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Parallel Quantum Solutions

Current Trends in Computational Chemistry 2002

*Jackson, Mississippi
November 1-2, 2002*



CONFERENCE AGENDA

Current Trends in Computational Chemistry 2002

Jackson, Mississippi

November 1-2, 2002

FRIDAY, NOVEMBER 1

7:30 – 9:00	Continental Breakfast	
8:00 – 12:00	Registration	
9:00 – 9:30	Opening Ceremony	Dr. Ronald Mason <i>Jackson State University, President</i>
		Dr. Jeffery Holland <i>US Army ERDC, Laboratory Director</i>
		Dr. William McHenry <i>Institutions for Higher Learning, Asst. Commissioner for Academic Affairs</i>
		Dr. Robert W. Whalin <i>U.S. Army Research Lab, Director</i>
9:30 – 10:30	1 st Session (S1)	Buckingham lecture
10:30 – 11:00	Coffee Break	
11:00 – 12:30	2 nd Session (S2)	2 Talks
12:30 – 12:40	Group photo	
12:40 – 2:00	Lunch	
2:00 – 3:30	3 rd Session (S3)	2 Talks
3:30 – 4:00	Coffee Break	
4:00 – 5:30	4 th Session (S4)	2 Talks
6:00 – 8:00	First Poster Session (P1)	
8:00 – 9:30	Dinner	
	After-dinner Noble Lecture Series	<i>Speaker: Magdolna Hargittai</i> Eötvös University

SATURDAY, NOVEMBER 2

8:00 – 9:00	Continental Breakfast	
8:30 – 11:00	Registration	
9:00 – 10:30	5 th Session (S5)	2 Talks
10:30 – 11:00	Coffee Break	
11:00 – 1:00	Second Poster Session (P2)	
1:00 – 2:30	Lunch	
2:30 – 4:00	6 th Session (S6)	2 Talks
4:00 – 4:30	Coffee Break	
4:30 – 6:30	Third Poster Session (P3)	
7:00 – 8:00	Cocktails	
8:00 – 11:00	Banquet	<i>Speaker: Dr. Roosevelt Johnson</i>
	Best Student Poster Award Presentation	<i>National Science Foundation</i>

BUCKINGHAM LECTURESession Chairman: **Peter Politzer**, *University of New Orleans***David Buckingham**
University of Cambridge

Polarizability and Hyperpolarizability

2ND SESSIONSession Chairman: **Andrzej Wierzbicki**, *University of South Alabama***David A. Case**
The Scripps Research Institute

Macromolecular Simulations Using Continuum Solvent Models

Andreas Klamt
COSMOlogic

COSMOtherm: The Bridge between Quantum Chemistry and Fluid Phase Thermodynamics

3RD SESSIONSession Chairman: **Jan Labanowski**, *Ohio Supercomputer Center***Roberto Car**
*Princeton Materials Institute
Princeton University*

First-principles Molecular Dynamics: Current Achievements and Perspectives

Yuko Okamoto
Institute for Molecular Science

Free Energy Calculations in Protein Folding by Generalized-Ensemble Simulations

4TH SESSIONSession Chairman: **Eric Fisher**, *University of Illinois at Springfield***Jean-Marie André**
University of Namur

Does Deterministic Chaos Play a Role in Chemistry?

Piotr Piecuch
Michigan State University

Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods

5TH SESSIONSession Chairman: **Jerome Karle**, *Naval Research Laboratory***Peter J. Rossky**
University of Texas

The Coupling of Environmental and Electronic Dynamics in Excited State Relaxation

**Srinivasan Iyengar /
Gregory A. Voth**
*University of Utah*Atom-centered Density Matrix Propagation (ADMP): A New Approach to *ab initio* Molecular Dynamics**6TH SESSION**Session Chairman: **Jiande Gu**, *Chinese Academy of Sciences***Kwang Soo Kim**
*Center for Superfunctional
Materials*

De novo Design of Functional Nano-materials and Molecular Devices

Margaret Hurley
US Army Research Laboratory

Organophosphorus Compounds, Cyanides, and Other Chemicals to Avoid

P1	M. Mohamed Naseer Ali and P.Kaliannan Enzyme Targetted Herbicide Design: A Molecular Modelling Studies	13
P1	R.N. Allen, M.K. Shukla and Jerzy Leszczynski A Theoretical Study of Structure and Properties of Uric Acid: A Potent Antioxidant	14
P1	Nada Amer, Eddie Reaves, Tracy P. Hamilton, and Morgan S. Ponder Substituent Effects on the Cyclopentadienyl Cation	15
S4	Jean-Marie André Does Deterministic Chaos Play a Role in Chemistry?	16
P1	Peter Babinec and Jerzy Leszczynski Visual Recurrence Analysis of Nonlinear Vibrational Dynamics in H_3^+ Molecule	17
P1	Víctor Bazterra, Marta B. Ferraro and Julio C. Facelli Modified Genetic Algorithm to Model Crystal Structures Allowing Molecular Geometry Relaxation	20
P1	Víctor Bazterra, Ofelia Oña, Marta B. Ferraro and María C. Caputo Modeling of Atomic Clusters Structures by Means of the Genetic Algorithm Using Semiempirical Methods	23
P1	Jean-Philippe Blaudeau, Douglas Dudis, Alan Todd Yeates, and Thomas M. Cooper Theoretical Studies of Air Force Material Projects	26
P1	Jessica Blundell, Chuanyun Xiao, Frank Hagelberg and William A.Lester, Jr Comparative Study of Small Silicon Clusters with Cu, Sc and Y Dopants	27
P1	Judge Brown, Diwakar Pawar, and Eric A. Noe Conformational Studies of cis - and trans - Cycloundecenes by Dynamic NMR Spectroscopy and Computational Methods	28
S1	A. D. Buckingham Polarizability and Hyperpolarizability	29
P1	Jaroslav V. Burda Some Aspects of cis/transplatin Coordination to the DNA Bases and a Comparison of the Pt and Pd Complexes: Quantum Chemical Computational Studies	30
P1	Edward F. C. Byrd and Cary F. Chabalowski Pseudopotential DFT Plane-wave Calculations on Unit Cell Structures for Energetic Organic Compounds	31
P1	R. Cammi, B. Mennucci, C.Cappelli, G.W. Trucks, M.J. Frish, J. Tomasi Analytical Second Derivatives of the MP2 Energy for Molecules in Solution: A Formulation within the Polarizable Continuum Model.	32
P1	Dalephine Cain, Diwakar Pawar, and Eric A. Noe Conformational Studies of trans - Cycloheptene, trans - Cycloheptene Oxide and trans - Bicyclo [5.1.0] Octane	33
P1	Dalephine Cain, Diwakar Pawar, and Eric A. Noe Conformational Studies of Cyano Formate (HCO_2CN) and Related Compounds	34
S3	Roberto Car First-principles Molecular Dynamics: Current Achievements and Perspectives	35
P1	Louis Carlacci, Mark Olson and Charles B. Millard Conformational Analysis of the Acyl Pocket Loop in Acetylcholinesterase Computed by Monte Carlo Methods with a Generalized Born Model of Solvation	36
S2	David A. Case Macromolecular Simulations Using Continuum Solvent Models	37

P1	David C. Chatfield, Alberto Augsten, and Stanislaw F. Wnuk Regioselectivity of Nucleophilic Addition to α,β Unsaturated Carbonyl Compounds with a π -Deficient Aromatic Substituent Attached to the β -Carbon	38
P1	Anthony Chuma, Dong Hee Kim and Peter Pulay Conformational Preferences of Small Polypeptides from Calculated and Experimental NMR Chemical Shifts	39
P1	David M. Close Oxidative Damage to Cytosine: Implication for Radiation Induced Damage in DNA	40
P1	Jiří Czernek On the Intermolecular ^{15}N NMR Chemical Shielding Surface for Nucleic Acids	41
P1	Y. Daoudi, P.J. Bonifassi Time Dependent Hartree Fock hyperpolarizabilities Calculations on Conjugated Chiral Nonlinear Optical Molecules. Correlation with Measurements by Hyper-Rayleigh Scattering(HRS)	42
P1	H. Dodziuk, G. Dolgonos Hydrogen Storage in Bundles of (5,5) Carbon Nanotubes	44
P1	Piotr M. Drożdżewski, Ewa Kordon, Szczepan Roszak The Studies of Metal Isotope and Deuteration Effects in Vibrational Spectra of Palladium(II) Complex with Histamine	46
P1	Jesse Edwards, Genzo Tanaka, April Anderson, Claudia Eybl, Henry Joung Lee, Zhengqing You Solvation Studies on Steroid-Nucleoside Conjugates	47
P1	Jesse Edwards, Claudia Eybl, Genzo Tanaka, and Betsy M. Rice Relationships between Impact Sensitivity and Molecular Properties in Nitramine Molecules	48
P1	Jesse Edwards, and Betsy M. Rice Bond Dissociation Energies for NO_2 in Some Nitroheterocyclic Explosives	49
P1	Jesse Edwards, Genzo Tanaka, Jason Ford-Green Conformational Analysis of Various Organophosphate Acetylcholinesterase Inhibitors to Provide Structure Activity Relationships	50
P1	Jesse Edwards, Genzo Tanaka, Dalelia Q. Davis Reactivities of Nerve Agents in the Gorge of Acetylcholinesterase	51
P1	Jesse Edwards, Genzo Tanaka, Makini Cobourne Bonding and Bond Energies of Various Nerve Agents Bound to Acetylcholinesterase	52
P1	Tarek M. El-Gogary and Koehler Gottfried Interaction of Psoralens with DNA-Bases. An ab initio DFT Study	53
P1	Lisa C. Fedoroff, Brian W. Hopkins, and Gregory S. Tschumper Ab initio Study of the Conformational Preferences of Tyrosine	54
P1	L. Feria and M. Castro Theoretical Study of the $\text{CH}_3\text{CH}_2\text{O}_2$ Self-Reaction	55
P1	Eric W. Fisher, Hei-Chi Chan, and Mark A. Lovik A Random-Move and Geometric-Optimization Procedure for Building Water Molecules into Protein Clefts for Molecular Structure Calculations	56
P1	Gareth Forde, Latasha Salter, Glake Hill, Leonid Gorb, and Jerzy Leszczynski Theoretical ab initio Study of the Effects of Methylation of Guanine (G), Cytosine (C) on GC Base Pair	57

P1	Gareth Forde, Pawel Kedzierski, Andrzej Sokalski, Robert Gora, Jolanta Grembecka, Glake Hill, and Jerzy Leszczynski Ab initio Study of the Physical Nature of Interactions between Neutral and Protonated Cytosine Transition States Structures and Enzyme Inhibitors with Cytosine-5-methyltransferase Active Site Constituents	58
P1	Angela Fortner, Gareth Forde, Aviane Flood, Alejandro Nazario, Adrian Ford, Glake Hill, and Jerzy Leszczynski Theoretical ab initio Study of Tautomeric Properties in Methylated Nucleic Acid Bases	59
P1	Aviane Flood, Gareth Forde, Glake Hill, Leonid Gorb and Jerzy Leszczynski Theoretical ab initio Study of the Effects of Methylation on the Nature of Hydrogen Bonding in AT Base Pair	60
P1	Ken Flurchick and Jan Labanowski Computational Portals for Chemistry	61
P2	H. A. Grebneva Some Problems to be Solved Under Subsequent Study of the Nature and Mechanisms for the Formation of Potential Mutations	63
P2	Jiande Gu and Jerzy Leszczynski Importance of the Bifurcated H-Bonding in the Formation of Iso-Guanine Tetrads	67
P2	Steven R. Gwaltney, Sergiy V. Rosokha, Martin Head-Gordon, and Jay K. Kochi Electron-Transfer in Nitration and Nitrosation	69
P2	F. Hagelberg, J. Fedor, S. Matt-Leubner, P. Scheier, T.D. Märk The Decay of Metastable Ne_2^+ : Experiment and Theory	70
NL	Magdolna Hargittai Conversations with Prominent Women Scientists	71
P2	Robert H. Higgins An ab initio Investigation of Alkylations of Cytosine	72
P2	Glake Hill, Nicholas Hill, Gareth Forde, Szczepan Roszak, and Jerzy Leszczynski Greater Insight into the Stacking Properties of Nucleic Acids	74
P2	Drahomir Hnyk and Bohumil Stibr "Free" Boranes and Heteroboranes in the Czech Republic	75
P2	Brian W. Hopkins and Gregory S. Tschumper Extending the ONIOM Integrated MO/MO Approach to Hydrogen Bonding in Biological Systems: The Serine-Water and Threonine-Water Dimers	76
P2	Ming-Ju Huang Ab initio Studies of Tamoxifen and Related Compounds	77
S6	Margaret M. Hurley, Jeffrey B. Wright, Alex Balboa, Gerald H. Lushington Organophosphorus Compounds, Cyanides, and Other Chemicals to Avoid	78
P2	Sheena M. Inge and Suely M. Black Modeling of 2-Methyl-4-Nitroaniline (MNA) Adsorption on the Si (100) Surface	79
P2	I.S. Irgibaeva Multidimension Vibration Hamiltonian of Methylamine	80
P2	Olexandr K. Isayev, Leonid Gorb, Igor Zilberberg and Jerzy Leszczynski One-Electron Reduction of Nitrobenzene by Iron (II) Compounds. A DFT Investigation	83
S5	Srinivasan Iyengar and Gregory A. Voth Atom-centered Density Matrix Propagation (ADMP): A New Approach to ab initio Molecular Dynamics	84
P2	Ping Jin, Jane S. Murray, and Peter Politzer Average Local Ionization Energy as a Measure of Local Polarizability	85

P2	Anna Kaczmarek, Leonid Gorb and Jerzy Leszczynski Structures and Properties of Sarin and Soman	86
P2	Anna Kaczmarek, Leonid Gorb, and Jerzy Leszczynski Post-Hartree-Fock Study of Guanine and Methylguanine	87
P2	Marc L. Kasner, Christine Bray, Mayuko Yokota, Fillmore Freeman, Warren J. Hehre A Computational Study of the Energy of Propylcyclohexane as a Function of the Exocyclic Torsional Angles	88
S6	Kwang S. Kim De novo Design of Functional Nano-materials and Molecular Devices	89
S2	Andreas Klamt, Frank Eckert COSMOtherm: The Bridge Between Quantum Chemistry and Fluid Phase Thermodynamics	91
P2	Kukueva V.V. Theoretical Investigation of Molecule's Destruction Way on the Silica Surface	92
P2	G.M. Kuramshina, Yu.A. Pentin, S.V. Syn'ko Vibrational Spectra and Molecular Force Fields of Ethane-Like Halogensubstituted Silanes	93
P2	C. H. Langley, J.-H. Liu, K. Chen and N. L. Allinger Studies of Carbonyl Compounds Using the MM4 Molecular Mechanics Force Field	95
P2	Yuguang Ma and Peter Politzer Calculation of Intermolecular Interaction Energies	96
P2	Krzysztof Maruszewski, Marek Rybaczuk, Marcin Grzegorzczak Ballistic Aggregation: An Alternative Approach to Modeling of Silica Sol-Gel Structures	97
P2	James L. Meeks Geometry of Bis(Pinacolato)Diboron and Related Molecules	98
P2	A. Michalkova, M. Ilchenko, L. Gorb, J. Leszczynski Adsorption of Sarin and Soman on the Surface of Clay Minerals – ab initio ONIOM Study	99
P2	Andrea Michalková, Daniel Tunega, Ladislav Turi Nagy Theoretical Study of Interactions of Dickite and Kaolinite with Small Organic Molecules	101
P2	S.E Nefediev, V.F Sopin, M.B. Zuev Quantum-chemical Study of the Basis Set Convergence for the Hyperpolarizabilities Calculations	103
P2	Alexander V. Mitin, Jon Baker, and Peter Pulay An Improved 6-31G* Basis Set for First-row Transition Metals	104
P2	Hans-Christian Müller, Axel Schulz, and Magdolna Hargittai Structure and Bonding in Silver Halides. A Quantum Chemical Study of Silver Mono- and Trihalides	105
S3	Yuko Okamoto Free Energy Calculations in Protein Folding by Generalized-Ensemble Simulations	106
P2	Okovyty S.I., Seferova M.F., L.K.Umrikhina, Kasjan L.I. Quantum-Chemical and NMR Spectral Investigation of the Epoxidic Derivatives of Tetrahydroindene Stereochemistry	107
P2	Okovytyy S.I., Kasyan L.I., Zvyagintseva T.V. Quantum-chemical Study of Amidoacids of Norbornene Row Lactonisation	108
P2	S.I. Okovytyy, L.I. Kasyan, V.A. Bakumov, J. Leszczynski Formation of Azabrendane Systems on the Basis of Substituted Endo-5-aminomethyl-exo-2,3-epoxybicyclo[2.2.1]heptanes	109

- P2 **Vladimir Rossikhin, Sergiy Okovytyy and Jerzy Leszczynski** In Relation to Efficiency of Magnetically Consistent Basis Sets for Nuclear Shieldings Calculations. HF, DFT and MP2 GIAO Comparative Studies 110
- P2 **Daniel A. Osborne and Abby L. Parrill** Docking Studies to Examine Immunosuppressive Phospholipid Binding Selectivity 113
- P2 **R.B. Pandey and Ray Seyfarth** Tracer Polymer Chain: Interface To Bulk 115
- S4 **Piotr Piecuch, Karol Kowalski, Ian S.O. Pimienta, Michael J. McGuire, Peng-Dong Fan** Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods 116
- P2 **Yevgeniy Podolyan, Leonid Gorb, Jerzy Leszczynski** Double Proton Transfer in the DNA Base Pairs. Post-Hartree-Fock Gas-Phase and Aqueous Solution Study 117
- P2 **Lawrence M. Pratt** Solvent Effects on Mixed Aggregate Formation between Lithium Dialkylamides and Alkylolithiums 118
- P2 **Mo Qasim, Dr. Herb Frederickson, Chris McGrath, Rakesh Bajpai** Modes of Degradation of Cyclic Nitramines: An Approximation Methods Comparison of the Relationships Between the Structures and Reactivities of CL-20, ONC, TNTAC, and RDX 121
- P2 **B. Ramachandran, Kirk A. Peterson, Tiao Xie and Joel M. Bowman** Potential Energy Surfaces for the $^3A''$ and $^3A'$ Electronic States of the $O(^3P) + HCl$ System and Calculations of Thermal Rate Constants 123
- P2 **Bakhtiyor F. Rasulev, Nasrulla D. Abdullaev, Kamila A. Eshbakova** The Conformational Analysis and Study by NMR of Sesquiterpene Lactone Gaillardine 124
- P3 **Pornpun Rattananakin, Svein Saebø, Willard Collier and Charles U. Pittman, Jr.** Push-Pull Electron Systems: An ab initio Study 128
- P3 **Ashley L. Ringer, Patricia L. Honea, and David H. Magers** Conventional Strain Energy in the Diazetidines and the Diphosphetanes 129
- P3 **Teri Robinson, Leonid Gorb, Valeri Poltev and Jerzy Leszczynski** Development of New Force Filed Taking into Account the Nonrigidity of Amino Group in DNA bases. Preliminary Data 130
- P3 **Teri Robinson, Glake Hill, Gareth Forde, Andrej Sokalski, and Jerzy Leszczynski** Calculation of Weak Interactions of Aromatic and Nucleic Acid Systems Using MP2 and Local MP2 Methods 131
- S5 **Peter J. Rossky** The Coupling of Environmental and Electronic Dynamics in Excited State Relaxation 132
- P3 **F. Ruetter, M. Sánchez, G. Martorell, C. González, R. Añez, A. Sierraalta, L. Rincón, and C. Mendoza.** A Parametric Quantum Method for Catalytic Reactions (CATIVIC) 133
- P3 **F. Ruetter, M. Sánchez, C. Mendoza, A. Sierraalta, G. Martorell, and C. González.** Calculation of One-Center Integrals in Parametric Methods Using Simulated Annealing and Simplex Methods 134

- P3 **Amar Saal and Ourida Ouamerli** Vibrational and Electronic Contributions to the Polarizability and First Hyperpolarizability of Mono-Substituted Acetylene: A Theoretical study. 135
- P3 **Julia Saloni-Szymczak, Szczepan Roszak, and Jerzy Leszczynski** Theoretical Studies on Structure and Thermodynamics of Dinuclear Tin Halide Clusters 136
- P3 **E. A. Salter and A. Wierzbicki** Quantum Mechanical Study of the syn and anti Conformations of Solvated Cyclic GMP 137
- P3 **Yinghong Sheng, Szczepan Roszak, and Jerzy Leszczynski** The Molecular Structures and Nature of Interactions in $N_2H^+-Ne_n$ ($n = 1 - 12$) Complexes 138
- P3 **Yinghong Sheng, Ramaiyer Venkatraman, Józef S. Kwiatkowski, Joanna Majewska and Jerzy Leszczynski** Theoretical Study on the Molecular Structures and Vibrational Spectra of Halogenosubstituted Phosphoryl and Their Thio-analogs 139
- P3 **Yinghong Sheng and Jerzy Leszczynski** A Comprehensive Theoretical Study on the Reaction Mechanisms of the Inversion Reaction between Spiropyrans and Merocyanines and the Racemization of Spiropyrans 140
- P3 **M.K. Shukla and Jerzy Leszczynski** Excited States of Nucleic Acid Bases: A Theoretical Study 141
- P3 **M.K. Shukla and Jerzy Leszczynski** Excited States of Hypoxanthine: An MCSCF and CIS Investigations 144
- P3 **Aníbal Sierraalta, Orlando Lisboa** Theoretical Study of the H_2 Interaction with CoMoS, NiMoS and MoS_2 Catalyst 147
- P3 **Vitali Solkan and Jerzy Leszczynski** Density Functional Studies of Dihydrogen and Methane Dissociative Adsorptions in High Silica Zn(2+) ZSM-5 Zeolite 148
- P3 **Vitali Solkan and Jerzy Leszczynski** Theoretical Study of Dihydrogen Adsorption on Co(II) and Zn(II) Exchanged ZSM-5 zeolites 149
- P3 **Vitali Solkan and Jerzy Leszczynski** MP2 and DFT Studies of Hydrogen Bonded Complexes of Several Superacids Taking into Account Solvation Effects 153
- P3 **Jiří Šponer, Judit E. Šponer, Ali Mokdad, Nada Spackova, Neocles B. Leontis, Jerzy Leszczynski** Unique Molecular Interactions and Conservation Patterns of Cis Watson-Crick G.A Base Pairs in RNA and DNA 154
- P3 **Judit E. Šponer, Frank Glahé, Jerzy Leszczynski, Bernhard Lippert, and Jiří Šponer** Quantum Chemical Description of the Nucleobase Rotation in $trans-[Pt(NH_3)_2(Cyt-N3)_2]^{2+}$ 156
- P3 **Arvydas Tamulis, Jelena Tamuliene, Vykintas Tamulis** Quantum-Mechanically Designed Hardware of Molecular Electronics Digital and NMR Quantum Computers 157
- P3 **Arvydas Tamulis, Jelena Tamuliene, Zilvinas Rinkevicius, Vykintas Tamulis** Quantum Mechanical Design of Single Supermolecule Photoactive Machines and Molecular Classical and Quantum Logic Devices 159
- P3 **Christina Turner, Hongbin Yuan and Abby L. Parrill** Docking Studies of Eleven Structural Types of HIV Integrase Inhibitors Demonstrate Two Non-Overlapping Binding Sites 162

- P3 **J. Urban, P. Mach, M. Probst, and J. Leszczynski** Theoretical Study of Ionized Argon Clusters 163
- P3 **V.F.Vargaljuk, L.V.Borshchevich, J.A. Holod** Quantum-chemical Investigation of the Influence of Electrolyte's Ionic Composition on the Reaction of Oxidation of Water Molecules 164
- P3 **Ramaiyer Venkatraman, M.K. Shukla and Jerzy Leszczynski** Tautomeric Equilibria and Electrostatic Potentials of Xanthopterin: A Theoretical Study 167
- P3 **Jing Wang, Jiande Gu, Jerzy Leszczynski** The Stability of the Sarin-Serine Complex: A DFT-based Molecular Dynamics Investigation 168
- P3 **Nanping Wang, Jiande Gu** Theoretical Study for the Association Constants for β -cyclodextrin with the Phenol Derivatives 171
- P3 **C.A. Weatherford, A. Wynn III, E. Red, and C. Mathis** Diagonalization of the Two-Electron Coulomb Operator, Geminals, and Helium 173
- P3 **Mary La'Françes Williams, and Suely M. Black** Comparative Study of the First Hyperpolarizabilities of Urea Clusters 174
- P3 **Adrian Wilson, Glake Hill, Gareth Forde, Leonid Gorb, and Jerzy Leszczynski** The Effects of cis-Pt(LH₃)₂Cl₂ (L = N, P, As) on the Structure of Nucleic Acid Bases 175
- P3 **Ilya Yanov and Jerzy Leszczynski** Quantum Transport in Nanostructures 176
- P3 **Yasunori Yoshioka, Hiroko Kawai, and Tomoko Sato** G-Selectivity of GGG Triplet toward One-Electron Oxidation Mediated by Cu(I). Ab initio Molecular Orbital Study 177
- P3 **R. Zaleśny, W. Bartkowiak, J. Leszczynski** Theoretical Study of the Two-Photon Absorption in Photochromic Indolylfulgides for Optical Memory Storage 180
- P3 **Michal Zeizinger, Jaroslav Burda, Jerzy Leszczynski** Ab initio Study of Cisplatin's Analogs 181
- P3 **Nurbosyn U. Zhanpeisov, Ayako Kawase, Masakazu Anpo** Adsorption of Products of Photooxidation of Methane on Silicalite Structures with and without Ti-impurities. Ab initio and DFT Study 182
- P3 **Nurbosyn U. Zhanpeisov, Kazuhiko Mizuno, Masakazu Anpo and Jerzy Leszczynski** C₁-C₂ Bond Cleavage in Vinylidenecyclopropanes: A Theoretical Density Functional Theory Study 183
- P3 **Nurbosyn U. Zhanpeisov, Yukiya Kanazawa, Hiromi Yamashita, Masakazu Anpo** Intrinsic Band Gap Shift in Ti-silicalites Modified by V Ion-Implantation: An ab initio and Density Functional Theory Study 184