis. The second uses a high temperature molecular dynamics simulation and then iteratively reduces the total energy of the simulation until a low temperature reactive trajectory is found. The third uses an orbital based bias potential to find a reactive trajectory and uses this trajectory to initiate an unbiased trajectory. In addition, we present a technique to use an auxiliary potential to sample trajectories more efficiently.

[P2-30]

Effect of Pressure on Hydrophobic Interactions

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Proteins are known to denature under the effect of high pressure. Upon denaturation, the hydrophobic residues of the protein are exposed to water. Hydrophobic forces are among the dominant driving forces in protein folding/unfolding. Studies of the effect of pressure on hydrophobic interactions provide insight into the effect of pressure on hydrophobic residues in proteins when subjected to high pressure. In this work, effect of high pressure on hydrophobic hydration and hydrophobic interactions amongst methane-like solutes is investigated by extensive constant-pressure simulations in a TIP4P model of water. Using test-particle insertion techniques, thermodynamic and volumetric properties of hydrophobic hydration and hydrophobic interactions are obtained at various pressures and temperatures. The results for this simple model systems are in agreement with results obtained in experiments.

[P2-31]

Orbital Optimalization with Density Matrix Renormalization Group Method in the Active Space.

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In modern quantum chemistry the quest for a general method which can capture cases where mean-field theory brakes down is still of high importance. "The state of the art" which is Full Configuration Interaction fulfills all needed criteria but is much too expensive to be an affordable method for standard quantum chemistry calculations. Different branches of *ab initio* methods like Coupled Cluster are incapable to describe in a satisfying way the non-dynamic correlation. Multi-reference methods have their share of problems and cannot be used with large active spaces.

The Density Matrix Renormalization Group Method can become a powerful method in chemistry. It was shown in the literature that it can capture non-dynamic correlation easily. The formulation of the method is general in principle, we can converge to any level of accuracy with single algorithm. One electron properties can be calculated without additional effort.

We present results of orbital optimization with the DMRG method in the active space. We compare our results to the standard CASSCF method. We discuss the calculation of the 2-body density matrix within the the DMRG scheme which allows us to couple the calculation of orbital rotations to the DMRG algorithm. We will present state-averaged as well as state-selective approach which becomes possible after inclusion of spatial and spin symmetry into our DMRG algorithm. We also will show a comparison between convergence for a spin-adapted and non-spin addapted DMRG method. Finally, we will present a scheme which will allows us to add the missing dynamical correlation to our current approach.

[P2-32]

Quantitative Docking: Prediction Of Binding Affinities and Novel Estrogen Receptor Agonists

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A new software has been developed for accurate prediction of ligand-receptor binding affinities. The platform was built using the SVL language of the Molecular Operating Environment (Chemical Computing Group, Montreal). The complete procedure of docking was re-examined, from preparation of protein structure and ligand conformer generation, to scoring methods, data analysis and interpretation. Some guidelines are established to monitor the efficiency of the docking procedure. The resulting method includes modified versions of some features from existing programs, plus some novel features, including a fast method for simulation of receptor flexibility and a couple of method to accelerate the docking procedure.

The software takes advantage of a calculation cluster which makes it scalable for the high volume of calculations needed on typical targets. Also, the docking procedure is modular, which makes it possible to optimize the method for studying different types of ligand-receptor targets. The scoring method uses pure energy terms, without introducing arbitrary descriptors.

Using the method, binding affinities of a series of agonists were calculated in human estrogen receptor (ERα and ERβ), with good agreement with experimental values. The software could also predict α/β selectivity of the ligands in good agreement with experimental data. Finally, we used the software to design novel non carcinogenic estrogen agonists. Prototype molecules are synthesized and tested positive for activity.

[P2-33]

Transition from molecular to hydrodynamic diffusion regimes: A molecular dynamics study

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The tracer diffusion of a hard sphere particle immersed in a hard sphere fluid is studied using molecular dynamics simulations. Over a wide range of fluid densities, the diffusion of tracers with sufficiently small diameters should be accurately described by Enskog theory (a kinetic theory) while that for those with large enough diameters should be accurately described by hydrodynamic theory (the Navier-Stokes equation). Diffusion coefficients for tracers of varying diameters are presented that connect each of these limits, and show the behavior in the transition region between them. This is shown for several fluid densities. It is found that the value of the diffusion coefficient is close to the sum of the Enskog and hydrodynamic predictions when slip boundary conditions are employed with the latter. A simple formula is proposed to estimate the calculated results, and is employed to predict when, for a given fluid density, the diffusion can be reasonably predicted using hydrodynamic theory. The calculated results should serve as a benchmark for future theories that aim to predict the diffusion coefficient in the transition from molecular to hydrodynamic regimes.

[P2-34]

Density Functional Theory Investigation into the Stereocontrol of the Syndiospecific Polymerization of Propylene Catalyzed by Cs-Symmetric Zirconocenes

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The mechanisms of the two most likely routes for the generation of stereodefects in the syndiospecific polymerization of propylene, mediated by C_s-symmetric zirconocenes, are explored in detail using Density Functional Theory. Double mm triads are generated mainly as a consequence of enantiomeric mis-insertions, while defective single m dyads are to be ascribed to site epimerization events. The frequency of enantiomeric mis-insertion is marginally affected by the counter-anion and by solvation, the most important factor being the structure of the ligand. Site epimerization is also influenced by the nature of the ligand system, but the bulk and the charge distribution of the anion also play a prominent role. Inclusion of solvent effects is critical to explaining reactivity and to affording qualitatively correct predictions of the selectivity.

Application of a two-parameter probabilistic scheme allows predicting pentad distributions from the computed selectivities. The good agreement found between experiment and computations for the basic unsubstituted system by Ewen et al. validates the proposed model and allows relying on the computed pentad distributions for assessing the effectiveness of ligand substitutions on syndioselectivity.

[P2-35]

QSPR Approaches to Calculating the pKa Values of Protonated Aliphatic Amines.

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Quantitative Structure-Property Relationships (QSPRs) relating quantum-mechanical properties ("descriptors") to experimentally-determined pK_a values are sought for a group of protonated aliphatic amines. These relationships may either provide a new theoretical method of pK_a calculation, or increase the accuracy of existing methods based on calculation of Gibbs free energies for the acid/base equilibrium. The descriptors examined computationally include a mix of orbitalic and electrostatic factors. All are calculated using a variety of electronic structure approaches. Calculations are carried out in the gas phase and using Polarizable Continuum Methods of solvent modeling with and without explicit inclusion of some solvent molecules. While the immediate goal is a rapid and accurate method of pK_a calculation, ultimately the intent is to use QSPR to illuminate the combination of electrostatic and orbitalic properties which control the acid/base equilibrium.

[P2-36]

Dissociation of Charged Protein Complexes in Gas Phase

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Electrospray ionization mass spectrometry (ESI-MS) has been used to study properties of protein complexes in the gas phase. Some of these experimental studies have pointed out that dissociation of protein clusters lead to asymmetric charge distributions in the resulting fragments. Molecular dynamics (MD) simulation was used to study this phenomenon in detail using cytochrome c dimers with different charge states. Various shape descriptors such as radius of gyration, asphericity and overcrossing number were calculated to determine structural changes in each monomer. Structural changes were observed only for the monomers with charges over +11. Moreover, only symmetrically charged dimers dissociated within the ps time scale. Results from this study will help to explain experimental evidence on asymmetric charge distributions in protein fragments during gas phase dissociation.

[P2-37]

Study of the Conformational Dynamics of HIV-1 Protease using Reversible Digitally Filtered Molecular Dynamics

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Reversible digitally filtered molecular dynamics (RDFMD) [1-3] is a method which enhances conformational dynamics through the application of digital filters to the internal velocities of a system to selectively enhance or suppress vibrational motion. This method has been applied to several protein systems, including the HIV enzymes.

HIV-1 protease is an aspartic protease and one of the three enzymes encoded by the HIV genome. Its role in the life-cycle of HIV involves the hydrolysis of viral polyproteins into functional proteins, which are essential for viral assembly and subsequent activity, making the enzyme an obvious target for drug development. However, mutations of this protein occur rapidly due to the high replication rate of the virus, heightened by selective pressure exerted by the current inhibitors which affects their long-term effectiveness.

The enzyme is a homodimer comprising of two 99 residue monomers with a substrate cleavage site located at the interface between them. The active site is capped by two identical beta-hairpin loops, known as the flaps, which form part of the substrate binding site and regulate substrate entry into the active site.

The methods of conventional molecular dynamics and RDFMD have been applied to both the wild-type and mutant HIV-1 protease in the apo [4] and inhibitor-bound forms to evaluate the effects of mutations and inhibitor binding on the conformational dynamics of the enzyme. The RDFMD simulations of the apo wild-type enzyme reveal numerous flap opening events. The effect of the enzyme mutation and ligand binding on the conformations accessible to protein will be described. The RDFMD simulations are able to accelerate infrequent large-scale conformational changes, thereby revealing new conformations which were not present in simulations carried out using conventional molecular dynamics.

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[P2-38]

Studies of APX_3 systems (A=O, S and X= Br and I)

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Computational studies of OPX_3 and SPX_3 (X = Br and I) molecules and the corresponding anions was carried out using DFT, MP2, and CCSD(T) methods with the newly developed model core potentials. $OPBr_3$ was used as a benchmark species to test the model core potentials and methods by comparing experimental and calculated results. With mcp-dzp1, mcp-tzp1 and mcp-qzp1 basis-sets we computed the geometric structure, electron affinities, and electrostatic moments. Infrared frequencies were calculated and compared with available experimental data. Wave functions were analyzed by the Natural Bond Orbital method.

[P2-39]

From Molecules to Properties: The Suite of Programs around COSMO-RS

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The quantum chemically based COSMO-RS method has developed to powerful approach toward the prediction of thermodynamics properties for chemistry, chemical engineering, medicinal chemistry and environmental chemistry. Various software tools have been developed in order to supplement the core program COSMotherm for the various application areas. In this poster the different programs and their modes of interaction will be discussed.

[P2-40]

Docking study of 3-(N,N-dimethylamino)-1,2-diphenyl-1-prpanone and other opioid analgesic

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Opioid analgesics offer reduction of severe pain, and for centuries opium and its extracts have been used for therapeutic purposes. Therapeutic potential and demand of opioid analgesics have initiated numerous amounts of scientific efforts, which have resulted in development of a number of new opioid analgesics. 3-(N,N-dimethylamino)-1,2-diphenyl- 1-prpanone recently synthesized and found to have opioid analgesic activity. In this report, we will present our results from a docking study of the title compound, morphine, methadone and met, leu-enkephalines with the μ, κ and δ-opioid receptors based on the agonist peptide-incorporated structural model of the opioid receptor reported by Mosberg et al. [Mosberg HI & Fowler CB; J. Peptide Res. 60, 329–335, 2002] using the Autodock 3 program. Formalin and tail-flick test were used to evaluate in vivo analgesic activity data. Docking energies, binding mode and structure of tested compounds correlate well with in vivo tests.

[P2-41]

On the Design of Raney-Type Catalysts: A Density Functional Study

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Raney-type catalysts, which have the form of skeletal or sponge metals and alloys, constitute an attractive catalyst form for direct conversion of methane. These metals are relatively cheap and less liable to sinter under milder conditions. The catalyst is prepared by selective dissolution of Al-based binary, ternary or even higher alloys of, e.g., Ni, Co, Cu, etc., in concentrated NaOH. After leaching out the Al, spontaneous structural collapse and rearrangement of the residual metal(s) leads to a porous material of high specific-surface-area for catalysis [1-3]. However, selection and preparation of the "appropriate" catalyst may involve tedious trial and errors. On the other hand, theoretical calculation and prediction of structural stability is now within many researchers' grasp via powerful and ubiquitous computational programs. In this work, a throughput-screening of the physico-chemical properties of several Raney-type catalysts, some of them are known and others are theoretically designed, has been carried out using density functional theory. While the calculation provided information on the stability and physico-chemical properties of the catalysts, a series of new catalysts has been proposed for experimental verification. Results of the calculations will be presented and discussed in the conference.

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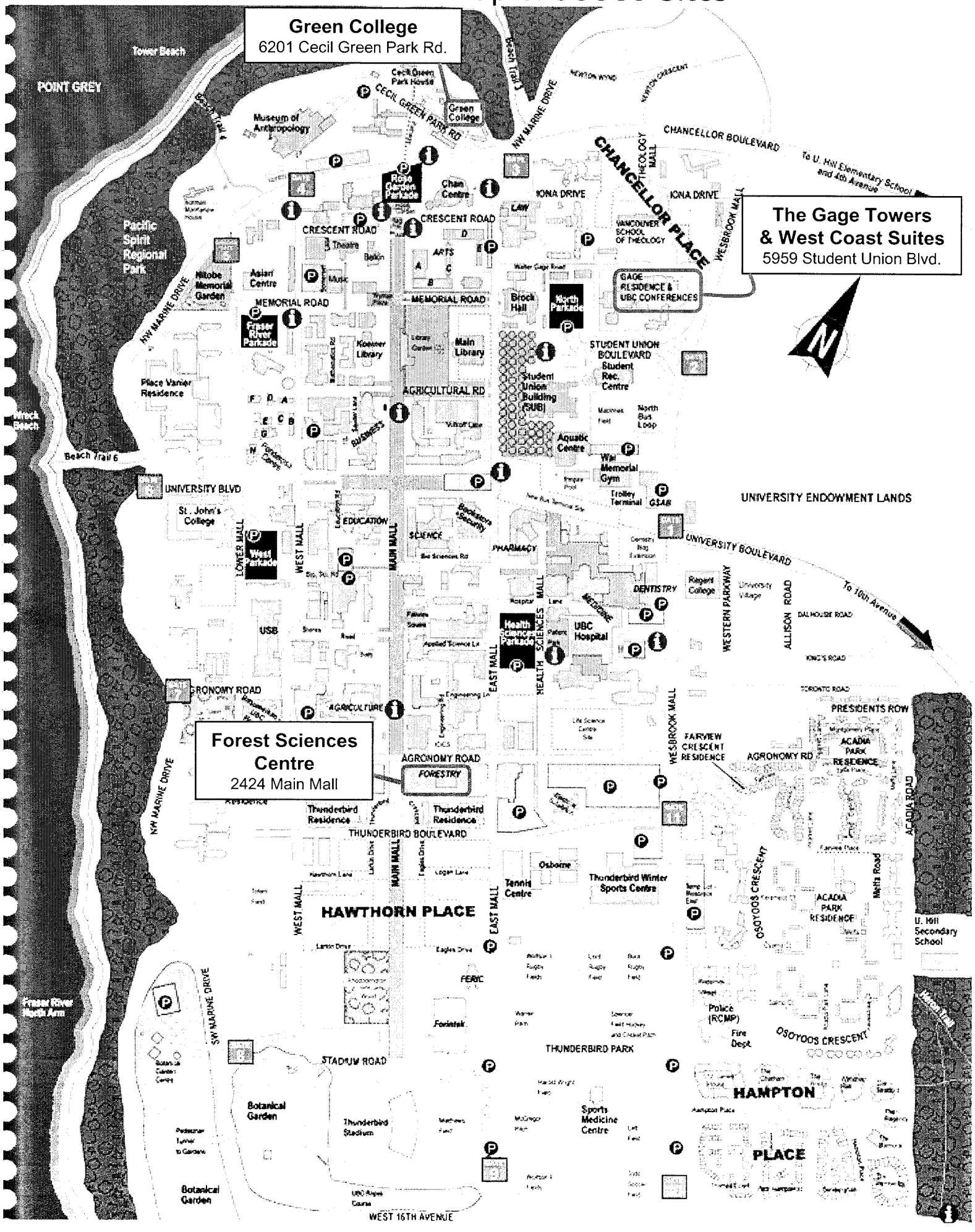
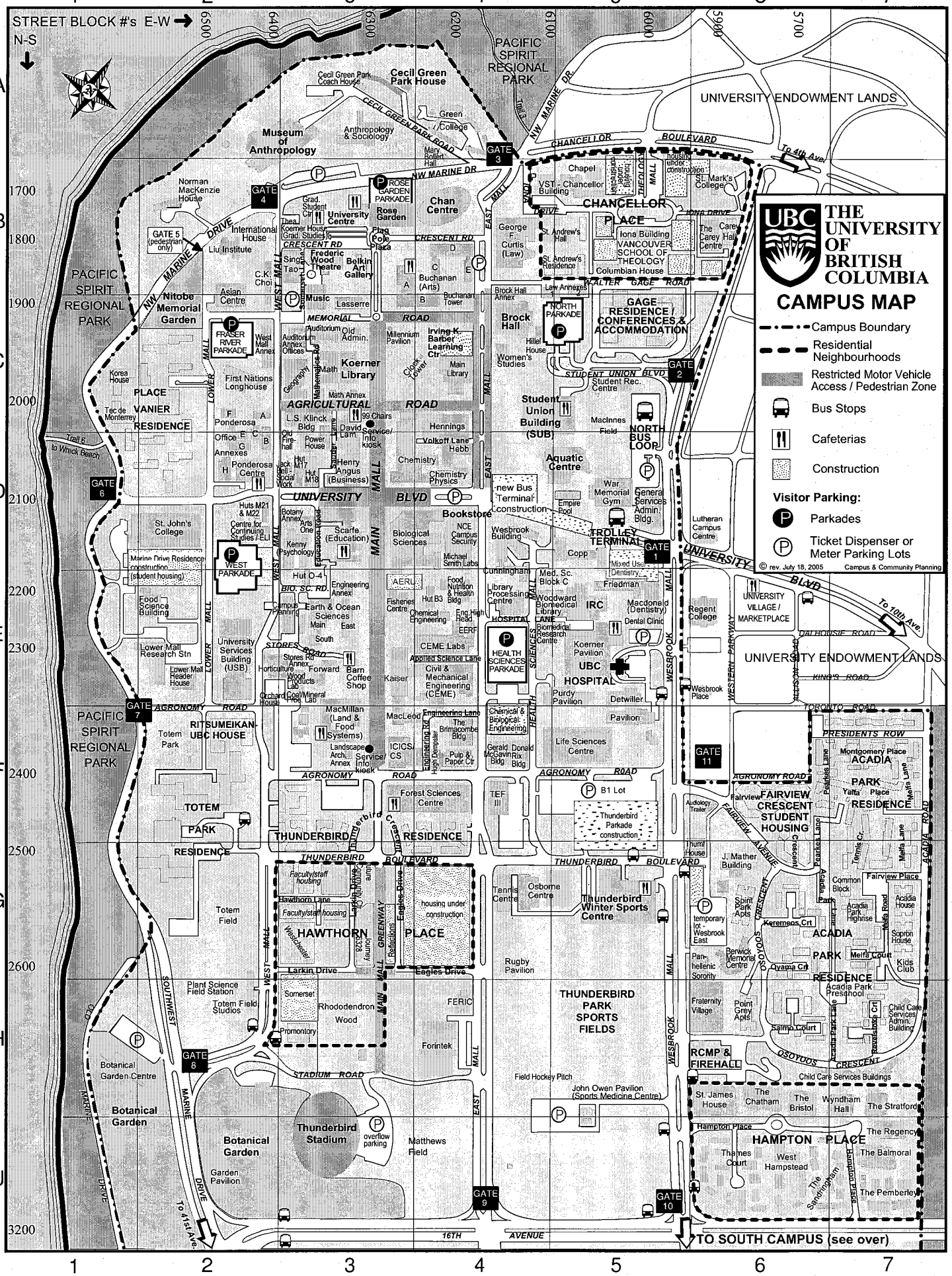
CCCC6 Information

UBC maps, accommodation, shops, food services, athletic facilities, and recreational activities on UBC campus

Detailed UBC Map & CCCC6 Sites




THE UNIVERSITY OF BRITISH COLUMBIA
CAMPUS MAP
Campus Boundary
Residential Neighbourhoods
Restricted Motor Vehicle Access / Pedestrian Zone
Bus Stops
Cafeterias
Construction
Visitor Parking:
Parkades
Ticket Dispenser or Meter Parking Lots
© rev. July 18, 2005 Campus & Community Planning
STREET BLOCK #'s E-W
N-S
PACIFIC SPIRIT REGIONAL PARK
UNIVERSITY ENDOWMENT LANDS
CHANCELLOR PLACE
GAGE RESIDENCE / CONFERENCES & ACCOMMODATION
Brock Hall
Student Union Building (SUB)
Koerner Library
Museum of Anthropology
Cecil Green Park House
Chan Centre
Rose Garden
Nitobe Memorial Garden
VANIER RESIDENCE
Aquatic Centre
UBC HOSPITAL
IRC
Bookstore
TROLLEY TERMINAL
new Bus Terminal construction
Thunderbird Winter Sports Centre
THUNDERBIRD PARK SPORTS FIELDS
THUNDERBIRD RESIDENCE
HAWTHORN PLACE
TOTEM PARK RESIDENCE
RITSUMEIKAN-UBC HOUSE
FAIRVIEW CRESCENT STUDENT HOUSING
ACADIA PARK RESIDENCE
HAMPTON PLACE
Thunderbird Stadium
Botanical Garden
RCMP & FIREHALL
UNIVERSITY VILLAGE / MARKETPLACE
TO SOUTH CAMPUS (see over)

Map Directory

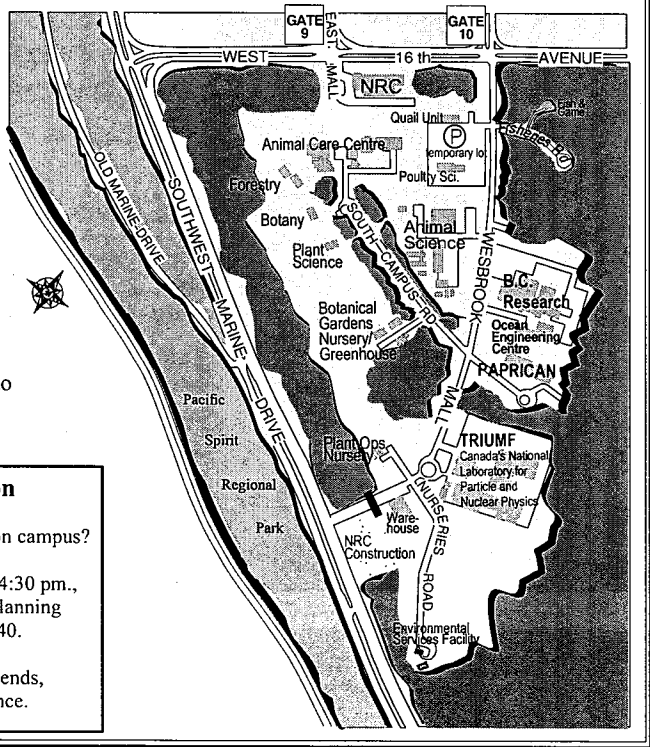
Site or Building Name & Address	Grid
Acadia/Fairview Common Block, 2707 Tennis Cres	G7
Acadia House, 2700-2720 Acadia Rd	G7
Acadia Park Residence	F/H-6/7
Acadia Park Highrise, 2725 Melfa Rd	G7
Acadia Park Preschool, 2750 Acadia Park Lane	H7
Animal Care Centre, 6199 S. Campus Rd	South Campus
Animal Science S. Campus Bldgs, 3473 Wesbrook Mall	South Campus
Anthropology & Sociology Bldg, 6303 NW Marine Dr	A3
Aquatic Centre, 6121 University Blvd	D5
Aquatic Ecosystems Research Lab (AERL) (under construc.), 2202 Main Mall	E3
Arts One Bldg, 6358 University Blvd	D3
Asian Centre, 1871 West Mall	B2
Audiology & Speech Sciences Classroom Trailer, 5830 Fairview Ave	F6
Auditorium, 6344 Memorial Rd	C3
Auditorium Annex Offices, 1924 West Mall	C3
Barn Coffee Shop, 2323 Main Mall	E3
B.C. Research Inc., 3650 Wesbrook Mall	South Campus
Belkin (Morris & Helen) Art Gallery, 1825 Main Mall	B3
Berwick Memorial Centre, 2765 Osoyoos Cres	G6
Biological Sciences Bldg [Science Faculty office], 6270 University Blvd	D3
Biomedical Research Ctr, 2222 Health Sciences Mall	E4
Biotechnology Laboratory, 2125 East Mall	D4
Bollert (Mary) Hall, 6253 NW Marine Dr	A4
Bookstore, 6200 University Blvd	D4
Botanical Garden Centre/Gatehouse, 6804 SW Marine Dr	H1
Botanical Garden Pavilion (enter at Gatehouse, 6804 SW Marine Dr)	J2
Botan. Gard. Greenhses/ Workshops, 6088 S. Campus Rd	South Campus
Botany Annex, 6386 University Blvd	D3
Botany Greenhouses & Trailer, 6182 S. Campus Rd	South Campus
Brimacombe Building, 2355 East Mall	F4
Brock Hall and Brock Hall Annex, 1874 East Mall	C4
Buchanan Building (Blocks A, B, C, D, & E) [Arts], 1866 Main Mall	B3/4
Buchanan Tower, 1873 East Mall	C4
C.K. Choi Building for the Institute of Asian Research, 1855 West Mall	B2
Campus & Community Planning, 2210 West Mall	E3
Campus Security, 2133 East Mall	D4
Carey Hall, 1815 Wesbrook Mall	B6
Carey Centre (The) 5920 Iona Drive	B6
Cecil Green Park Coach House, 6323 Cecil Green Park Rd	A3
Cecil Green Park House, 6251 Cecil Green Park Rd	A3
CEME — *see Civil & Mechanical Engineering Building*	
Centre for Continuing Studies [English Language Inst], 2121 West Mall	D2
Centre for Rsrch in Women's Studies & Gender Relations, 1896 E. Mall	C4
Chan Centre for the Performing Arts, 6265 Crescent Rd	B4
Chancellor Place	B5
Chemical & Biological Engineering Bldg (under construction), 2360 East Mall	F4
Chemical Engineering Building, 2216 Main Mall	E4
Chemistry Building, 2036 Main Mall	D3
Chemistry Physics Building, 6221 University Blvd	D4
Child Care Services Admin. Bldg, 2881 Acadia Rd	H7
Child Care Services Bldgs, 5580-5690 Osoyoos Cresc	H7
Civil & Mechanical Engineering Bldg (CEME), 6250 Applied Science Lane	E4
Civil & Mechanical Eng. Labs, 2275 East Mall	E4
Coal & Mineral Processing Lab, 2332 West Mall	E3
Copp (D.H.) Building, 2146 Health Sciences Mall	D5
Cunningham (George) Building [Pharmaceutical Sc.], 2146 East Mall	E4
Curtis (George F.) Building [Law], 1822 East Mall	B4
David Lam Learning Centre, 6326 Agricultural Rd	C3
David Lam Management Research Ctr, 2033 Main Mall	C3
Donald Rix Building, 2389 Health Sciences Mall	F4
Earth & Ocean Sciences (EOS) - East, 2219 Main Mall	E3
Earth & Ocean Sciences (EOS) - Main and South, 6339 Stores Rd	E3
Earthquake Engineering Research Facility (EERF), 2235 East Mall	E4
Engineering Annex, 6298 Biological Sciences Rd	E3
Engineering High Head Room Lab, 2225 East Mall	E4
Environmental Services Facility, 6025 Nurseries Rd	South Campus
Faculty of Law Annexes 1 and 2, 6050 and 6020 Walter Gage Rd	B4/5
Fairview Crescent Student Housing, 2600-2804 Fairview Cres	F6
FERIC (Forest Eng. Res. Institute), 2601 East Mall	H4
Fire Department, 2992 Wesbrook Mall	H6
First Nations Longhouse, 1985 West Mall	C2
Fish & Game Branch Workshops, 5773 Fisheries Rd	South Campus
Fisheries Centre - Hut B-8, 2204 Main Mall	E3
Flag Pole Plaza (Main Mall & Crescent Rd)	B3
Food, Nutrition and Health Bldg, 2205 East Mall	E4
Food Science Building, 6640 NW Marine Dr	E2
Forest Sciences Centre [Faculty of Forestry], 2424 Main Mall	F4
Forest Sciences Greenhouse, 6186 S. Campus Rd	South Campus
Forestry Field House, 6186 S. Campus Rd	South Campus
Forintek Western Research Facility, 2665 East Mall	H4
Forward (Frank) Building, 6350 Stores Rd	E3
Fraternity Village, 2880 Wesbrook Mall	H6
Frederic Wood Theatre, 6354 Crescent Rd	B3
Friedman Bldg, 2177 Wesbrook Mall	E5
Gage Residence, 5959 Student Union Blvd	C5
General Services Administration Bldg (GSAB), 2075 Wesbrook Mall	D5
Geography Building, 1984 West Mall	C3
Gerald McGavin Building, 2386 East Mall	F4
Graduate Student Centre (Thea Koerner House), 6371 Crescent Rd	B3
Green College, 6201 Cecil Green Park Rd	A4
Hampton Place	H/J-6/7
Hawthorn Place	G/H3
Hebb Building, 2045 East Mall	D4
Hennings Building, 6224 Agricultural Rd	C4
Henry Angus Building [Sauder School of Business], 2053 Main Mall	D3
Hillel House, 6145 Student Union Blvd	C4
Horticulture Building/Greenhouse, 6394 Stores Rd	E2/3
Hospital, UBC, 2211 Wesbrook Mall	E5
Hugh Dempster Pavilion, 6245 Agronomy Rd	F4
Hut B-3 - Fisheries Ctr, 6248 Biological Sciences Rd	E4
Hut M-17, 6373 University Blvd	D3
Hut M-18, 6361 University Blvd	D3
Hut M-21 & Hut M-22, 2109 West Mall	D2
Hut O-4, 6365 Biological Sciences Rd	E3
ICICS/CS (Institute for Computing, Information & Cognitive Systems/ Computer Science - formerly CICSR/CS), 2366 Main Mall	F4
Instructional Resource Centre (IRC), 2194 Health Sciences Mall	E5
International House, 1783 West Mall	B2
Irving K. Barber Learning Ctr (former Main Library)	C4
Jack Bell Building for the School of Social Work, 2080 West Mall	D3
John Owen Pavilion & Allan McGavin Sports Medicine Centre, 3055 Wesbrook Mall	H5
Kaiser (Fred) Building [Faculty of Applied Science], 2332 Main Mall	E3
Kenny (Douglas T) Building, 2136 West Mall	D3
Kids Club, 2855 Acadia Rd	G7
Klinck (Leonard S.) Bldg, 6356 Agricultural Rd	C3
Koerner (Walter C.) Library, 1958 Main Mall	C3
Korea House (in Place Vanier), 1935 Lower Mall	C1
Landscape Architecture Annex, 2371 Main Mall	D4
Lasserre (Frederic) Building, 6333 Memorial Rd	C3
Leon and Thea Koerner University Centre, 6331 Crescent Rd	B3
Library Processing Centre, 2206 East Mall	E4
Life Sciences Centre, 2350 Health Sciences Mall	F5
Liu Institute for Global Issues, 6476 NW Marine Dr	B2
Lower Mall Header House, 2269 Lower Mall	E2
Lower Mall Research Station, 2259 Lower Mall	E2
Macdonald (J.B.) Building [Dentistry], 2199 Wesbrook Mall	E5
MacLeod (Hector) Building, 2356 Main Mall	F3
MacMillan (H.R.) Bldg [Faculty of Land & Food Systems], 2357 Main Mall	F3
Main Library (new Irving K. Barber Learning Ctr), 1956 Main Mall	C4
Marine Drive Residence (for students, under construction), 2205 Lower Mall	D2
Mathematics Annex, 1986 Mathematics Rd	C3
Mathematics Building, 1984 Mathematics Rd	C3
Mather (James) Building, 5804 Fairview Ave	G6
Medical Sciences Block C, 2176 Health Sc. Mall	E4
Michael Smith Laboratories, 2185 East Mall	D4
Museum of Anthropology, 6393 NW Marine Dr	A2/3
Music Building, 6361 Memorial Rd	B/C3
Networks of Ctrs of Excellence (NCE), 2125 East Mall	D4
99 Chairs/Trek Express, 2015 Main Mall	C3
Nitobe Memorial Garden, 1903 West Mall	B/C2
Norman MacKenzie House, 6565 NW Marine Dr	B2
NRC Institute for Machinery Research, 3250 East Mall	South Campus
Ocean Engineering Centre, 3760 Wesbrook Mall	South Campus
Old Administration Building, 6328 Memorial Rd	C3
Old Firehall, 2038 West Mall	D3
Orchard House (formerly Header House), 2336 West Mall	E2
Osborne (Robert F.) Centre/Gym, 6108 Thunderbird Blvd	G4
Panhellenic Sorority House, 2770 Wesbrook Mall	G6
PAPRICAN Building, 3800 Wesbrook Mall	South Campus
Place Vanier Residence, 1935 Lower Mall	C/D2
Plant Ops Nursery/Greenhouses, 6116/6136 Nurseries Rd	South Campus
Plant Science Field Building, 6182 S. Campus Rd	South Campus
Plant Science Field Station & Garage, 2613 West Mall	H2
Point Grey Apartments, 2875 Osoyoos Cresc	H6
Police (RCMP) & Fire Department, 2990/2992 Wesbrook Mall	H6
Ponderosa Centre, 2071 West Mall	D2
Ponderosa Office Annexes: A, B, & C, 2011-2029 West Mall	C/D2
Ponderosa Office Annexes: E to H, 2008-2074 Lower Mall	C/D2
Power House, 2040 West Mall	D3
Pulp and Paper Centre, 2385 East Mall	F4
Ritsumeikan-UBC House, 6460 Agronomy Rd	F2
Rodney Graham Millennium Pavilion	C3
Rose Garden	B3
Rugby Pavilion, 2584 East Mall	G4
Scarfe (Neville) Building [Education], 2125 Main Mall	D3
Sing Tao Building, 6388 Crescent Rd	B3
Sopron House, 2730 Acadia Rd	G7
South Campus Warehouse, 6116 Nurseries Rd	South Campus
Spirit Park Apartments, 2705-2725 Osoyoos Cresc	G8
St. Andrew's Hall/Residence, 6040 Iona Dr	B5
St. John's College, 2111 Lower Mall	D2
St. Mark's College, 5935 Iona Dr.	B6
Stores Road Annex, 6368 Stores Rd	E3
Student Recreation Ctr, 6000 Student Union Blvd	C5
Student Union Bldg (SUB), 6138 Student Union Blvd	C4
Tec de Monterrey (in Place Vanier), 1935 Lower Mall	C1
Technology Enterprise Facility III, 6190 Agronomy Rd	F4
Thea Koerner House [Graduate Studies], 6371 Crescent Rd	B3
Thunderbird Residence, 6335 Thunderbird Cresc	F3/4
Thunderbird Stadium, 6288 Stadium Rd	J3
Thunderbird Winter Sports Ctr, 6066 Thunderbird Blvd	G5
Totem Field Studios, 2613 West Mall	H2
Totem Park Residence, 2525 West Mall	F/G2
TRIUMF, 4004 Wesbrook Mall	South Campus
Triumf House (TRIUMF Visitor's Residence), 5835 Thunderbird Blvd	G6
UBC Hospital, 2211 Wesbrook Mall	E5
UBC Tennis Centre, 6160 Thunderbird Blvd	G4
University Centre (Leon & Thea Koerner), 6331 Crescent Rd	B3
University Services Building (USB), 2329 West Mall	E2
Vancouver School of Theology, 6000 Iona Drive	B5
Walter H. Gage Residence, 5959 Student Union Blvd	C5
War Memorial Gymnasium, 6081 University Blvd	D5
Wesbrook Bldg, 6174 University Blvd	D4
Wesbrook Place, 2250 Wesbrook Mall	E6
West Mall Annex, 1933 West Mall	C2
West Mall Swing Space Bldg (under construction), 2175 West Mall	D2
Wood Products Laboratory, 2324 West Mall	E3
Woodward Biomedical Library, 2198 Health Sciences Mall	E4/5

SOUTH CAMPUS MAP

Campus & Community Planning
www.planning.ubc.ca

Note:

▬ Road blocked — No through traffic along Wesbrook Mall on South Campus from/to SW Marine Drive



Map Information

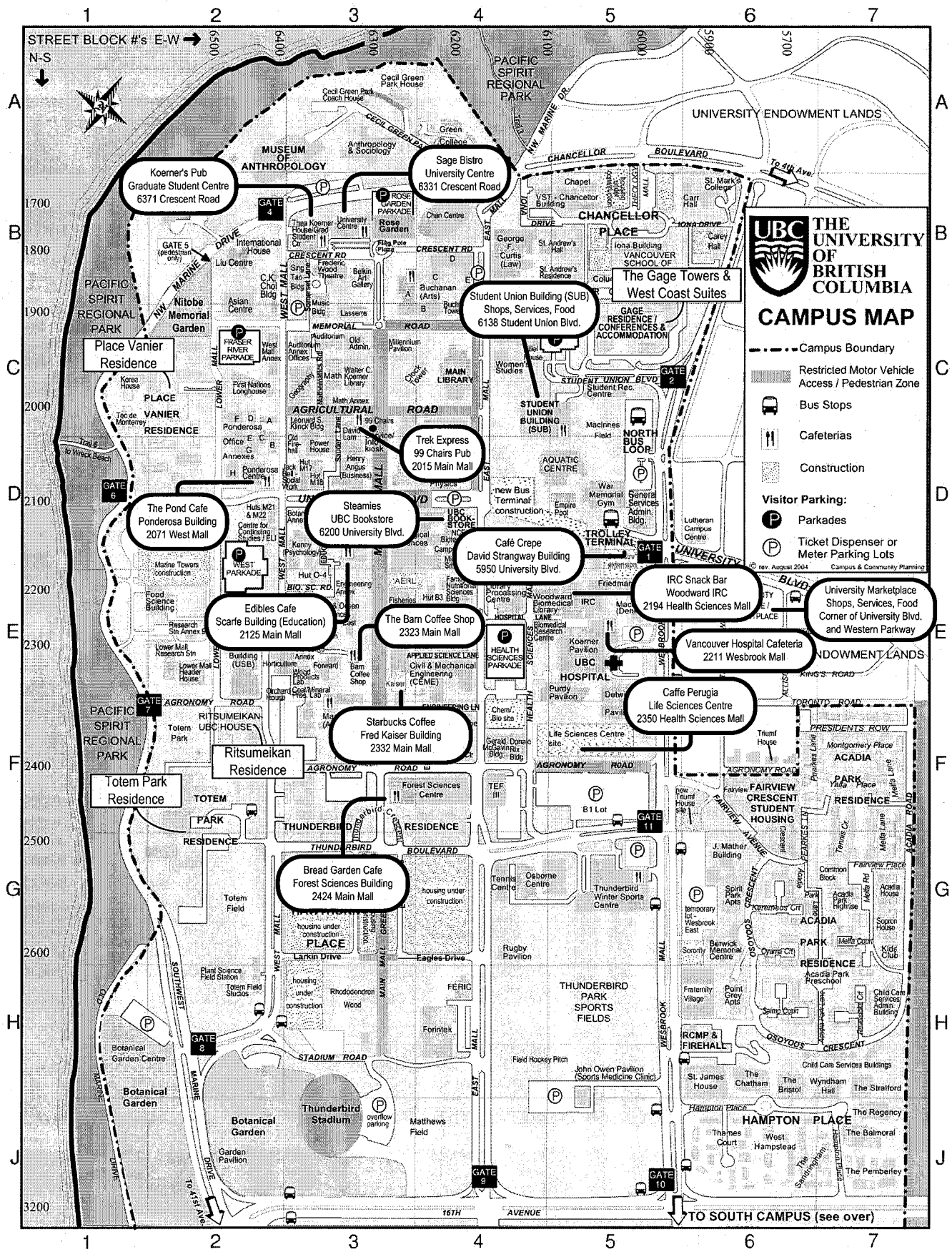
Need help finding your way on campus?

Monday to Friday, 8:30 am - 4:30 pm., call Campus & Community Planning Map Info Line at 604-827-5040.

After hours, holidays or weekends, call 604-822-8609 for assistance.

UBC Conferences and Accommodation
at The University of British Columbia
A DIVISION OF HOUSING AND CONFERENCES

Accommodation and Food Services
at the University of British Columbia



Summer 2006 Campus Dining Hours

at the University of British Columbia

UBC Conferences and Accommodation
at The University of British Columbia
A DIVISION OF HOUSING AND CONFERENCES

Name	Type of cuisine	Monday-Friday Hours	Weekend Hours
University Village/Marketplace			
Aji Taro Kanpai Japanese Bistro	Japanese Food	11am-3pm & 5pm-10pm	11am-3pm & 5pm-10pm
Blenz	Coffee, Snacks	6am-11pm	7am-11pm
McDonald's	Burgers, Fries, Shakes	M/T 6am-12am, W/Th/F 6am-3am	Sat 6am-3am, Sun 6am-12am
Mio Japan	Japanese Food	11am-9pm	11am-9pm
One More Sushi* *(upstairs)*	Japanese Food	11am-3pm, 5pm-10pm	Sat and Sun 12pm-10pm
Only U Café*	Deli Style Foods	8am-8pm	Sat and Sun 9am-3pm
Oven Fresh Bakery*	Baked Goods-fresh daily	7:30am-7pm	Sat 8:30am- 6pm
Pearl Fever Tea House	Blended Drinks	11am-11pm	12pm-11pm
Pita Pit	Pitas, Salads	M-F 6am-11pm	Sat 6am-11pm, Sun 7am-11pm
Starbucks Coffee	Coffee, Snacks	6am-11pm	Sat 6am-11pm, Sun 7am-11pm
University Pizza	Pizza & Pasta	M-Th 11am-11pm, F 11am-2am	Sat 11am-2am, Sun 4pm-11pm
University Village Restaurant	Chinese Food	11am-10pm	Sat 11am-10pm, Sun 4pm-10pm
Vera's Burger Shack*	Burgers & Fries	11am-11pm	11am-11pm
International Food Court *(downstairs)*			
A1 Vietnamese Food	Vietnamese Food	10am-8pm	Sat 10am-8pm
Donair Town	Persian, Mediterranean	11am-8pm	Sat 12pm-7pm
Combo Express	Taiwanese-Style Food	10am-9pm	Sat 10am-9pm
Curry Point*	East Indian Cuisine	11am- 9pm	Sat and Sun 12pm- 7pm
Hong Kong Chinese Food	Chinese Food	10am-10pm	10am-10pm
My Home Cuisine	Chinese Food	10am-10pm	10am-10pm
Osaka Sushi	Sushi	10:30am-9:30pm	11:30am-9pm
Yi Kou Xiang Foods	Northern Chinese Food	10am-10pm	10am-10pm
Student Union Building			
Bernoulli's Bagels	Montreal-Style Bagels	Closed for renovations until Aug- 1	
Blue Chip Cookies	Cookies, Coffee	Until August 1: 7am- 4:00pm	Closed weekends until August 1
		As of Aug- 1: 7am- 9:00pm	As of Aug-1: Sat 8am- 7pm, Sun 9am- 4pm
The Delly*	Sandwiches, Samosas, Baked Goods	7am-6pm	Closed
The Honour Roll	Sushi	10am-6pm	Sat 11am-4pm
The Moon Noodle House	Chinese Take-out	11am-7pm	Closed
The Pit Pub	Pub Style. Licensed.	M/T 12pm-12am, W-F 12pm-2am	Sat 12pm-2am
The Pendulum*	Breakfast, Lunch & Dinner Menus	M-Th 8am-8pm, F 8am-7pm	11am-3pm
Pacific Spirit Place Cafeteria	Grill, Salads, Sandwiches	7:30am-2pm	Closed
A&W *at Pacific Spirit Place*	Burgers, Fries	7:30am-4:00pm	Closed
Starbucks *at Pacific Spirit Place*	Coffee, Snacks	7am-6:45pm	Sat 8am-3pm
Subway *at Pacific Spirit Place*	Sandwiches, Salads	9:00am-6:00pm	Closed
Pie R Squared	Pizza	M/ T 11am-9pm, W-F 11am-11pm	11am-9pm
Snack Attack	Wraps, Hot Dogs, Frozen Yogurt	10:30am-5pm	Closed
Food Outlets Around Campus			
99 Chairs	Pub Style. Licensed.	8am-4pm	Closed
Barn Café	Coffee, Snacks	7:45am- 3:30pm	Closed
Bread Garden Café*	Sandwiches, Snacks	7:45am- 3:30pm	Closed
Café Crêpe *at David Strangway*	Crêpes, Dessert, Coffee	7am-12am	7am-12am
Caffé Perugia	Coffee, Light Dining	7:30am- 4:30pm	Closed
Edibles	Coffee, Soup, Sandwiches	As of Jul-1: 7:45am-2:45pm	Closed
IRC Snack Bar	Soup, Salads, Sandwiches	7:45am-3:00pm	Closed
Koerner's Pub	Drinks, Light Snacks	12pm-1am	Sat 7pm-12am
Pond Café	Coffee, Snacks	7:30am-2:30pm	Closed
Sage Bistro*	Fine Dining. Licensed.	Breakfast 7:15-9am Lunch 11:30am-2pm Dinner 3:30pm-8pm	Closed
Starbucks Coffee *at Fred Kaiser*	Coffee, Snacks	7am-3pm	Closed
Steamies	Coffee, Snacks	9:30am-4:45pm	Closed
Trek Express *Pizza Pizza, Tim Hortons*	Soup, Sandwiches, Pizza	Pizza Pizza 10:30am-2:30pm Tim Hortons 7:30am-3:30pm	Closed

*Staff recommended.

Please note that hours are subject to change without notice. Updated May 2006

AMS Food Outlets & Meal Tickets

at the Student Union Building
UBC, Vancouver

The AMS features a variety of food outlets all under one roof and conveniently located at the heart of campus. Purchase meal tickets for your group to use at any of the nine AMS Food outlets (and the Patio BBQ operating Monday to Friday, weather permitting!). You can set the maximum value and we will reimburse you for any unredeemed tickets that you return.

Please see the reverse side for Meal Ticket Ordering and helpful information.

Blue Chip Cookies

Proudly serving organic, Fair Trade coffees, cappuccinos & lattés.
All our cookies & fabulous baked goods are made in-house and baked fresh every day.

Mon - Fri 7 am - 4 pm
Regular hours resume Aug 1st

Pie R Squared

Great pizza slices, great prices, cold drinks

Mon/Tues 11 am - 9 pm
Wed/Thurs/Fri 11 am - 11 pm
Sat/Sun 11 am - 9 pm

The Pit Pub Burger Bar

Charbroiled hamburger specials, veggie burgers, hot wings, beer battered fish & chips and more
**no trans fats used in our frying!*

Mon - Sat 11 am - 9:30 pm
Sunday CLOSED

The Patio BBQ

On the South Concourse
¼lb burgers, veggie burgers, smokies, drinks

Mon - Fri 11 am - 200 pm
Sat/Sun CLOSED
weather permitting

The Pit Pub

Satellite big screen sports, pool tables, NTN Trivia & Poker tournaments

Mon/Tues 12 pm - 12 am
Wed/Thurs/Fri/Sat 12 pm - 2 am
Sunday CLOSED

Snack Attack

Wonderful spit-roast chicken and Halal beef
Lots of healthy, low-fat items to choose from and ice-cream, slurpees & frozen yogurt

Mon - Fri 10:30 am - 5 pm
Saturday/Sunday CLOSED

The Honour Roll

Maki rolls, nigiri, sushi, Donburi rice bowls, bento boxes are made fresh throughout the day.
Ask about our party platters and catering.

Mon - Fri 10 am - 6 pm
Saturday 11 am - 4 pm

The Pendulum Restaurant

Excellent breakfast, salads, pasta, quesadillas and delicious desserts. Lots of vegetarian and vegan dishes
Outdoor seating on our private patio - Licensed

Mon - Thurs 8 am - 8 pm
Friday 8 am - 7 pm
Sat - Sun 11 am - 3 pm

The Moon Noodle House

Great wonton, daily specials, fresh steamed veggies, combos, hot and sour soup

Mon - Fri 11 am - 7 pm
Sat/Sun CLOSED

Bernoulli's Bagels

Montreal style bagels made fresh daily on the premises
Great sandwiches, soup, Calzones, subs
Freshly squeezed fruit and veggie juices

is CLOSED until August 1st

Need Catering? For catered events or meals on the go, AMS Catering offers a multitude of menu ideas to meet every occasion, and a range of dietary needs. We pride ourselves on our knowledgeable and friendly staff, professional service and quality ingredients.

For more information on meal tickets or catering, please visit **www.amscatering.com** or contact us at:
Phone: 604-822-4617 catering@ams.ubc.ca

The Student Union Building (SUB) is located at 6138 Student Union Boulevard
at the University of British Columbia, Vancouver

Summer Dining 06

For more information visit www.foodserv.ubc.ca

We accept the Meal Plans & Dining Convenience Plan at all UBC Food Services Locations.

Effective May 1 - August 31, 2006

LOCATIONS	HOURS
SAGE at the University Centre	
Breakfast	7:15am - 9:00am (M - F)
Lunch	11:30am - 2:00pm (M - F)
Evening Dining	3:30pm - 8:00pm (Th - F)
Pacific Spirit Place at SUB	7:30am - 2:00pm (M - F)
PIZZA PIZZA, ManchuWok, Koya Japan - Closed	
A&W	7:30am - 4:00pm (M - F)
SUBWAY	9:00am - 6:00pm (M - F)
Cafés & Snack Bars	
BARN on Main Mall	7:45am - 3:30pm (M - F)
BREAD GARDEN at the Forest Science Centre	7:45am - 3:30pm (M - F)
CAFFÉ PERUGIA at Life Sciences Centre	7:30am - 4:30pm (M - F)
EDIBLES (open July 4)	7:45am - 2:45pm (M - F)
IRC Snack Bar at IRC	7:45am - 3:00pm (M - F)
MOA Cafe at The Museum of Anthropology	
99 CHAIRS at David Lam	8:00am - 4:00pm (M-F)
Pub style menu - Licensed	
TREK EXPRESS at David Lam	
PIZZA PIZZA	10:30am - 2:30pm (M-F)
Tim Hortons at Trek	7:30am - 3:30pm (M - F)
Starbucks Coffee	
Fred Kaiser on Main Mall	7:00am - 3:00pm (M - F)
Pacific Spirit Place at SUB	7:00am - 6:45pm (M - F) 8:00am - 3:00pm (Sat)
We Proudly Brew Starbucks Locations	
STEAMIES at Bookstore	9:30am - 4:45pm (M - F)
POND CAFÉ at Ponderosa Ctr	7:30am - 2:30pm (M - F)

RESIDENCE DINING ROOMS - *Conference Dining and Bed & Breakfast*

Totem Park & Vanier's Dining Rooms
Conference Dining Service - Bed & Breakfast, May to August
Contact: 604-822-6828

Hours subject to change. visit www.foodserv.ubc.ca for updates

Catering for Everyday and Special Events Call
UBC Catering at 604-822-2018
www.ubccatering.ubc.ca

PACIFIC SPIRIT PLACE

pizza pizza

KOYA JAPAN

ManchuWOK

SUBWAY eat fresh.

A&W

The Trek EXPRESS Tim Hortons

99 CHAIRS

THE BARN

Edibles

CAFFÈ PERUGIA

REBOOT CAFÉ

BREAD GARDEN BAKERY·CAFÉ

We Proudly Brew STARBUCKS COFFEE

At these Coffee Bars

Steamies at the Bookstore

The Pond Cafe at the Ponderosa

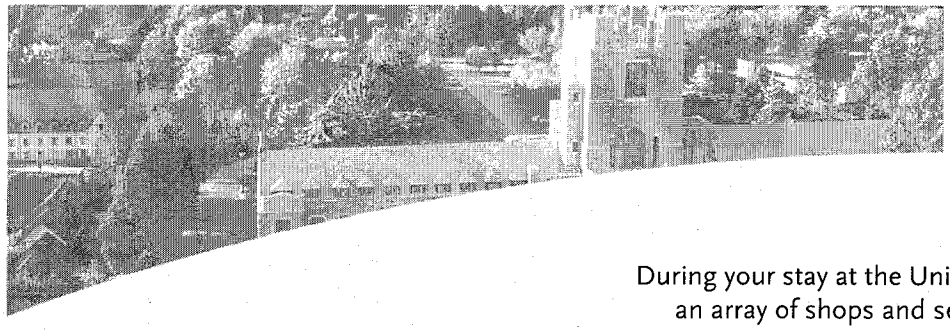
Full Service Starbucks at Pacific Spirit Place & Fred Kaiser

SAGE

at The University Centre

Operated by UBC FOOD SERVICES

Use your reusable mug and container for all your take-outs. Save 15cents per transaction at all participating Food Service Outlets on Campus. Reusable container are available for $2.50 each.



SHOPS AND SERVICES

During your stay at the University of British Columbia, take advantage of an array of shops and services conveniently located right on campus. Whatever your needs, you will find what you are looking for right here.

UBC Bookstore

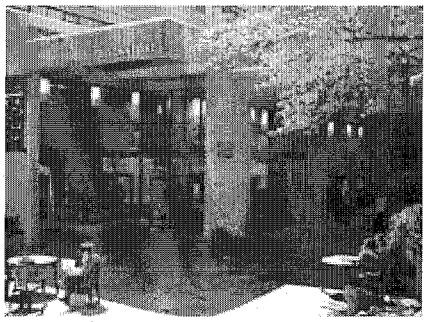
UBC Clothing and Gifts, Computer Shop, General Books, and UBC Textbooks. Ask your Sales Representative about group discounts.

Student Union Building

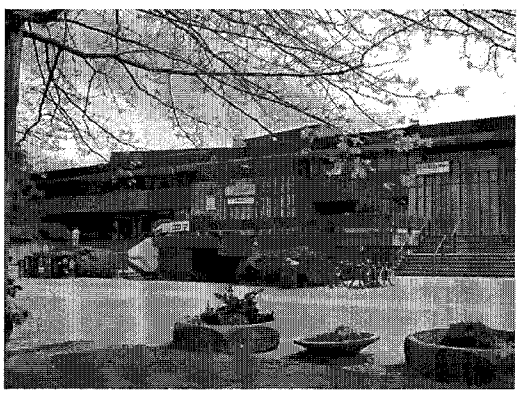
Canada Post.....Full Service Postal Outlet
CopyRight.....Full Service/Self-Serve Photocopying
"The Norm" Cinema.....Movie Screenings
On the Fringe.....Hair Studio
The Outpost.....Stationery, UBC Clothing and Gifts
Perpetual Insurance.....Insurance Services
Sprouts.....Organic Food Co-Op
SUB Arcade.....Gaming Room
SUBcetera.....Bus Tickets, Candy, Lottery
TravelCUTS.....Discount Travel Agency

University Marketplace

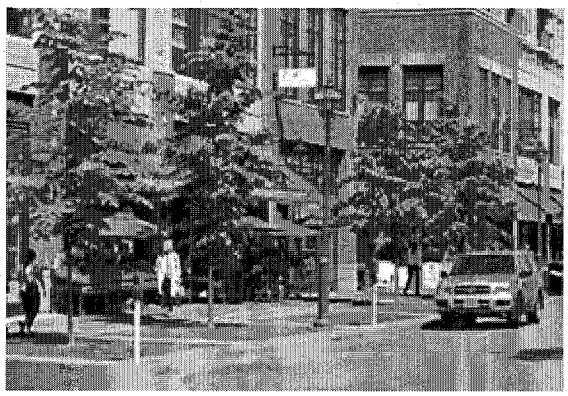
BC Liquor Store.....Beer, Wine, Spirits
Bank of Montreal.....Full Service Banking
CIBC.....Full Service Banking
Copiesmart.....Photocopy and Fax Service
Damask Designs.....Gifts, Housewares
Del Sol Tanning.....Tanning Studio
Discount Textbooks.....Used Textbooks
Dollar 'N' Plus Store.....Household Items
Granville Island Produce.....Fresh Produce, Groceries
Helly Hansen Outlet.....Outdoor Clothing, Sportswear
Hollywood DVD Zone.....Video and DVD rental
House of Vision Optical.....Designer Eyewear, Contacts
Lucky Market.....Groceries
Paloma Hair Design.....Hair Studio
Prime News.....Newsstand, Cigars, Lottery
Rogers/AT&T.....Cell Phone Sales and Plans
Staples Business Depot.....Office Supplies
Thriller.....Active Lifestyle Clothing
University Dry Cleaners.....Dry Cleaning and Alterations
University Grocery.....Groceries
University Pharmacy.....Drugstore
University Village Medical and Dental Clinic.....Full Service



UBC Bookstore
at the corner of University Boulevard and East Mall



Student Union Building (SUB)
at the corner of Student Union Boulevard and East Mall



University Marketplace
at the corner of University Boulevard. and Western Parkway

ATHLETIC FACILITIES

at the University of British Columbia

"One Location. For Every Sport Imaginable."

It doesn't matter whether you're hosting a national sporting event, a conference, a team-building event, a training camp or a retreat. You'll find everything you need at UBC.

War Memorial Gymnasium	War Memorial Gymnasium features 15,000 square feet of flat space, permanent seating for more than 2,300 spectators and retractable bleachers for an additional 600 spectators.
Student Recreation Centre	The Upper Gymnasium has 17,713 square feet of flat space that can be configured for three basketball courts and up to four championship volleyball courts. The lower level houses a full-service fitness and weight room and a traditional martial-arts dojo.
Thunderbird Stadium	Open-air stadium with natural turf surface and a level area of approximately 550 feet long by 350 feet wide in an oval configuration. Covered seating for 3200 spectators and additional grass seating for 1500 spectators. The stadium has television quality lighting and is adjacent to the Whit Matthews field, a full-size practice football field.
Thunderbird Park	Thunderbird Park is comprised of 13 playing fields and can accommodate 24 ultimate fields, 11 rugby fields or 11 soccer fields.
Artificial Surface on Wright Field	This 92 x 55 metre artificial turf field was completed in May 2002. Specifically designed for field hockey using the newest innovations in "Astro-Turf" technology, the field is lit for evening games and has an automatic artificial irrigation system to reduce friction from the field surface.
Aquatic Centre	The Aquatic Centre's open-air swimming pool is 50 feet wide by 165 feet long and features a diving tower for both five and ten metre events. The main pool of the indoor aquatic complex has eight 50-metre lanes, eight 25-metre lanes and six 25-yard lanes. It also includes a five-metre diving platform, as well as one-metre and three-metre diving boards.
Thunderbird Winter Sports Centre	The Thunderbird Winter Sports Centre houses three ice rinks, with the largest measuring 85 by 200 feet and offering seating for 1284 people. The centre also features four squash courts, two handball courts, dressing and ancillary rooms as well as a lounge and snack bar.
Robert Osborne Centre	The Osborne Centre has five large gymnasiums and is located only a short walk from Totem Park Residence.
Coast Club Tennis Centre	Offering a covered four-court tennis complex, the Coast Club Tennis Centre also has 10 additional outdoor courts (6 lit for evening play).

RECREATIONAL ACTIVITIES

at the University of British Columbia

MUSEUM OF ANTHROPOLOGY - 6393 NW Marine Drive 604 822 5087

The Museum of Anthropology is one of North America's premier museums. School programs focusing on the Northwest Coast First Nations are available. All programs encourage discussion, observation and hands-on experience with touchable objects to learn about people and cultures. School programs must be arranged in advance.

SUMMER HOURS: Daily 10:00 am - 5:00 pm
Tuesdays 10:00 am - 9:00 pm *(Free admission Tuesdays 5:00 – 9:00 pm)*

ADMISSION:

Adult:	$9.00	Children (6 and under):	Free
Student:	$7.00	Group Rates: Call (604) 822-4643	
Senior:	$7.00	*(Available for groups of ten or more)*	

BOTANICAL GARDEN - 6804 SW Marine Drive 604 822 9666

Established in 1916, the UBC Botanical Garden has an outstanding collection of temperate plants displayed according to their geographic areas. Exhibits of regional plants include the Native Garden, Alpine Garden, and the Nitobe Memorial Japanese Garden. The Nitobe Garden is located at 1903 Lower Mall.

SUMMER HOURS: Daily 10:00 am - 6:00 pm

ADMISSION:

Botanical Garden		Nitobe Garden	
Adult:	$6.00	Adult:	$4.00
Senior (65+):	$4.00	Senior (65+):	$3.00
Student:	$3.00	Student:	$2.50

Double-Entry Pass: $8.00
Children (6 and under): Free

Group rates: Call (604) 822-4208
(Available for groups of ten or more)

STUDENT RECREATION CENTRE - 6000 Student Union Blvd. 604 822 6000

The SRC is one of Canada's premier University fitness facilities.

SUMMER HOURS: Monday to Thursday 7:00 am –10:00 pm
Fridays 7:00 am – 8:00 pm
Weekends 10:00 am – 7:00 pm

ADMISSION: "BirdCoop" Weight Room: $8.00 drop-in fee.

RENTALS: The smaller upstairs gym is available for booking; items may be borrowed. Outdoor volleyball nets and balls are available to rent. Please call to reserve.

PACIFIC SPIRIT REGIONAL PARK - 4915 West 16th Avenue 604 224 5739

The Pacific Spirit Regional Park encompasses 763 hectares of forest and foreshore surrounding UBC, and boasts 35 kilometres of walking trails. Experience a variety of landscapes, from estuary marshes, rock and cobble beaches, wooded ravines, ancient bog and upland forests. Regional Park Interpreters offer customized group programs on themes ranging between edible plants, birds, and bog ecology. Call for more information.

TENNIS COURTS - 2525 West Mall & 6160 Thunderbird Boulevard 604 822 2505

All guests staying at the University of British Columbia are welcome to use the tennis courts located at Place Vanier and Totem Park Residences. In addition to this, there are ten courts at the UBC Coast Club located at 6160 Thunderbird Blvd. Please call (604) 822-2505 for information on reservations, fees and special packages.

THE PACIFIC MUSEUM OF THE EARTH - 6339 Stores Road — 604 822 6992

The Geology Department maintains a significant collection of rocks, minerals and fossils that are displayed to the public throughout much of the first floor of the building. The museum also features real Lambeosaurus dinosaur fossils.

SUMMER HOURS: Monday to Friday 8:30 am - 4:30 pm (Closed Weekends)

ADMISSION: Free Admission

UBC AQUATIC CENTRE - 6121 University Boulevard — 604 822 4522

The UBC Aquatic Centre features a 50-metre indoor pool, seasonal 55-yard outdoor pool, whirlpool, fitness/weight room, sauna/steam rooms, seasonal patio area and diving boards from one to ten metres.

SUMMER HOURS: Please call for public swim times, lessons, birthday parties and pool rentals.

ADMISSION:

Children (3-12):	$2.55
Youth (13-17):	$3.20
Adult (18-64):	$4.20
Senior (55+):	$2.50

UBC THUNDERBIRD WINTER SPORTS CENTRE – 6066 Thunderbird Boulevard — 604 822 6121

This sports complex offers a variety of athletic facilities including four hockey rinks, four squash courts and two racquetball courts. After a day of exercise, enjoy a relaxing evening in the licensed lounge and restaurant.

SUMMER HOURS:	7 Days a week	Mon- Fri 8:30 am, Sat 9:00 am, Sun 9:30 am- close; closing times vary.
ADMISSION:	Public:	$10.00 / 45 minutes of court time
	Student:	$7.00 / 45 minutes of court time

THE NORM THEATRE– Main floor of the Student Union Building — Office 604 822-3698, Movie Hotline 604 822 3697

The Norm shows second-run movies for a great price!

2 Shows Nightly at 7 & 9pm (subject to change)
ADMISSION: $3.00

MAIN LIBRARY – 1956 Main Mall — 604 822 6375

KOERNER LIBRARY – 1958 Main Mall — 604 822 2406

SUMMER HOURS:	Main Library	Monday/Thursday/Friday	9:00 am – 5:00 pm
		Tuesday/Wednesday	9:00 am – 9:00 pm
		Saturday	10:00 am – 5:00 pm
	Koerner Library	Monday to Thursday	9:00 am – 10:00 pm
		Friday	9:00 am – 5:00 pm
		Saturday	10:00 am – 5:00 pm

KOERNER'S PUB - 6371 Crescent Road — 604 822 3203

Koerner's is a friendly, relaxing campus bar with a large patio and daily barbeque. Everyone is welcome. Operated by the Graduate Student Society.

SUMMER HOURS:	Monday to Friday	12:00 pm – 1:00 am
	Saturday	4:00 pm – 1:00 am
	BBQ:	5:00 pm – 7:00 pm (Wednesday – Friday)

PLEASE NOTE: RATES AND SCHEDULES ARE SUBJECT TO CHANGE.

The University of British Columbia, Vancouver, BC, Canada

6th Canadian Computational Chemistry Conference

July 26 – 30, 2006