

<i>Session[†]</i>	<i>Presentation</i>	<i>Page</i>
P1	Exploring the Nature of the Solubility Properties of Soluble and Insoluble Fractions of Asphaltenes Using Molecular Dynamic Simulations <i>Yosslen Aray, Jesus Rodriguez, Jesus E. Montenegro, Raiza Hernandez and D. Vega</i>	21
P1	Nature of Small Nickel Sulfide Particles Supported on Acid-Mordenite: an Atom in Molecules Theory and Electrostatic Potential Studies <i>Yosslen Aray, David Vega, Jesus Rodriguez and Santiago Coll</i>	24
P1	Nature of the NiMoS Catalyst Edge Sites: an Atom in Molecules Theory and Electrostatic Potential Studies <i>Yosslen Aray, Jesús Rodríguez, Alba Beatriz Vidal and Santiago Coll</i>	28
P1	The Efficiency of the Conversion of Translational Energy into Internal Energy of the Molecules at Inelastic Collisions in the System CsCl + RbJ <i>V.M. Azriel, L.Yu. Rusin</i>	31
P1	TDDFT Investigation of the Absorption Spectra of a Cyanine Dye <i>A. Bamgbelu, J. Wang, I. Shukla, L. Sitole, T. Wheat, J. Gu, and J. Leszczynski</i>	32
S1	Coupled-Cluster Theory in Quantum Chemistry: the Emergence of a New Paradigm <i>Rodney J. Bartlett</i>	33
P1	The New CEP-31G ^{##} Basis Set: DFT Calculations of Static Polarizability and Magnetic Susceptibility <i>Vladimir I. Bolshakov, Vladimir V. Rossikhin, Eugene O. Voronkov, Sergiy I. Okovytyy, Jerzy Leszczynski</i>	34
P1	Static Hyperpolarizability of Dimer, Trimer and Tetramers Porphyrins with Different Substituents between the Porphyrin Rings. Dynamic Hyperpolarizability(CPHF) for the Dimer Porphyrins Containing the Same Substituents <i>P.Bonifassi, Paresh.C.Ray and J.Leszczynski</i>	36
P1	Static and Dynamic Hyperpolarizability Calculation in Vacuum and in CHCL ₃ of the Four Tetranitro Tetrapropoxy Calix[4] Arene Conformers. Static Hyperpolarizability in Vacuum of Some Donors and Acceptors for the Conic Conformer <i>P.Bonifassi, Paresh.C.Ray and J.Leszczynski</i>	39
P1	Static and Dynamic Hyperpolarizability Calculation in Vacuum of the Four p-Nitrophenylazo Calix[4] Arenes <i>P.Bonifassi, Paresh.C.Ray and J.Leszczynski</i>	42
P1	Theoretical Studies of Adsorption Mode of 2-cylohexenone on Surface Rh(111) <i>A. Bouferguene, R. Ghomari, R. Bachir, M. Mekelleche, A. Choukchou-Braham</i>	45
P1	Theoretical Study of Ethylene Polymerization for Ziegler-Natta Catalyst <i>A. Bouferguene, A. Rebabti, M. Bensitel</i>	46
P1	A Computational Study of the Vibrational Spectrum of Crystalline RDX <i>Sylke G Boyd, Kevin J. Boyd</i>	47
P1	Bond Length and Bond Distortion of Ferroelectric BaTiO ₃ <i>Shemekia Braddock, Brent Melot, Katharine Page, Ram Seshadri, and Glake Hill</i>	48

P1	Theoretical DFT Study of Solvent Effects on Platinum Complexes Interactions with Cysteine and Methionine <i>Jaroslav V. Burda, T. Zimmermann, and Jerzy Leszczynski</i>	49
S6	Structure and Properties of Molecular Solutes in Electronic Excited States <i>Roberto Cammi</i>	50
P1	Towards the Elaboration of a QM Method to Describe Molecular Solutes under the Effect of a Very High Pressure <i>Roberto Cammi, Vincenzo Verdolino, Benedetta Mennucci, Jacopo Tomasi</i>	51
P1	The Validation of a Novel Secretary Domain of HIV-1 Nef using Cohort Sequence Analysis and Computational Chemical Analysis <i>P. Campbell, S. Ali, M.-B. Huang, M. Khan, T. Campbell, M. Powell, V. Bond</i>	52
P1	Relative Aromaticity in Pentacene Derivatives <i>Bei Cao and David H. Magers</i>	53
P1	Theoretical Investigation of Ligand Interaction in Ni-Organometallic Compounds <i>M. A. Cato, H. P. Hratchian, J. Sonnenberg, H. B. Schlegel, J. Montgomery</i>	54
P1	Theoretical and Experimental Study of the Osmium (IV) Derivatives of 2,6-Dimercapto-3-Methyl-4H-Thiopyran-4-One <i>Chmilenko F.A., Hudjakova S.N., Chmilenko T.S., Olefir D.A.</i>	55
P1	The Influence of Microhydration on the Ionization Energy of Thymine: Comparisons of Theoretical Calculations with Experimental Values <i>David M. Close, Carlos E. Crespo-Hernández, Leonid Gorb, and Jerzy Leszczynski</i>	56
P1	Can DFT Dissolve CO ₂ in Water? <i>Jessica Cross, Mauricio Cafiero</i>	58
P1	Novel Density Functional Theory Methods for Describing Dispersion Interactions <i>Lori Marie Culberson, Mauricio Cafiero</i>	59
NL	A Brief History of Carbon <i>Robert Curl</i>	60
P2	Homology Modeling of CYP2B6 and Insights into Mechanism-Based Inactivation of Phenyl Diaziridines <i>Pankaj R. Daga, John M. Rimoldi, Robert J. Doerksen</i>	61
P1	Gold-Nanoparticle-Based Probe for the Simultaneous Detection of E-Coli and Anthrax <i>Gopala Krishna Darbha, Anandhi Ray, William Hardy, Joshua Walker, Paresh Chandra Ray</i>	63
P1	¹⁹ F- ¹⁹ F and ¹⁹ F- ¹ H Spin-Spin Coupling Constants in Cyclic FH Polymers (FH) _n , n = 2-6 <i>Janet E. Del Bene</i>	65
P1	Continued Development of the Correlation Consistent Composite Approach (ccCA) <i>Nathan J. DeYonker, Thomas R. Cundari, Angela K. Wilson</i>	66
P1	Theoretical Investigation of C-C Bond Cleavage in (3,3) Armchair Single-Walled Carbon Nanotubes by Chemisorption of Hydrogen Atoms <i>T. C. Dinadayalane, Anna Kaczmarek, Jerzy Łukaszewicz, and Jerzy Leszczynski</i>	67
P1	Theoretical Calculation of Electronic Circular Dichroism of the Rotationally Restricted 3,8''-Biflavonoids <i>Yuanqing Ding, Xing-Cong Li, and Daneel Ferreira</i>	69

P1	Ab Initio Electron Propagator Studies of Porphyrins <i>O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz</i>	70
P1	Preliminary Molecular Dynamic Simulations of the Estrogen Receptor from Antagonist to Agonist <i>Jesse Edwards, T. Dwight McGee, Adrian E. Roitberg</i>	71
P1	Prediction of Electronic Excited States for Homonuclear Diatoms using Quantum Monte Carlo Theory <i>Floyd Fayton Jr, Ainsley Gibson, William A. Hercules, and John A.W. Harkless</i>	72
P1	New Developments in Electron Propagator Methods <i>Roberto Flores-Moreno and J. V. Ortiz</i>	73
P1	Theoretical Comparison of Parathion and Paraoxon for the Discernment of Acetylcholinesterase-Phosphorothionate/Phosphate Inhibition in Mammalian Systems <i>Jason Ford-Green, D. Majumda, Jerzy Leszczynski</i>	74
P1	Substituent Effects on the 1,2-Rearrangements (Thia-Wolff) and C—H Insertion Reactions of C-4-X-Arylsulfinyl Carbenes <i>Fillmore Freeman and Nha Thi Bich Nguyen</i>	75
P1	Tautomerization Mechanisms in 2-Pyrimidinethiols <i>Fillmore Freeman, Henry N. Po</i>	76
P1	The Hydrogen Bonding of DNA Bases in Aqueous Solution. Ab Initio Molecular Dynamics Study <i>A. Furmanchuk, O. Isayev, L. Gorb and J. Leszczynski</i>	77
P1	Novel Derivatives of Bicyclo[2.2.2]octane and Their Strain Energies <i>Earl Chauncey Garrett, Edward J. Valente, and David H. Magers</i>	78
P1	Chemistry in Acetone Complexes of Metal Dications: A Remarkable Ethylene Production Pathway <i>Frank Hagelberg, Jianhua Wu, Sung Soo Park, Alexandre A. Shvartsburg</i>	79
S4	Nuclear-Electronic Orbital Approach: Including Nuclear Quantum Effects in Electronic Structure Calculations <i>Sharon Hammes-Schiffer</i>	81
P1	Comparative Theoretical Study on the Interactions of Alkali Metal Ions (Li^+ , Na^+ and K^+) with Benzene: Effect of Sequential Ring Annulation of Six-Membered Aromatic Ring and Bicyclo[2.1.1]Hexene to Benzene. <i>Ayorinde Hassan, T. C. Dinadayalane and Jerzy Leszczynski</i>	83
P1	Using ab initio/GIAO/NMR Structural Tool for Molecular Structure Determination of Various Macropolyhedral Boron Clusters. Their Possible Interaction with Biomolecules <i>D. Hnyk, J. Macháček, J. Fanfrlík, P. Hobza, M. Kolaski, K. S. Kim</i>	85
P2	Theoretical Study of the Interactions of Perfluorinated Fatty Acids with Cysteine <i>Tiffani Holmes, Jacek Dosckoz, Terrance Wright, Jerzy Leszczynski, Glake Hill</i>	88
P2	Structures and Electronic Properties of Cu@Sin (n= 9-15) Nano-clusters <i>Delwar Hossain and Steven R. Gwaltney</i>	89
P2	Theoretical Characterization of the Phosphaalkenes $\text{Ar}_\text{F}\text{P}=\text{C}(\text{CH}_3)_2$ ($\text{Ar}_\text{F} = 2,6\text{-(CF}_3)_2\text{C}_6\text{H}_3$) <i>Ming-Ju Huang, David J. Watts, and John D. Watts</i>	90

P2	Surface Interactions of Graphitic Sheets and Water: A Study of the Hydrophobic Effect <i>Estelle M. Huff, Peter Pulay</i>	91
P2	Building Transferable Hamiltonians with localized Correlated Orbitals <i>Thomas F. Hughes and Rodney J. Bartlett</i>	92
P2	Relative Stability of Isomers of a Dipseudoacid <i>Peter J. Huwe, Dmitriy V. Liskin, Edward J. Valente, and David H. Magers</i>	93
P2	An ab initio Molecular Dynamics Study of the Initial Chemical Events in Nitramines: Thermal Decomposition of CL-20 <i>Olexandr Isayev, Leonid Gorb, M. Qasim, and Jerzy Leszczynski</i>	95
P2	Structure of Liquid Water from <i>ab initio</i> Molecular Dynamics at the Complete Plane Wave Basis Set Limit <i>Olexandr Isayev, Leonid Gorb, Jerzy Leszczynski</i>	96
S3	A Combined Direct Molecular Dynamics/Density-Functional Theoretical Study of the Electrochemical Hydrogen Oxidation Reaction and Underpotential Deposition of H on Pt(111) <i>Yasuyuki Ishikawa, Juan J. Mateo, Donald A. Tryk, and Carlos R. Cabrera</i>	98
P2	Quantum Electron Transport in Toroidal Carbon Nanotubes <i>Mark A. Jack and Mario R. Encinosa</i>	100
P2	An Efficient Parallel Implementation of Triples Contribution to CCSD(T) Energies <i>Tomasz Janowski and Peter Pulay</i>	102
P2	Electron Impact Ionization Cross Sections for Beryllium-Isoelectronic Sequences <i>D.C. Joseph, M.F. Gu, B.C. Saha</i>	104
P2	Electric Dipole (Hyper)Polarizabilities of Aluminum Phosphide Clusters Al_nP_n ($n=2-9$) <i>Panaghiotis Karamanis and Jerzy Leszczynski</i>	105
P2	The Mechanism of RDX Hydrolysis in Alkaline Solutions <i>Yana Kholod, Leonid Gorb, Sergiy Okovytyy, Mohammad Qasim, and Jerzy Leszczynski</i>	109
S3	Magic Structures and Quantum Conductance of Linear Ultrathin Nanowires and Negative Differential Resistance of Molecular Wires <i>Kwang S. Kim</i>	110
P2	Modeling of Time-Dependent Spatial Distribution of Multi-Component Reacting System. Implication for Prebiotic Evolution <i>Dmytro Kosenkov, Yana Kholod, Andrea Michalkova, Leonid Gorb and Jerzy Leszczynski</i>	113
P2	Quantum-Chemical Research of Flame Inhibition Mechanism <i>V. Kukueva</i>	114
P2	New Approach for the Correction of <i>ab initio</i> Molecular Force Fields in Cartesian Coordinates <i>G.M.Kuramshina, I. V. Kochikov, A.V.Stepanova</i>	116
P2	A System of Informational Fractal Parameters for Developing Quantitative Structure-Activity Relationships. Antihyperthermic activity of N,N'-(bis-5-nitropyrimidyl)dispirotriperazine derivatives <i>V.E. Kuz'min, N.A. Kovdienko</i>	121

P2	Structure and Properties of Perfluoroalkylated Phthalocyanines. A Theoretical Study <i>Meng-Sheng Liao, John D. Watts, and Ming-Ju Huang</i>	124
P2	Intermolecular Electron Transfer in Dimetallofullerenes Based on C ₈₄ and C ₈₆ <i>Dan Liu and Frank Hagelberg</i>	125
S2	Development of a Polarizable Force Field Based on the Classical Drude Oscillator <i>Alexander D. MacKerell, Jr.</i>	127
P2	Relative Stability of Isomers of 1,2-Disubstituted 3-Aminoindenes <i>Andrew K. Magers and David H. Magers</i>	128
P2	Strain Energies in Isomers of 1,3-Cycloheptadiene and Bicyclo[3.2.0]hept-6-ene <i>D. Brandon Magers, Steven R. Davis, and David H. Magers</i>	129
P2	Binding Energies in Dimers of N-methyl methyl carbamate, N-methylS-methyl thiocarbamate, and N-methyl methyl dithiocarbamate <i>Harley R. McAlexander and David H. Magers</i>	130
P2	Adapted <i>ab initio</i> Theory: KS-DFT Based Semiempirical Theory <i>Joshua J. McClellan and Rodney J. Bartlett</i>	131
P2	Computational Study on the Flap Dynamics of HIV-1 Protease Subtype B vs. C <i>T. Dwight McGee Jr., Jesse Edwards, Adrian E. Roitberg</i>	132
P2	Truncation of the Correlation Consistent Basis Sets for Hydrogen: Extension to the Hydrogen Containing Molecules of the G3/99 Test Suite <i>Benjamin Mintz, Sage Driskell, Amy Shah, and Angela K. Wilson</i>	133
P2	A Comparative Computational Study of Nitroaromatic Explosives and Their Related Derivatives <i>Brett Moore, Lyssa Taylor, Frances Hill, Mohammad Qasim</i>	134
P2	New QSAR Equations for Predictions of an Aqueous Solubility for Military Compounds: Preliminary Results <i>E. N. Muratov, V. E. Kuz'min, A. G. Artemenko, L. Gorb, M. Qasim, J. Leszczynski</i>	137
P2	The Nonuniform Nature of Electrostatic Potentials on Bonded Atom Surfaces <i>Jane S. Murray, Monica C. Concha, Pat Lane, and Peter Politzer</i>	140
P2	Chemistry of Hydrated Cations: Part II. Linearity of Total Energy on [M(H ₂ O) _n] ⁺ (n=1,2,3,4,5,6), M=Li, Na, K Species <i>Jamshid Najafpour, Abdolreza Sadjadi, Ng Seik Weng</i>	142
S5	Large-Scale Molecular Theory <i>Takahito Nakajima</i>	145
P2	A Coupled-Cluster Analysis of H ₂ SN ₂ Molecules Using Conventional and the cc-pV(X+d)Z Basis Sets <i>Brian Napolion and John D. Watts</i>	148
P2	Moderate-Size Basis Sets for Correlated Calculations of the (Hyper)Polarizability at MP2 Level <i>Sergey E. Nefediev</i>	149
P2	Conformational Studies of Thirteen-Membered Rings <i>Eric A. Noe, Frank R. Fronczek, Diwakar M. Pawar, and Judge Brown</i>	152
P2	The Quantum-Chemical Investigation of Nucleophilic Substitution Mechanism in Reaction of Methylamine with Methylsulfochloride <i>S.I. Okovytyy, G.V. Gryn'ova, A.V. Tokar, L.I. Kasyan</i>	153

S6	Three Approaches to a Nonlocal, Energy-Dependent Correlation Potential in Electron Propagator Theory <i>J. V. Ortiz</i>	155
P2	pKa of TEPA and THIOTEPA Antitumor Drug : A Computational Study <i>O. Ouamerali, D. Kheffache, U. Rothlisberger</i>	156
S4	The Linear and Nonlinear Optical Properties of a Series of Derivatives Involving One or More Noble Gas Atoms <i>Manthos G. Papadopoulos and Aggelos Avramopoulos</i>	157
P2	Investigation of Optical Polymers with Improved Chemical Properties <i>Sung Soo Park, Frank Hagelberg</i>	158
P2	Theoretical Study of the Adsorption of Organophosphorus Compounds on Metal Oxide Surfaces <i>Y. Paukku, A. Michalkova, and J. Leszczynski</i>	159
P2	Computational DFT Study of the Mechanisms for the Ethanolysis of Epoxyendic Imides in Polar Solution <i>T. Petrova, S. Okovytyy, L. Gorb, J. Leszczynski</i>	161
P3	The Impact of Systematic Basis Set Truncation and Recontraction on Density Functional Theory Computations <i>Brian P. Prascher, Brent R. Wilson, Angela K. Wilson</i>	163
P3	Calculation of the Solvation State of Organolithium Compounds: Effects of Basis Sets and Electron Correlation Methods <i>L. M. Pratt, D. Jones, A. Sease, D. Busch, E. Faluade, S. C. Nguyen, B. T. Thanh</i>	164
P3	Radiative and Nonradiative Decay Rates of Molecular Fluorophore Layer Adsorbed at Noble-Metal Nanoparticle <i>V. N. Pustovit and T. V. Shahbazyan</i>	166
P3	Gold and Silver Nanosystems: Synthesis, Characterization And Study Of Size And Shape Dependent Optical Properties, Application Towards Biology <i>U. S. Rai, G. K. Darbha, A. Ray, O. Tovmachenko, W. Hardy, J. Walker, J. Griffin, P. Ray</i>	167
P3	Na,K-ATPase Inhibition Activity Predicting: A Comparative Computational Study By CoMFA, CoMSIA, GA-MLRA and GA-PLS Methods <i>B. F. Rasulev, F. T. Umarov, M.P. Yuldashev, Z. A. Khushbaktova, and J. Leszczynski</i>	168
P3	Transition State Verification between the Transformation of Parathion to Paraoxon within Cytochrome P450 (CYP) <i>Kevin L. Reese, Jason Ford-Green, Jerzy Leszczynski</i>	169
P3	Lattice Energy Determination for Crystalline Benzene <i>Ashley L. Ringer and C. David Sherrill</i>	171
P3	Theoretical Study of Adsorption of Selected Tautomers of Uracil and Thymine on Dickite <i>T. L. Robinson, A. Michalkova, L. Gorb, and J. Leszczynski</i>	172
S3	The Bonding and Structural and Thermodynamic Properties of Metal-Carbon and Metal-Silicon Compounds – Building Blocks of Same Nanomaterials <i>Szczepan Roszak and Pawel Wielgus</i>	174
P3	MP2/6-31+G** Calculations of Complexes of Adenine Tautomers with Zn(II), Cu(II) and Ag(I) <i>Yu.V. Rubin, G.M. Kuramshina, M. Shukla and Jerzy Leszczynski</i>	175

P3	Topological Analysis and Quantum Mechanical Structure of C ₅ Pure Carbon Clusters <i>Abdolreza Sadjadi, Gholam Hossein Shafiee, Jamshid Najafpour, Shant Shahbazian</i>	177
P3	Analytical and Numerical Treatment of Overlap-Like Quantum Similarity Integrals over Exponential Type Functions <i>H. Safouhi and A. Bouferguene</i>	179
P3	K-shell Ionization of Neutral Targets $1 \leq Z \leq 92$ by Electron Impact <i>B. C. Saha, M. A. R. Patoary, M. A. Uddin, A. K. Basak</i>	180
S5	Self-Interaction Corrected Local Spin Density Calculations in Strongly Correlated Electron Materials <i>Thomas C. Schulthess</i>	183
P3	Structures and Properties of C ₆₀ -Gold Nanocontacts: A Theoretical Investigation <i>M.K. Shukla, Madan Dubey and Jerzy Leszczynski</i>	184
P3	A Theoretical Study of the Chemisorptions of H ₂ with Stone-Wales Defect Armchair (5, 5) Single-Walled Carbon Nanotubes <i>Tomekia Simeon, T. C. Dinadayalane and Jerzy Leszczynski</i>	185
P3	Manzamine A Interaction with CDK5: Docking, Molecular Dynamics Simulations and Binding Free Energy Calculations <i>Prasanna Sivaprakasam, Mark T Hamann, Robert J. Doerksen</i>	186
P3	The Singlet Oxygen Activation in Zn(2+)/ZSM-5 Zeolites: A DFT Study of the Adducts of Activated Singlet Oxygen with Propene or Propyne. Does Exist Dioxetanes in Triplet State? <i>Vitaly Solkan and Jerzy Leszczynski</i>	188
P3	A DFT Study of the Methane Activation by Univalent Transition-Metal Ion Structures in Co(1+)/ZSM-5, Ni(1+)/ZSM-5, and Cu(1+)/ZSM-5 Zeolites <i>Vitaly Solkan</i>	192
P3	Theoretical Study of Nitrous Oxide Decomposition Catalysed by Ga/ZSM-5 Using Post-Hartree-Fock and Density Functional Theory Calculations <i>Vitaly Solkan</i>	196
P3	A DFT Study of Stability and Chemical Activity of Binuclear Gallium-Oxide Nanocluster Adsorbed at Channel Surface in ZSM-5 Zeolite <i>Vitaly Solkan</i>	200
P3	Enthalpies of Formation of TNT Derivatives by Homodesmotic Reactions <i>Amika Sood, Patricia Honea, and David H. Magers</i>	204
P3	B _n Si _m (n+m=5) Microclusters – The Precursors of Boron/Silicon Nanomaterials <i>Chi-Cobi Speaks, Julia Saloni, Szczepan Roszak, and Glake Hill</i>	205
P3	Hydrazinolyses of 4-Methyl-1,3-Dihydro-2H-1,5-Benzodiazepin-2-Thione <i>Liudmyla K. Sviatenko, Sergiy I. Okovytyy, Alexandr A. Gaponov, Igor Tarabara, and Jerzy Leszczynski</i>	206
P3	Theoretical Studies of Corannulene Dimers <i>Andrzej Sygula and Svein Saebo</i>	207
P3	Quantum Processes of Self-Assembly, Photosynthesis and Molecular Computing in Artificial Minimal Living Cells <i>Arvydas Tamulis and Vykintas Tamulis</i>	210
P3	Quantitative Bond-Breaking with Coupled-Cluster Theory: Brueckner Λ CCSD(T) <i>Andrew G. Taube and Rodney J. Bartlett</i>	213

P3	Additive SMILES based Optimal Descriptors: QSPR modeling of Fullerene C ₆₀ Solubility in Organic Solvents <i>Andrey A. Toropov, Bakhtiyor F. Rasulev, Danuta Leszczynska and Jerzy Leszczynski</i>	215
P3	Shape and Size Dependent SERS Effect of Silver Nanoparticles <i>O. Tovmachenko, G. K. Darbha, U. S. Rai, A. Ray, W. Hardly, P. C. Ray</i>	217
P3	Recasting the 2-Body: n-Body Treatment for Weakly Bound Clusters in the ONIOM Formalism: Efficient and Accurate QM:QM Methods for Hydrogen Bonding and n Interactions <i>Gregory S. Tschumper</i>	218
P3	Accuracy and Fast Topological Analysis of Gridded Electron Densities Functions:A Powerful Algorithm Implemented in C++ <i>David Vega, Jesus Rodriguez and Yosslen Aray</i>	219
P3	Quadrature Scheme for Higher-Order Energy Derivative of Density Functional Theory <i>Prakash Verma and Rodney J. Bartlett</i>	225
P3	Absorption and Emission Study of a Conjugated Polymer <i>J. Wang, J. Gu, A. Bamgbelu, L. Sitole, T. Wheat, I. Shukla, and J. Leszczynski</i>	226
P3	Critical Assessment of Coupled Cluster Methods for Core Ionization Potentials of Small Molecules <i>Thomas Watson and Rodney J. Bartlett</i>	227
P3	A Coupled-Cluster Study of Isomers of H ₂ SO ₂ <i>John D. Watts, Brian Napolion and Ming-Ju Huang</i>	228
P3	Molecular Dynamics Simulation Studies of Hydrophobic Solvation of Winter Flounder Antifreeze Protein <i>Andrzej Wierzbicki, Keith Battle, Jeffry D. Madura</i>	229
P3	Hartree-Fock Energy Convergence of Transition Metal Species <i>T. Gavin Williams, Angela K. Wilson</i>	230
P3	Quantum Transport throughout the DNA Bases Located Between Gold Electrodes <i>Ilya Yanov, Juan José Palacios and Glake Hill</i>	231
S2	Molecular Simulation and Quantum Chemical Studies of Ribozyme Catalysis <i>Darrin M. York</i>	232
P3	Electron Propagator Calculations on the C ₇₀ Photoelectron Spectra <i>V. G. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz</i>	233
P3	Ionization Constant (pKa) Prediction for Drug-Like Molecules <i>Shuming Zhang, Jon Baker, and Peter Pulay</i>	235
P3	Alkanethiol Molecule on Copper (111) Substrate <i>Jian-Ge Zhou and Quinton L. Williams</i>	236
P3	Molecular Dynamics Simulations of DNA-Polycation Complexes <i>Jesse Ziebarth and Yongmei Wang</i>	237
P3	Influence of Exocyclic Proton Donor/Acceptor on Tautomerism, Aromaticity and Intramolecular Resonance-Assisted Hydrogen Bonds <i>Roman I. Zubatyuk, Oleg V. Shishkin</i>	238

[†]S* – Oral presentation (* denotes session number); P* – Poster presentation (* denotes poster session number);
NL – After Dinner Nobel Lecture