TECHNICAL PROGRAM - CERMACS 2008

Tuesday, June 10, 2008

Tuesday, June 10, 2008, 5:30 PM - 7:30 PM
Reception and Sci-Mix Poster Session
First Floor Atrium (Center of Science and Industry (COSI))

Organizer: Claudia Turro, The Ohio State University

1 Aromatic Hydroxylation of 1-Benzylpiperazine by a Carbonyl Oxide, a Chemical Model of Monooxygenase Enzymes. **Shailendra Kumar** and Ajaykumar Mallesha, Governors State University

2 Magic-Angle Spinning Solid-State NMR Studies of Paramagnetic Proteins. **Philippe S. Nadaud**, Jonathan J. Helmus, Nicole Hoefer and Christopher P. Jaroniec, The Ohio State University

3 Review of Recent Applications of Photocycloaddition Reactions of Nonracemic Compounds. **Wendell L. Dilling**, Central Michigan University

4 Dewetting of Polystyrene Thin Films on Poly(ethylene glycol) Modified Surfaces as a Simple Approach for Patterning Proteins. **Yangjun Cai** and Bi-min Zhang Newby, The University of Akron

5 Cytotoxicity and Anti-Inflammatory Activity of Polyphenolics. **Kimberly N. Wisman**, Akeysha A. Perkins and Ann E. Hagerman, Miami University

6 Synthetic Studies of Spiro[Cycloalkane-1,3'-Indolenine] Derivatives. **Sureshbabu Narayanasamy**, Eric Schwartz, Pratiq Akshay Patel and James R Fuchs, College of Pharmacy, The Ohio State University

7 Vanadate Salts as Potential Pigments: Synthesis, Structure, and Band Gaps. **Derek Decker**, Graham King, Matthew W. Stoltzfus and Patrick Woodward, The Ohio State University

8 Rhodium(II)-Catalyzed Decomposition of Furanose-Derived Diazoesters. **Jennie Patton**, Ashley Malich, Calvin Austin, Matthias Zeller and Peter Norris, Youngstown State University

9 Structure and Preliminary Biological Evaluation of N-Glycosides. **Erin Schuler**, Steve Knapp, Matthias Zeller, Peter Norris and Nina Stourman, Youngstown State University

10 Methionine Aminopeptidase Inhibitors as Antibacterial Agents. **Wenlong Wang** and Qi-Zhuang Ye, Indiana University School of Medicine

11 Thermo-Optical Properties and Characterization of Heat Generation of Single Gold Nanoparticles Embedded in Ice. **Alyssa C. Thomas**, Hugh H. Richardson, Michael C. Carlson and Alexander O. Govorov, Ohio University

12 Block Copolymers Via RAFT Polymerization and Click Chemistry: Designing New Biomaterials. **Thirumamagal B.T.S.** and Scott Schricker, College of Dentistry

13 Thermal Effects of Electromagnetic Stimulation of Nanoparticles. **Michael T. Carlson**, Hugh H. Richardson and Martin E. Kordesch, Ohio University

14 Developing Novel Photoprotecting Groups. **Stephen A. Sims** and Anna Gudmundsdottir, University of Cincinnati

15 A One-Step, One-Pot Gewald Reaction for Alkyl-Aryl Ketones Via Mechanochemistry. **William C. Shearouse** and James Mack, University of Cincinnati

16 Ultrafast UV-Vis/ir Studies on the Photochemistry of Phenyldiazirine. **Yunlong Zhang**, Gotard Burdzinski, Jacek Kubicki, Shubham Vyas and Matthew S. Platz, The Ohio State University

17 Investigating the Role of Vibrational Excitation on the Dynamics of the $F(^2P)$ + HCl --> FH + $Cl(^2P)$ Hydrogen-Transfer. **Sara E. Ray**, Ge W.M. Vissers and Anne B. McCoy, The Ohio State University

18 Effect of Axial Halide Coordination on Electronic Properties and Photochemistry of Dirhodium Complexes. **Robert Garner** and Claudia Turro, The Ohio State University

19 Novel Functionalized Core/shell Nanocapsules for Imaging and Drug Delivery. **Duangruthai Sridaeng**, Tejal Deodhar, Jacob J. Weingart and Jun J. Hu, University of Akron

20 Can My GC-MS Be Sharper Than My Nose?. **John A. Milo**, Roland Riesen and Brian D. Leskiw, Youngstown State University

21 Highly Stable Dendritic Trityl Radicals as Oxygen and pH Probe. **Yangping Liu**, Frederick A. Villamena and Jay L. Zweier, The Ohio State University

22 Integration of Structurally and Compositionally Diverse Metal Oxide Semiconductor Nanomaterials for Photovoltaic Applications. **Gayatri Natu**, Yanguang Li, Mario Alpuche-Aviles and Yiying Wu, The Ohio State University

23 Substrate Specificity of IPP Isomerase in Moths. **Ryan Denton**[1], Stephanie Sen[1], Michel Cusson[2], Catherine Béliveau[2] and Dring Crowell[1], (1)IUPUI, (2)Natural Resources Canada

24 Asymmetric Hydrogenation Over Folding Dendrimer Rhodium(I) Complexes. **Jianfeng Yu**, T.V. RajanBabu and Jon Parquette, The Ohio State University

25 A Single Amino Acid Residue Mutation of the Human Islet Polypeptide Completely Suppresses Its Toxicity. **Kevin M. Hartman**, Jeffrey R. Brender and Ayyalusamy Ramamoorthy, University of Michigan

26 High Temperature Internal Reference Oxygen Sensors Using a Conducting Metal Oxide Electrode. **Julia Rabe**, Prabir K. Dutta and John Spirig, The Ohio State University

27 4-Aryl-1,3,2-Oxathiazolylium-5-Olates as pH-Controlled NO-Donors: The Next Generation of S-Nitrosothiols. **Dongning Lu**, Janos Nadas, Jay Zweier, Frederick Villamena and Peng George Wang, the Ohio State University

28 Studies on the Binding and Iron Delivery of Human Frataxin to Its Partners. **Jia Huang**, The Ohio State University and J. a. Cowan, Ohio State University

29 Flexible and Precise Control of Multi-Phase Laminar Flow for 3D in-Channel Microfabrication. **Yunxiang Gao** and Liwei Chen, Ohio University

30 Preparation and Characterization of Reversibly Photochromic Polydiacetylenes. **Nathan A. Furr**, Robert E. Minto and Michael Akers, IUPUI

31 Total Synthesis of Histone H3 Acetylated at Lysine 56. **John C. Shimko**, Tiffany V. Sommers and Jennifer J. Ottesen, The Ohio State University

32 Preparation of New Polymerizable Dithienylethene Chromophores and Their Photochromic Polymer Films. **Thilini K. Mudiyanselage** and Douglas C. Neckers, Bowling Green State University

33 Phenylacetylene Based Materials: Enhanced Emission in Nanoparticles and Solid-State. **Sujeewa S. Palayangoda** and Douglas C. Neckers, Bowling Green State University

34 Title: A Study of the Barrier to Free Rotation in Tetramethylurea. **Xiaojian Mao**, West Virginia University

35 A Gated Guest Entrance in Command of the Encapsulation Thermodynamics. Molecular Baskets at Work. **Baoyu Wang**[1], Jovica Badjic[1], Zhiqing Yan[2], Xiaoguang Bao[1] and Christopher Baddeley[1], (1)The Ohio State University, (2)Eastern Illinois University

36 Hemeproteins and Enzymes in Bilayer Structures Bathed in Ionic Liquids: The Role of WATER in Electron Transfer and Protein Function. **John J. Moran**, Noufissa Zanati, Jeremiah Bolden and Mekki Bayachou, Cleveland State University

37 Electron Transfer Dynamics Between 9-Anthracenecarboxylic Acid and TiO2 Nanoparticles with Applications for Novel Photovoltaic Devices. **Lynetta M. Mier**, Yagnaseni Ghosh, Austin R. Carter, Malcolm H. Chisholm, Arthur J. Epstein and Terry L. Gustafson, Ohio State University

38 Binding Modes of Pyridinium Oximes with Acetylcholinesterase: Importance of Aromatic Residues Elucidated by Ligand-Receptor Docking Studies. **Jeremy M. Beck**, Shubham Vyas and Christopher M. Hadad, The Ohio State University

39 Solid-State NMR of Rare-Earth Aluminosilicate Glasses and Nanocrystals. **Shay M. Smith**, Celeste Savitski, Alexanne Holcombe and Joseph R. Sachleben, Otterbein College

Tuesday, June 10, 2008, 7:30 PM - 9:00 PM
Welcome and Lecture by Prof. Lonnie Thompson
Traveling Exhibits Hall (Center of Science and Industry (COSI))

Presider: Malcolm H. Chisholm, The Ohio State University

7:30 Welcoming Remarks by James A. Cowan.

7:40 Introductory Remarks by CAS and COSI.

8:00 **40** Retreating Glaciers, Abrupt Climate and Our Future. **Lonnie G. Thompson**, The Ohio State University

Wednesday, June 11, 2008

Wednesday, June 11, 2008, 8:30 AM - 9:15 AM
Plenary Lecture: Carl Kohrt, Battelle, CEO
Franklin A (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: James A. Cowan, The Ohio State University

8:30 **41** Solutions, Science, and the Synthesis of Disciplines. **Carl Kohrt**, Battelle

Wednesday, June 11, 2008, 9:30 AM - 12:30 PM
ACS Career Services Workshops
Franklin D (Hyatt Regency Columbus)

Organizers: Theresa Huston, Chemical Abstracts Service, Columbus, OH, Garretta Rollins, American Chemical Society

9:30 **42** Job Searching Strategies. **Garretta Rollins**, American Chemical Society

10:30 **43** Résumé Preparation for the Chemical Professional. **Garretta Rollins**, American Chemical Society

11:30 **44** Interviewing Skills for the Chemical Professional. **Garretta Rollins**, American Chemical Society

Wednesday, June 11, 2008, 9:30 AM - 5:45 PM
Biomolecular Solid-State NMR Spectroscopy I
Sponsors: Bruker Corporation, Varian, Cambridge Isotopes Laboratories, ISOTEC/Sigma-Aldrich, and ACS Division of Physical Chemistry
Harrison (Hyatt Regency Columbus)

Organizer: Christopher Jaroniec, The Ohio State University

9:30 **45** Magic Angle Spinning NMR Spectroscopy of Microtubule-Associated Protein and Thioredoxin Reassemblies. **Tatyana Polenova**[1], Shangjin Sun[1], Sivakumar Paramasivam[1], Jun Yang[1], John C. Williams[2], Christine Lightcap[2] and Amanda Roberts[2], (1)University of Delaware, (2)Thomas Jefferson University

10:00 **46** Solid State NMR Studies of Integral and Peripheral Membrane Proteins. **Vladimir Ladizhansky**, University of Guelph

10:30 **47** Structural Studies of Alpha-Synuclein Fibrils by Solid-State NMR. **Kathryn D. Kloepper**, Andrew J. Nieuwkoop, Julia M. George and Chad M. Rienstra, University of Illinois at Urbana Champaign

10:45 Break.

11:00 **48** Unusual Spin Dynamics in Solid-State NMR of Proteins Experiencing Ultra-Fast MAS and Low-Power Radio-Frequency Fields. **Joseph R. Sachleben**[1], Segolene Laage[2], Guido Pintacuda[2] and Lyndon Emsley[2], (1)Otterbein College, (2)Université de Lyon

11:30 **49** High Resolution Spectra and Structures of Solid Proteins by NMR. **Chad M. Rienstra**, University of Illinois at Urbana-Champaign

12:00 **50** Comparative & Combined Analyses of Protein Relaxation Data from Solid- and Solution-State NMR. Veniamin Chevelkov[1], Yi Xue[2], Vipin Agarwal[1], Anne Diehl[1], Anastasia Zhuravleva[2], Nathan Benjamin[2], Bernd Reif[1] and **Nikolai R. Skrynnikov**[2], (1)Leibniz-Institut für Molekulare Pharmakologie (FMP), (2)Purdue University

12:30 Lunch Break.

1:30 **51** Structure Determination of Dynamic Membrane Peptides by Solid-State NMR. **Mei Hong**, Ming Tang and Sarah Cady, Iowa State University

2:00 **52** Effect of Substrate on Supported Lipid Bilayers. **Megan M. Spence**, University of Pittsburgh

2:30 **53** Structure Elucidation Using Oriented Solid State NMR Methods: The Case Study of Filamentous Bacteriophage. **Suzana K. Straus**[1], Walter R.P. Scott[1], Martyn Symmons[2] and Don A. Marvin[2], (1)University of British Columbia, (2)University of Cambridge

3:00 **54** Structure and Topology of the Phospholamban/ca-ATPase (SERCA) Complex by Solid-State NMR. **Gianluigi Veglia**, Nathaniel J. Traaseth, Lei Shi and Raffaello Verardi, University of Minnesota

3:30 Break.

3:45 **55** Toward Variable Angle Spinning NMR for Membrane Systems. **Rachel W. Martin**, Pierre Thureau, Rebecca Shapiro and Ilya Litvak, University of California, Irvine

4:15 **56** Furanose Ring Dynamics in Damaged DNA from 2H Solid-State NMR. **Nathan Oyler**[1], Crystal Ferguson[2] and Gary A. Meints[2], (1)University of Missouri-Kansas City, (2)Missouri State University

4:45 **57** Solid-State NMR and EPR Spectroscopic Studies of Integral Membrane Proteins. Shadi Abu-Baker and **Gary A. Lorigan**, Miami University

5:15 **58** Dynamical Structures of Protein-Protein and Peptide-Peptide Interactions in the Membrane Interface by NMR. **Ayyalusamy Ramamoorthy**, Jiadi Xu, Kazutoshi Yamamoto, Jeffrey Brender and Ravi Nanga, University of Michigan

Wednesday, June 11, 2008, 9:30 AM - 5:30 PM
Frontiers In Protein and Peptide Engineering I
Sponsor: ACS Divisions of Biochemical Technology and Biological Chemistry
Franklin B (Hyatt Regency Columbus)

Organizers: Dennis Bong, The Ohio State University, Thomas J. Magliery, The Ohio State University

Session Overview: The session will include talks on protein engineering and design, peptide design for therapeutic and materials applications, and biomolecular recognition.

9:30 Welcome (Morning).

9:35 **59** Optimization of Protein Folding in Vivo. **James Bardwell**, Howard Hughes Medical Institute

10:10 **60** Uncoupling the Active Sites of the I-SceI Homing Endonuclease to Create DNA Nicking Enzymes with High Specificity. **Frederick S. Gimble**[1], Kristen Tenney[1], Hongye Li[2] and Yan Niu[1], (1)Purdue University, (2)Institute of Biosciences & Technology, TAMHSC

10:45 **61** Covariation Analysis on Two Families of Dimeric Proteins - Triosephosphate Isomerase and Cu Zn Superoxide Dismutase. **Venuka Durani**[1], Brandon Sullivan[1], Hatice Gulcin Ozer[2], William C. Ray[2] and Thomas J. Magliery[2], (1)The Ohio State Univeristy, (2)The Ohio State University

11:05 Break (Morning).

11:20 **62** Fuzzy Substrate Recognition in Neuropeptidases. **David W. Rodgers**, Nicholas Noinaj, Sowmya Sampath and Eun Jeong Lim, University of Kentucky

11:55 **63** Protein Stability from Combinatorial and Statistical Approaches. **Thomas J. Magliery**, The Ohio State University

12:30 Lunch Break.

1:30 Welcome (Afternoon).

1:35 **64** Engineering Conformational Peptide Epitopes as Cancer Vaccines. **Pravin Kaumaya**, OSU

2:10 **65** Fluorous Amino Acids: A New Element in Protein Design. **E. Neil G. Marsh**, Lindsey M. Gottler, Hwang-Yeol Lee and Roberto de la Salud Bea, University of Michigan

2:45 **66** Monitoring Protein Stability and Ligand Binding by Pulse Proteolysis without Purifying Proteins. **Chiwook Park**, Purdue University

3:05 **67** All Domains of Cry1A Toxins Insert into Insect Brush Border Membranes. **Manoj S. Nair** and Donald H. Dean, The Ohio State University

3:25 Break (Afternoon).

3:40 **68** De Novo Designed Heterochromic and Diasteromeric Metallopeptides. **Vincent L. Pecoraro**, Olga Iranzo, Anna Peacock, Debra Touw and Saumen Chakraborty, University of Michigan

4:15 **69** Controlling Collagen Triple Helix and Fiber Formation. **Jean Chmielewski**, Purdue University

4:50 **70** Functional Deteminants of a Synthetic Membrane Fusion System. **Dennis Bong**, The Ohio State University

Wednesday, June 11, 2008, 9:30 AM - 12:30 PM
General Analytical Chemistry I - Contributed Talks
Sponsor: GFS Chemicals
Garfield (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: William J. Clark, Capital University

9:30 **71** Evaluation of a Single Temperature Model for Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) and Semi-Quantitative Elemental Analysis. **Josh R. Dettman**, John W. Olesik and Susan V. Olesik, The Ohio State University

9:55 **72** Comparative Study Between 5 Micron Particle-Packed C18 and Monolithic C18 Columns for the Separation of Algal Pigments by High-Performance Liquid Chromatography with Fluorescence Detection. **Aaron R. Roerdink**, National Center for Water Quality Research, Heidelberg College

10:20 **73** ICP-MS Isotope and Elemental Ratio Precision Improvement by Temporal Homogenization in a Pressurized Reaction Cell. **Patrick J. Gray**, John W. Olesik and Susan V. Olesik, The Ohio State University

10:45 Break.

11:05 **74** Persistent Self-Assembled Monolayers for Micro/Nano Electro-Mechanical Device Fabrications. **Jun J. Hu**, Jiang Zhe and Yong Ma, University of Akron

11:30 **75** Zeolite-Based Impedance Type Sensor for Selectively Detecting Highly Toxic Organophosphate-Bearing Nerve Agents. **Xiaogan Li** and Prabir K. Dutta, The ohio State University

11:55 **76** Comparison of Derivatized Polysaccharide Phases for Separation of Warfarin and Related Drugs. **Kahsay Gebre-Yohannes** and Victoria McGuffin, Michigan State University

Wednesday, June 11, 2008, 9:30 AM - 5:30 PM
General Inorganic Chemistry I - Contributed Talks
Marion (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presiders: Jeffrey J. Rack, Ohio University, Michael Jensen, Ohio University

9:30 **77** Biocatalytic Electrodes Based on Single-Walled Carbon Nanotube Network Thin Films. **Dan Wang** and Liwei Chen, Ohio University

9:55 **78** Construction of Metal-Organic Framework with Permanent Porosity Based on Hexatopic Ligand. **Dan Zhao**, Daqiang Yuan and Hongcai Zhou, Miami University

10:20 **79** Nanowire Self-Alignment with Graphene Oxide. **Yanguang Li**, The Ohio State University and Yiying Wu, Ohio State University

10:45 Break.

11:05 **80** Negative Thermal Expansion Caused by a Bifurcated H-Bonding Network in Zirconium Phosphate. **Robert T. Hart Jr.**, The Shepherd Chemical Company

11:30 **81** Effect of Synthesis Conditions of Nano-Ruthenium Oxide as a NOVEL Platform for Low Temperature Carbon Monoxide Detection. **Adedunni D. Adeyemo** and Prabir K. Dutta, The Ohio State University

11:55 **82** A Scanning Probe Assay for Metallic and Semiconducting Contents in Single-Walled Carbon Nanotube Mixtures. **Yao Xiong**, Ohio university

12:20 Lunch.

1:30 **83** Photoinduced Catalysis by Cis-$[Rh_2(\mu\text{-}O_2CCH_3)_2(CH_3CN)_6]^{2+}$. **Lauren E. Joyce**, Craig R. Smith and Claudia Turro, The Ohio State University

1:55 **84** Non-Adiabatic Picosecond Linkage Isomerization in Chelating Ruthenium(II) Sulfoxides. **Beth Anne McClure**[1], Eric Abrams[1], Jeffrey L. Petersen[2] and Jeffrey J. Rack[1], (1)Ohio University, (2)West Virginia University

2:20 **85** Nickel in N3S2 Ligand Fields Inspired by Nickel Superoxide Dismutase. **Huaibo Ma**[1], Swarup Chattopadhyay[1], Jeffrey L. Petersen[2] and Michael Jensen[1], (1)Ohio University, (2)West Virginia University

2:45 **86** Mixed Cyano-Thiolato-Complexes of Gold(III) and Gold(I): Relevance to Chrysotherapy Metabolites. **C. Frank Shaw III**, Philip M. Yangyuoru, Adam Manthey, Jennifer O'Neill, Kelly Anne Teske and Julie Minser, Illinois State University

3:10 Break.

3:30 **87** Mechanism of Hydrogen Production by [Fe-Fe]-Hydrogenase in DdH and CpI: A QM/MM Study. **Steven Trohalaki** and Ruth Pachter, Air Force Research Laboratory

3:55 **88** New Catalysts for Electroreduction of Oxygen. **Sachin Kumar** and Shouzhong Zou, Miami University

4:20 **89** Application of Conducting Polymer – to Repair CdS - CdTe Photovoltaic Devices. **Misle Tessema**, University of Toledo

4:45 **90** Reducing CO2 to Methane Under Visible Light Illumination by Non-Stoichiometric Mixed Phase Titania Thin Films. **Le Chen**[1], Gonghu Li[2], Michael.E Graham[1], Paul DeSario[1] and Kimberly. A Gray[1], (1)Northwestern Univ., (2)Yale University

Wednesday, June 11, 2008, 9:30 AM - 5:30 PM
General Organic Chemistry I - Contributed Talks
Madison (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presiders: Arthur Winter, The Ohio State University, Jordan L. Fantini, Denison University

9:30 **91** Biotinylated Bi- and Tetra-Antennary Glycoconjugates for Escherichia Coli Detection. **Duane M. Hatch**, Ramesh Kale, Alison A. Weiss and Suri Iyer, University of Cincinnati

9:55 **92** Synthesis of Glycoconjugates for Capturing Shiga Toxins. **Ashish A. Kulkarni**, Cindy Fuller, Michael Flagler, Alison A. Weiss and Suri S Iyer, University of Cincinnati

10:20 **93** Unexpected Cu-Mediated Tandem Cyclization. **Hwan Jung Lim** and T. V. RajanBabu, The Ohio State University

10:45 Break.

11:05 **94** Synthesis of Mono- and Bi-Antennary Biotinylated Carbohydrates for the Study of Carbohydrate-Protein Binding Interactions. **Dan M. Lewallen**, David Siler and Suri S. Iyer, University of Cincinnati

11:30 **95** Structure Activity Relationship Studies towards the Understanding of Active Site Residues in Paraoxonase-1: Experimental and Computational Studies. **Siva Muthukrishnan**, Vivekanand Shete, Toby T. Sanan, Lauren M. Porter, Thomas J. Magliery and Christopher M. Hadad, The Ohio State Unversity

11:55 **96** Synthesis and Antibiotic Testing of 5-Aryl-3-Oxo-δ-Lactones. **David Baudo**, Elizabeth Nguyen and Brad Andersh, Bradley University

12:20 Lunch.

1:30 **97** Synthesis and Biological Evaluation of Digallates and Related Tannins. **Jennifer J. Vogel**[1], Maria M. Puscau[1], Mark Warnock[2], Jacqueline M.

Cale[2], Daniel A. Lawrence[2] and Cory D. Emal[1], (1)Eastern Michigan University, (2)University of Michigan Medical School

1:55 **98** Chemical Exploration of the 9-(2,2,2-Triphenylethylidene)-Fluorene Moiety. **Daniel J. Phillips**, Melanie D. Ward, Dino R. Phillippi, Shannon L. Smuck, Jennifer C. Miller, Amanda M. Law and Tiffany R. Furbee, Bethany College

2:20 **99** Synthesis of the C31-C46 Domain of 45,46-Dehydrobromo-33-*O*-Methoxy Phorboxazole a. **Lynn M. Weyer** and Craig J. Forsyth, Ohio State University

2:45 **100** Synthesis of a Panel of Glycoconjugates for Capture of Shiga Toxins. **Sujit S. Mahajan** and Suri Iyer, University of Cincinnati

3:10 **101** Facile Approach to the Total Synthesis of Largazole. **Bo Wang** and Craig J. Forsyth, The Ohio State University

3:35 Break.

3:50 **102** Synthesis of ABO Blood Group Saccharides. **Chengfeng Xia**, Yalong Zhang and Peng George Wang, The Ohio State University

4:15 **103** Novel Microbial Transformations of Bioactive Natural Products. **Athar Ata** and Jordan Betteridge, The University of Winnipeg

4:40 **104** Total Synthesis of Azaspiracid-3. **James Xu**[1], Yue Ding[1], Son T. Nguyen[2] and Craig J. Forsyth[1], (1)The Ohio State University, (2)University of Illinois Urbana-Champaign

5:05 **105** Glycomacromolecules in Medical Applications:. **Yalong Zhang**, Peng George Wang and Andre F. Palmer, The Ohio State University

Wednesday, June 11, 2008, 9:30 AM - 5:30 PM
Homogeneous Catalysis
Sponsor: ACS Division of Organic Chemistry
Franklin A (Hyatt Regency Columbus)

Organizer: James P. Stambuli, The Ohio State University

9:30 Introductory Remarks.

9:35 **106** Effects of Ligand Steric and Electronic Properties on Metal-Catalyzed Cross-Coupling Reactions. **Kevin H. Shaughnessy**, The University of Alabama

10:05 **107** Development of Transition Metal-Catalyzed Synthetic Methodologies. **Vladimir Gevorgyan**, University of Illinois at Chicago

10:35 **108** N-Heterocycle Carbenes (NHC) - Copper Complexes Synthesis and Theoretical Studies. **Hector Palencia** and James S. Poole, Ball State University

10:55 Break.

11:10 **109** Capitalizing on Terphenyl Scaffolds for Ligands and Catalysts. **John Protasiewicz**, Case Western Reserve University

11:40 **110** Ruthenium-Catalyzed Cross-Metathesis Reactions of Directly Functionalized Olefins. **Marc J. A. Johnson**, Marisa L. Macnaughtan, J. Brannon Gary, Kuei-Nin Tseng, Stephen R. Caskey and Jeff W. Kampf, University of Michigan

12:10 **111** Gold-Catalyzed Double Migration Cascades toward Naphthalenes and 1,3-Dienes. **Alexander S. Dudnik**, Todd Schwier and Vladimir Gevorgyan, University of Illinois at Chicago

12:30 Lunch Break.

1:30 Introductory Remarks.

1:35 **112** Catalyzed Cyclization Reactions Leading to Enrichment of Functionality and Chirality. **T.V. RajanBabu** and Ramakrishna Reddy Singidi, The Ohio State University

2:05 **113** Copper Nitrenes in Catalytic C-H Bond Amination. **Timothy H. Warren**, Yosra M. Badiei, Raymond T. Gephart and Mohammad Ali, Georgetown University

2:35 **114** New Palladium Catalyzed Reactions for the Stereoselective Synthesis of Heterocycles. **John P. Wolfe**, University of Michigan

3:05 Break.

3:20 **115** Solving the Mysteries of Catalyst Deactivation in Palladium-Catalyzed Cyanation of Haloarenes: An Illustration of How Mechanistic Understanding Can Benefit Practical Catalysis. **Vladimir V. Grushin**[1], William J. Marshall[1], D. Cristopher Roe[1], Stefan Erhardt[2], Alison H. Kilpatrick[2] and Stuart A. Macgregor[2], (1)E. I. DuPont de Nemours and Co., Inc., (2)Heriot-Watt University

3:50 **116** Developing An Asymmetric Hydroboration Catalyst Using Supramolecular Self-Assembly. Shin Moteki[1], Andrea E. Holmes[2] and **James M. Takacs**[1], (1)University of Nebraska-Lincoln, (2)Doane College

4:20 **117** PEPPSI-Like Vs. Palladium Allyl-Chloride Monomeric Complexes in the Suzuki- Miyaura Coupling of Aryl Halides. Hector Palencia, Bruce N. Storhoff and **Randall T. Short**, Ball State University

4:40 **118** Sila Morita-Baylis-Hillman Reaction of Cyclopropenes. **Alexander Trofimov**, Stepan Chuprakov, Denis Malyshev and Vladimir Gevorgyan, University of Illinois at Chicago

5:00 **119** Calcium-Catalyzed Pictet-Spengler Reactions. **James P. Stambuli**, The Ohio State University and Matthew J. Vanden Eynden, Ohio State University

Wednesday, June 11, 2008, 9:30 AM - 5:30 PM
Women In Science
Sponsor: Procter & Gamble and Cincinnati Local Section of the ACS
Franklin C (Hyatt Regency Columbus)

Organizer: Samantha Horvath, The Ohio State University

9:30 **120** Title: Is It Possible to Reconcile Your Role as a Scientist and as a Woman: Successes and Challenges. **Valeriana Moeller**, Columbus State Community College

10:15 **121** Impact of Solvent-Solute Interactions upon the Photophysical Properties of Sunscreen Active Ingredients. **Sarah J. Schmidtke**, College of Wooster

11:00 Break.

11:15 **122** Women Chemistry Students' Perceptions of Academic Careers. **Megan L. Grunert** and George M. Bodner, Purdue University

11:45 **123** Exploring the Mechanics of Microtubules by Molecular Simulations. **Ruxandra Dima**, University of Cincinnati

12:30 Women in Science Luncheon (Peppercorn Room).

1:30 **124** Science That Really Matters to P&G's Global Consumers. **Sherrie A. Campbell**, Procter & Gamble

2:15 **125** Preparation and Distillation of Medicines by Early Modern Women. **A. L. Wilson**, Oolong Informatics

2:45 Break.

3:00 Panel Discussion. Breaking Down Barriers and Finding Opportunities. Discussion Leader: Deb Ballam. Panelists: Valeriana Moeller, Ruxandra Dima, Rosemary Loza, Sarah Schmidtke, Sherrie Campbell, Raquel Diaz-Sprague.

4:30 Break.

4:45 **126** The Women in Science Day Experience - Reflections along the Way. **Raquel Diaz-Sprague**, The Ohio State University

Wednesday, June 11, 2008, 12:30 PM - 1:30 PM
Women In Science Luncheon
Sponsor: Procter & Gamble and Cincinnati Local Section of the ACS
Peppercorn (Hyatt Regency Columbus)

Organizer: Samantha Horvath, The Ohio State University

Wednesday, June 11, 2008, 1:30 PM - 5:30 PM
ACS Career Services
Franklin D (Hyatt Regency Columbus)

Organizers: Theresa Huston, Chemical Abstracts Service, Columbus, OH, Garretta Rollins, American Chemical Society

Wednesday, June 11, 2008, 1:30 PM - 5:30 PM
Emerging Concepts In Polymer Science and Plastics Engineering I: Synthesis, Modeling and Design
Garfield (Hyatt Regency Columbus)

Organizer: Gustavo A. Carri, University of Akron

Session Overview: The purpose of this session is to present novel concepts and discoveries in the fields of Polymer Science and Plastics Engineering. Contributions in the areas of synthesis, modeling and design will be discussed.

1:30 Introductory Remarks.

1:35 **127** Effect of Silica NANOPARTICLES on the Local Segmental Dynamics in Polyvinylacetate. **Amy Randall**[1], C. G. Robertson[1], C. M. Roland[2] and R. Bogoslovov[2], (1)Bridgestone Americas Center for Research and Technology, (2)Naval Research Laboratory

2:00 **128** Smart Nanocomposite Coatings for Multifunctional Usage. **Mark Soucek**, University of Akron

2:25 **129** Crystallization of Polymers and Influence of Nanofillers. **Rahmi Ozisik** and Xiaofeng Chen, Rensselaer Polytechnic Institute

2:50 Break.

3:05 **130** Conformations, Dynamics and Surface Forces in Self-Assembled Monolayers of Alkanethiols on Au(111). **Taner E. Dirama**, Universal Technology Corporation and Joel A. Johnson, Air Force Research Lab

3:30 **131** Peptide Binding to Inorganic Surfaces and Thermal Transitions of Alkyl Chains on Nanoparticle Surfaces: Computation and Experiment. **Hendrik Heinz**[1], Richard A. Vaia[2], Rajesh R. Naik[2] and Barry L. Farmer[2], (1)University of Akron, (2)Air Force Research Laboratory

3:55 **132** Controlled Free Radical Polymerization of Functional Block Copolymers. **Kevin Cavicchi**, University of Akron

4:20 Break.

4:35 **133** Non-Synthetic Polymer Bio-Modification Using Gold Nanoparticles. **Craig Buckley**, J. T. Westerfield, Michael Boehm, Dr. Kurt W. Koelling and Dr. Jessica O. Winter, The Ohio State University

5:00 **134** Synthesis and Characterisation of a Novel N-Vinylcaprolactam (NVC) Containing Acrylic Acid Terpolymer for Applications in Glass-Ionomer Dental Cements (GIC). **Alireza Moshaverinia**[1], Nima Roohpour[2], Sahar Ansari[2], Ihtesham U. Rehman[2] and Scott R. Schricker[1], (1)Ohio State University, (2)Queen Mary University of London

Wednesday, June 11, 2008, 5:30 PM - 7:30 PM
General Poster Session I
McKinley/Hayes (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University

135 Title: A Study of the Barrier to Free Rotation in Tetramethylurea. **Xiaojian Mao**, West Virginia University

136 Diastereopeptides: A New Approach to Controlling Metal Coordination. **Anna Peacock**[1], Cherilyn E. Pascoe[1], Jeanne A. Stuckey[1], Lars Hemmingsen[2] and Vincent L. Pecoraro[1], (1)University of Michigan, (2)University of Copenhagen

137 Review of Recent Applications of Photocycloaddition Reactions of Nonracemic Compounds. **Wendell L. Dilling**, Central Michigan University

138 Total Synthesis of Histone H3 Acetylated at Lysine 56. **John C. Shimko**, Tiffany V. Sommers and Jennifer J. Ottesen, The Ohio State University

139 Design and Synthesis of Enantiomeric Phosphoramidate Derivatives of Cis Methylene Cylcopropane Analogue of Nucleosides as Prodrugs for Oral Bioavailable Antiviral Agent. **Wei Shen**, John Hilfinger and Jae-Seung Kim, Therapeutic Systems Research Laboratories (TSRL), Inc.

140 Chemically Modified Histones to Study Acetylation at the Nucleosome Dyad. **Mridula Manohar**, Michael G. Poirier and Jennifer J. Ottesen, The Ohio State University

141 Methionine Aminopeptidase Inhibitors as Antibacterial Agents. **Wenlong Wang** and Qi-Zhuang Ye, Indiana University School of Medicine

142 Development of Multi-Turnover Metallopeptides for Efficient Cleavage of HIV-1 mRNA Rev Response Element. **Jeffrey C. Joyner** and James A. Cowan, The Ohio State University

143 Lead Concentrations in Soils at Fruit Orchards in the Grand Rapids Area. **Elizabeth Jensen** and Shannon Henderson, Aquinas College

144 Effects of Oxygen Radicals on Chymotrypsin. **Nathan A. Lubertazza**, Cleveland State University

145 Highly Stable Dendritic Trityl Radicals as Oxygen and pH Probe. **Yangping Liu**, Frederick A. Villamena and Jay L. Zweier, The Ohio State University

146 A De Novo Designed Cu(I) Metalloprotein Having a Strongly pH-Dependent Luminescence. **Xianchun Zhu** and Michael Y. Ogawa, BGSU

147 Measurements of Effective Vapor Diffusion Coefficients in Porous Substrates. **Hongyang Li**, Ali R. Zand, Jennifer Meyers, Elizabeth Bowden, Lars Beholz, Bojan Markicevic, Yuri Sikorski, Matthew S. Sanders and Homayun Navaz, Kettering University

148 Cytotoxicity and Anti-Inflammatory Activity of Polyphenolics. **Kimberly N. Wisman**, Akeysha A. Perkins and Ann E. Hagerman, Miami University

149 Activity Coefficients and Molecular Interactions in Binary Solutions Using a Virial Equation. **S. Alex Studniarz**, Penn State University

150 Variation in Proanthocyanidin Composition with Environmental Conditions. **Michael A. Schmidt**, Melissa A. Moore, Ashley N. Scioneaux and Ann E. Hagerman, Miami University

151 Design, Synthesis, and Biological Activity of Fungicidal Triazin-3-Ones. **Michael T. Sullenberger**, James E. Hunter and Yelena A. Adelfinskaya, Dow AgroSciences

152 Characterization of Soluble Polyphenolic-Protein Complexes. **John D. Trombley**, Megan L. Albertz, Ann E. Hagerman and Neil D. Danielson, Miami University

153 Synthetic Studies of Spiro[Cycloalkane-1,3'-Indolenine] Derivatives. **Sureshbabu Narayanasamy**, Eric Schwartz, Pratiq Akshay Patel and James R Fuchs, College of Pharmacy, The Ohio State University

154 Catalytic Oxidation of Ethanol Vapor Over CuO/Fe2O3 Catalysts. **Guy Litt** and Catherine Almquist, Miami University

155 Block Copolymers Via RAFT Polymerization and Click Chemistry: Designing New Biomaterials. **Thirumamagal B.T.S.** and Scott Schricker, College of Dentistry

156 Developing Novel Photoprotecting Groups. **Stephen A. Sims** and Anna Gudmundsdottir, University of Cincinnati

157 Gas Phase Rearrangements of Some Transition Metal Hetero-Ligand β-Diketonate Complexes; Examining Ligand and Metal Center Effects. **Jordan O. Lerach**, Tara M. Cruickshank and Brian D. Leskiw, Youngstown State University

158 Roles of the TPLH Network in Maintaining the Global Structure of Gankyrin. **Yi Guo**, Chunhua Yuan, Ming-Daw Tsai and Junan Li, The Ohio State University

159 Synthesis of Terphenyl-Based Pincer Ligands. **Paul R. Challen**[1], Man Lung Kwan[1], Thomas F. Spilker[1], Paul M. Schroder[1], James B. Updegraff III[2] and John D. Protasiewicz[2], (1)John Carroll University, (2)Case Western Reserve University

160 Chemoenzymatic Analysis of Bacterial Polysaccharide Biosynthesis. **Robert L. Woodward Jr.**, Wen Yi, Ramu Perali and Peng George Wang, The Ohio State University

161 Synthesis of Pyrimidopyrimidoindole Nucleosides for Use as Fluorescent Probes for Abasic DNA Sites. **Deepa Perera** and Craig J. Miller, Muskingum College

162 To Dissociate or Decompose: A Comparison of Thermal Analysis and Mass Spectrometry. **Calvin Austin** and Brian D. Leskiw, Youngstown State University

163 Aromatic Hydroxylation of 1-Benzylpiperazine by a Carbonyl Oxide, a Chemical Model of Monooxygenase Enzymes. **Shailendra Kumar** and Ajaykumar Mallesha, Governors State University

164 Synthesis and Antimicrobial Comparison of NHC Gold Complexes and Their NHC Silver Precursors. **Tammy Siciliano**, Khadijah Hindi, Doug Medvetz, Matthew Panzner, Amy Milsted and Wiley J. Youngs, University of Akron

165 Progress in the Formation of a Labeled Thialysine Residue to Study the Pka of a Lysine Residue in a Rhodopsin Mimic Using NMR. **Montserrat Rabago-Smith**[1], Sarah Yoon[1], David LeCronier[1], Laci Beltz[1] and Babak Borhan[2], (1)Kettering University, (2)Michigan State University

166 Electrochemical Corrosion Testing of Aluminum Alloys Coated with a Thin-Film Trivalent Chromium Coating. **Ben Lee**, Michigan State University

167 Can My GC-MS Be Sharper Than My Nose?. **John A. Milo**, Roland Riesen and Brian D. Leskiw, Youngstown State University

168 Measurement of Polycyclic Aromatic Hydrocarbons in Dayton, Ohio Using Pine Needles as Passive Samplers. **Timothy A. Tomashuk**, Madhavi Mantha and Audrey E. McGowin, Wright State University

169 Progress towards the Synthesis of 2-Substituted Adenosine Analogs and Their Application in Photochemical Study. **Biswajit Saha** and Matthew S. Platz, The Ohio State University

170 Synthesis and Structure-Activity Relationships of a Series of Polyphenolic Inhibitors of Plasminogen Activator Inhibitor-1. **Paul R. North**[1], Nadine C. El-Ayache[1], Maria M. Puscau[1], Kristi L. Henricks[1], Nicolas R. Stoyanovich[1], Seo J. Oh[1], Mark Warnock[2], Jacqueline M. Cale[2], Daniel A. Lawrence[2] and Cory D. Emal[1], (1)Eastern Michigan University, (2)University of Michigan Medical School

171 Substrate Specificity of IPP Isomerase in Moths. **Ryan Denton**[1], Stephanie Sen[1], Michel Cusson[2], Catherine Béliveau[2] and Dring Crowell[1], (1)IUPUI, (2)Natural Resources Canada

172 The Synthesis of Fmoc-TAG Phosphoramidite and Its Application in Solid Phase DNA Library Synthesis. **Lihua Nie**, Mohosin Sarkar and Thomas J. Magliery, The Ohio State University

173 The Design and Synthesis of Pyridine Bisphosphonates as Selective Inhibitors of Lepidopteran Fpps. **Corey Trobaugh** and Stephanie Sen, IUPUI

174 Molecular Conformation and Dynamics of the Y145Stop Variant of Human Prion Protein in Amyloid Fibrils. **Jonathan J. Helmus**[1], Krystyna Surewicz[2], Philippe S. Nadaud[1], Witold K. Surewicz[2] and Christopher P. Jaroniec[1], (1)Ohio State University, (2)Case Western Reserve University

175 Magic-Angle Spinning Solid-State NMR Studies of Paramagnetic Proteins. **Philippe S. Nadaud**, Jonathan J. Helmus, Nicole Hoefer and Christopher P. Jaroniec, The Ohio State University

176 Synthesis and Structure-Activity Relationship Study of Isoglobotrihexosylceramide Analogues. **Wenlan Chen**, The Ohio State University

177 Studies on the Binding and Iron Delivery of Human Frataxin to Its Partners. **Jia Huang**, The Ohio State University and J. a. Cowan, Ohio State University

178 ATCUN-Metal Complexes as Catalytic Inactivators of RNA and Enzymes. **Seth S. Bradford**, The Ohio State University

179 Fenton-Type Chemistry in the Ascorbate-Benzoate System. **Roderick M. Macrae** and Ryan J. Bernhardt, Marian College

180 Vibrationally-Corrected Hyperfine Parameters for Isotopically Substituted Group 6A Hydride Radicals: Computational Studies. **Roderick M. Macrae**, Marian College

181 Structure-Function Studies on B. Anthracis N5-Carboxyaminoimidazole Ribonucleotide Mutase (PurE), a Critical Purine Biosynthesis Pathway Enzyme. **Anjali Mahajan**, Shahila Mehboob and Michael E. Johnson, University of Illinois at Chicago

182 The Oxidation of Tyrosine Mediated by Metal-ATCUN Complexes. **Lalintip Hocharoen** and James A. Cowan, the Ohio State University

183 Re-Engineering a Split-GFP Reassembly Screen to Examine RING-Domain Interactions Between BARD1 and BRCA1 Mutants Observed in Cancer Patients. **Mohosin Sarkar** and Thomas J. Magliery, The Ohio State University

184 Flexible and Precise Control of Multi-Phase Laminar Flow for 3D in-Channel Microfabrication. **Yunxiang Gao** and Liwei Chen, Ohio University

185 Expression of α1,2-Fucosyltransferase from *Escherichia Coli* O128:B12 and Applied in Enzymatic Synthesis of Fucosylated Lactose. **Xianwei Liu** and Guangyan Zhou, The Ohio State University

186 Large Scale Enzymatic Synthesis of Oligosaccharides. **Guangyan Zhou**, Xianwei Liu, Doris Su, Lei Li and Peng George Wang, The Ohio State University

187 Elucidation of the Proton Pumping Mechanism for Cytochrome bo_3 Oxidase Using Solid-State NMR. **Heather L. Frericks Schmidt**[1], Myat T. Lin[1], Lai Lai Yap[2], Gautam J. Shah[1], Robert B. Gennis[1] and Chad M. Rienstra[1], (1)University of Illinois at Urbana-Champaign, (2)A-Star Institute for Molecular and Cell Biology

188 Chemical Shift Assignments and Functional Dynamics Measurements of Microcrystalline DsbA, a 21 kDa *E. Coli* Enzyme. **Lindsay J. Sperling**, Deborah A. Berthold, Benjamin J. Wylie and Chad M. Rienstra, University of Illinois at Urbana-Champaign

189 NMR Studies of the cAMP-Regulated Phosphoprotein Endosulfine-Alpha. **John M. Boettcher**, Kevin L. Hartman, Daniel T. Ladror, Wendy S. Woods, Julia M. George and Chad M. Rienstra, University of Illinois Champaign-Urbana

190 Small Molecule Interactions with Alpha-Synuclein Characterized by Fluorescence and Solid-State NMR Spectroscopy. **Luisel Rodriguez**, Kathryn Kloepper and Chad M. Rienstra, University of Illinois at Urbana Champaign

191 A Single Amino Acid Residue Mutation of the Human Islet Polypeptide Completely Suppresses Its Toxicity. **Kevin M. Hartman**, Jeffrey R. Brender and Ayyalusamy Ramamoorthy, University of Michigan

192 Magic-Angle Spinning Solid-State NMR Spectroscopy of Nanodisc–Embedded Human CYP3A4. **Aleksandra Z. Kijac**, Ying Li, Stephen G. Sligar and Chad M. Rienstra, University of Illinois at Urbana-Champaign

193 Comparative Investigation of Forest Soil Organic Matter and Natural Plant Inputs as Determined by High Resolution Magic Angle Spinning Nuclear Magnetic Resonance. **Jeffrey W. Turner**, The Ohio State University - Marion and Patrick G. Hatcher, Old Dominion University

194 Overexpression, Purification and Characterization of Human HscA. **Wen-I Luo**, Eric Dizin, Taejin Yoon and James A. Cowan, The Ohio State University

195 Synthesis of α,α - Difluoroalkenes Using Cross-Metathesis and Wittig Approaches. **Matthew L. Barchok**, Alexander J. Seed and Paul Sampson, Kent State University

196 Preparation of New Polymerizable Dithienylethene Chromophores and Their Photochromic Polymer Films. **Thilini K. Mudiyanselage** and Douglas C. Neckers, Bowling Green State University

197 Behavior of a Class II Small Heat Shock Oligomeric Complex from Maize. **Hannah S. Tims**[1], Virginia B. Pett[1], Tamutenda C. Chidawanyika[1] and Robert A. Bouchard[2], (1)The College of Wooster, (2)OARDC

198 Controlling Metal Coordination Number and Metal Exchange in *De Novo* Designed Three-Stranded Coiled Coil Peptides. **Saumen Chakraborty**[1], Olga Iranzo[1], Lars Hemmingsen[2] and Vincent L. Pecoraro[1], (1)University of Michigan, (2)University of Copenhagen

199 Phenylacetylene Based Materials: Enhanced Emission in Nanoparticles and Solid-State. **Sujeewa S. Palayangoda** and Douglas C. Neckers, Bowling Green State University

200 In Vivo Incorporation of An Unnatural Amino Acid to Trap Protein Interactions in Yeast. **Christina K. Harsch** and Thomas J. Magliery, The Ohio State University

201 Novel Mixed-Anion Colossal Magnetoresistive Materials. **Anita Dasu** and Timothy R. Wagner, Youngstown State University

202 Characterization of Bacterial ProRS and Its Editing Domain Homologues in Vitro and in Vivo. **Mom Das**, Ohio State Biochemistry Program, The Ohio State University and Karin Musier-Forsyth, The Ohio State University

203 Studies in Mixed Anionic Systems. **Harry A. Seibel II**, The Ohio State University

204 Formaldehyde and Sulfur Dioxide Detection by Using Laser-Induced Fluorescence. **Ravi K. Boddeti**, Anand Matta and Josef B Simeonsson, Youngstown State University

205 Formaldehyde and Sulfur Dioxide Detection by Using Laser Induced Fluorescence Technique. **Anand Matta**, Ravi K. Boddeti and Joseph B Simeonsson, Youngstown State University

206 Synthesis of Globo-H Hexasaccharide, a Tumor-Associated Carbohydrate Antigen, by Glycosyltransferases. **Doris M. Su**, Hironobu Eguchi, Wen Yi, Chengfeng Xia and Peng George Wang, The Ohio State University

207 Fabrication and Characterization of Substrate Materials for Trace Analytical Measurements by Surface Enhanced Raman Scattering (SERS) Spectroscopic Techniques. **Naresh Kumar Boddu**, Pratima Vabbilisetty and Josef B. Simeonsson, Youngstown State University

208 "Fabrication and Characterization of Substrate Materials for Trace Analytical Measurements by Surface Enhanced Raman Scattering Techniques". **Pratima Vabbilisetty**, Naresh Kumar Boddu and Josef B Simeonsson, Youngstown State University

209 Solid-State Photolysis of Arylazides Produces Trans-Arylazo Dimers in High Stereoselective Yield. **Qian Li** and Anna D. Gudmundsdottir, University of Cincinnati

210 Hydrogen Abstraction in Triplet Nitrenes. **Jagadis Sankaranarayanan**, Sridhar Rajam and Anna D. Gudmundsdottir, University of Cincinnati

211 Hydride Generation and Laser Spectroscopy for Trace Measurements of Antimony, Selenium and Tellurium. **Sandeep Kunati**, Sangeetha Chari and Josef Simeonsson, YOUNGSTOWN STATE UNIVERSITY

212 Hydride Generation and Laser Spectroscopy for Trace Analytical Measurements of Antimony, Selenium and Tellurium. **Sangeetha Chari**, Sandeep Kunati and Josef Simeonsson, YOUNGSTOWN STATE UNIVERSITY

213 Hunting for Physiologically Relevant Inhibitors of Methionine Aminopeptidase. **Sergio C. Chai** and Qi-Zhuang Ye, Indiana University School of Medicine

214 Electron Transfer Dynamics Between 9-Anthracenecarboxylic Acid and TiO2 Nanoparticles with Applications for Novel Photovoltaic Devices. **Lynetta M. Mier**, Yagnaseni Ghosh, Austin R. Carter, Malcolm H. Chisholm, Arthur J. Epstein and Terry L. Gustafson, Ohio State University

215 Synthesis, Photolysis and Characterization of Products and Intermediates of 1-(4-Diazidomethyl-phenyl)-Ethanone. **R. A. A. Upul Ranawera**, Bruce S. Ault and Anna D. Gudmundsdottir, University of Cincinnati

216 Direct Detection of Triplet Alkene 1,2 Biradicals in β,γ Unsaturated Ketones by Laser Flash Photolysis. **Sridhar Rajam**, Erin McGreevy, Michelle Masnovi and Anna D. Gudmundsdottir, University of Cincinnati

217 Analysis of Hydrogen Peroxide-Fe (II)-Mediated Linoleic Acid Peroxidation Products by GC-MS: Development of a Biochemistry Lab Experiment. **Michael A. Nichols** and Devin C. Hale, John Carroll University

218 In Vitro Continuous Amperometric Measurement of 5-Hydroxytryptamine Using Diamond Microelectrodes. **A. Bryan Davis**, Michigan State University

219 Binding Modes of Pyridinium Oximes with Acetylcholinesterase: Importance of Aromatic Residues Elucidated by Ligand-Receptor Docking Studies. **Jeremy M. Beck**, Shubham Vyas and Christopher M. Hadad, The Ohio State University

220 Mechanism of Photochemical Ring Opening of Bicyclopentyl and Oxabicyclopentyl Aryl Ketones. **Krishna Panthi** and Thomas H. Kinstle, Center for Photochemical Sciences, Bowling Green State University

221 Isolation and Purification of a Secondary Alcohol Dehydrogenase (3-hydroxyacyl CoA dehydrogenase) from Micrococcus Luteus WIUJH20. **J. -K Huang**, Nicholas Youngblut, Babu Ram Dhungana, J. K. Park and Lisa Wen, Western Illinois University

222 Photolysis of Cis-1-Azido-1-Phenyl-1-Propene. **Xiaoming Zhang**, Sridhar Rajam and Anna Gudmundsdottir, University of Cincinnati

223 Structural Analysis of the Critical Role of His18 in the Toxicity of Islet Amyloid Polypeptide. **Stephanie V. Le Clair**, Khoi Nguyen, Jeffrey Brender, Ravi Nanga, Zhan Chen and Ayyalusa Ramamoorthy, University of Michigan

224 Regioselective Synthesis of Furans and Pyrones Via Ionic Liquid Catalysis. **Jeanne L. Kuhler**, Robey T. Brooks, Krystal D. Holley and Brandi L. Inman, Auburn University

225 Solid-State NMR of Lanthanide Acetylacetonates. **Janet H. Gaba** and Joseph R. Sachleben, Otterbein College

226 Solid-State NMR of Rare-Earth Aluminosilicate Glasses and Nanocrystals. **Shay M. Smith**, Celeste Savitski, Alexanne Holcombe and Joseph R. Sachleben, Otterbein College

Thursday, June 12, 2008

Thursday, June 12, 2008, 7:00 AM - 8:00 AM
ACS Directors Breakfast
Peppercorn (Hyatt Regency Columbus)

Organizer: Diane Schmidt, Procter & Gamble Co.

Thursday, June 12, 2008, 8:00 AM - 8:45 AM
Plenary Lecture: Robert Massie, Chemical Abstracts Service, President
Franklin A (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Prabir K. Dutta, The Ohio State University

8:00 **227** Chemical Information: Yesterday, Today and Tomorrow. **Robert J. Massie**, Chemical Abstracts Service

Thursday, June 12, 2008, 8:45 AM - 9:15 AM
Plenary Lecture on Education - Desmond Stubbs
Franklin A (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Prabir K. Dutta, The Ohio State University

8:45 **228** Advancing STEM Education Capacity to Build a Competitive Future for America. **Desmond D. Stubbs**, Battelle and Oak Ridge National Laboratories

Thursday, June 12, 2008, 9:30 AM - 5:30 PM
Advances toward Green Chemistry
Sponsor: ACS Divisions of Environmental Chemistry, Polymer Chemistry, and Inorganic Chemistry
Harrison (Hyatt Regency Columbus)

Organizer: Darcy Culkin, Ashland Inc.

9:30 Welcoming Remarks.

9:35 **229** Ohio BioProducts Innovation Center. **Stephen Myers**, Ohio State University

10:00 **230** Development of Polyurethane and Unsaturated Polyester Resins from Soy Oil. **Dwight A. Rust**, Omni Tech International, LTD

10:25 **231** Biomaterials from Vegetable Oils. **Dejan D. Andjelkovic**[1], Mark Hanson[2], Fengqui Li[2], Yongshang Lu[2], Phillip Henna[2], Marlen Valverde[2], Daniel P. Pfister[2], Jeffrey R. Baker[2], Patit P. Kundu[2] and

Richard C. Larock[2], (1)Ashland Performance Materials, (2)Iowa State University

10:50 Break.

11:05 **232** Unsaturated Polyester Resins Derived from Renewable Resources. **Roman Loza**, Darcy A. Culkin and Dejan D. Andjelkovic, Ashland Performance Materials, Division of Ashland Inc.

11:30 **233** Low Cost and Reactive Biobased Polyols: A Co-Product of the Emerging Biorefinery Economy. **Herman P. Benecke**, Bhima R. Vijayendran, Daniel B. Garbark and Katherine P. Mitchell, Battellle Memorial Institute

11:55 **234** Renewably Sourced Materials Based on 1,3-Propanediol: Cosmetics, Functional Fluids, Textiles, and Plastics. **Judith J. Van Gorp**, DuPont

12:20 Lunch.

1:30 **235** Polyesters and Polycarbonates from Renewable Resources: Challenges in Catalysis. Malcolm H. Chisholm and **Ruaraidh D. McIntosh**, Ohio State University

1:55 **236** A Green Continuous Reaction to Modify Biodegradable Polylactic Acid (PLA). **James H. Wang**, Kimberly-Clark Corporation

2:20 **237** Alkyds for the 21st Century. **Mark Soucek**, University of Akron

2:45 **238** Ionic Liquids as Unconventional Media for Carbocation and Onium Ion Chemistry. **Kenneth K. Laali**, Kent State University

3:10 Break.

3:25 **239** Chemistry of Neutralization of Red Mud Using H2S. **Rajkishore Patel**, NIT

3:50 **240** Mechanochemistry: Past, Present and Future. **James Mack**, Dennis A. Fulmer, Daniel C. Waddell, William C. Shearouse, Maxwell Shumba and Philip A. Vogel, University of Cincinnati

4:15 **241** Aqueous-Phase Palladium-Catalyzed Cross-Coupling: Seeking Highly Active, Easily Recovered, and Recyclable Catalyst Systems. **Kevin H. Shaughnessy**, The University of Alabama

4:40 **242** Aerobic Oxidation of Alcohols and Amines by a Nickel-Organic Redox Hybrid. **Michael J. Baldwin**, University of Cincinnati

5:05 **243** The Green Organic Laboratory Curriculum at Marian College: Implementation, Integration, and Sustainability. **Carl S. Lecher**, Marian College

Thursday, June 12, 2008, 9:30 AM - 12:30 PM
Biomolecular Solid-State NMR Spectroscopy II
Sponsors: Bruker Corporation, Varian, Cambridge Isotopes Laboratories, ISOTEC/Sigma-Aldrich, and ACS Division of Physical Chemistry

Franklin A (Hyatt Regency Columbus)

Organizer: Christopher Jaroniec, The Ohio State University

9:30 **244** Solid-State NMR Structural Measurements of (1) Membrane-Associated Viral Fusion Peptides and Proteins and (2) Inclusion Body Proteins. Wei Qiang, Jaime Curtis-Fisk, Ryan M. Spencer and **David P. Weliky**, Michigan State University

10:00 **245** Determination of 13C Shift Tensor Orientations Using Heteronuclear Dipolar Recoupling MAS NMR. **Manish Mehta**, Oberlin College and Anil Mehta, Emory University

10:30 **246** Atomic Resolution Protein Structure Determination through the Use of TEDOR Solid-State NMR Spectroscopy. **Andrew J. Nieuwkoop**, Benjamin J. Wylie, W. Trent Franks, Gautam J. Shah and Chad M. Rienstra, University of Illinois at Urbana-Champaign

10:45 Break.

11:00 **247** Exploring Boundaries of Solid-State NMR: Structure and Spectroscopy of Amyloid Proteins and Paramagnetic Systems. **Yoshitaka Ishii**, University of Illinois at Chicago

11:30 **248** Dipolar Recoupling with a Switched-Angle Probe. **Terry Gullion** and Eugene Mihaliuk, West Virginia University

12:00 **249** New Techniques and Applications in Biomolecular Solid State NMR. **Robert Tycko**, National Institutes of Health

Thursday, June 12, 2008, 9:30 AM - 12:30 PM
Emerging Concepts In Polymer Science and Plastics Engineering II: Synthesis, Modeling and Design
Franklin B (Hyatt Regency Columbus)

Organizer: Gustavo A. Carri, University of Akron

Session Overview: The purpose of this session is to present novel concepts and discoveries in the fields of Polymer Science and Plastics Engineering. Contributions in the areas of synthesis, modeling and design will be discussed.

9:30 Introductory Remarks.

9:35 **250** Bio-Inspired Dynamic Nanocomposites. **Stuart J. Rowan**, Jeff Capadona, Kadhiravan Shanmuganathan and Christoph Weder, Case Western Reserve University

10:00 **251** Poly (ethylene glycol)-Poly (caprolactone) Hydrogels for Drug Delivery. **Elise Ferguson**, Mike Owens and Dr. Jessica O. Winter, The Ohio State University

10:25 Break.

10:40 **252** Engineering Design of Polyhydroxyalkanoates with Controlled Properties. **Yvonne Akpalu**, Rensselaer Polytechnic Institute

11:05 **253** Achieving High Proton Conductivities In Polymer Electrolyte Membranes for Fuel Cells Applications. **Thuy D. Dang**, Wright-Patterson AFB

Thursday, June 12, 2008, 9:30 AM - 12:30 PM
Frontiers of Protein and Peptide Engineering II
Sponsor: ACS Divisions of Biochemical Technology and Biological Chemistry
Garfield (Hyatt Regency Columbus)

Organizers: Dennis Bong, The Ohio State University, Thomas J. Magliery, The Ohio State University

9:30 **254** Enzymatic Synthesis of Protein Conjugates. **Mark D. Distefano**, University of Minnesota

10:05 **255** Redox Tuning Over Almost 1 V with Retention of Structure. **Anne-Frances Miller**[1], Emine Yikilmaz[1], Laurie E. Grove[2], Gloria E. O. Borgstahl[3], David W. Rodgers[1] and Thomas C. Brunold[2], (1)University of Kentucky, (2)University of Wisconsin, (3)University of Nebraska Medical Center

10:40 **256** Correlation of Glide® Docking Energies with Spectroscopic Kinetic Assays of Xanthine Oxidase and Potential Inhibitors. Tarek Mahfouz, Brad Petersen, Rajvi Patel and **Amy Stockert**, Ohio Northern University

11:00 Break (Morning).

11:15 **257** Design of Metalloproteins: The Effect of Secondary Structure and Biosensing Applications. **David E. Benson**, Calvin College

11:50 **258** Synthetic Tools to Probe Histone Modifications in the Nucleosome Core. **Jennifer J. Ottesen** and Michael G. Poirier, The Ohio State University

12:25 Farewell (Morning).

Thursday, June 12, 2008, 9:30 AM - 12:30 PM
General Organic Chemistry II - Contributed Talks
Franklin C (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Ksenija D. Glusac, Bowling Green State University

9:30 **259** Low Temperature Nitrile Oxide Cycloadditions. **David G.J. Young**, Ophilia Toh and James W. Hickerson, East Tennessee State University

9:55 **260** Recent Developments in the Allene INOC Reaction. **David G.J. Young**, East Tennessee State University, Dongxiang Zeng, University of Tennessee, Knoxville and Joseph A. Burlison, Synta pharmaceuticals

10:20 **261** Corannulene Based Materials. **Praveen Bachawala**[1], James Mack[1] and Felicia Fullilove[2], (1)University of Cincinnati, (2)Butler University

10:45 Break.

11:05 **262** Polymer-Bound Hydroxybenzotriazole-Based Synthesis and GC Analysis of Benzylamides from Biogenic Amines. **Smitha Vokkaliga**[1], William LaCourse[1] and Aristotle Kalivretenos[2], (1)University of Maryland, Baltimore County, (2)Aurora Analytics LLC

11:30 **263** Efficient, Catalytic and Green: Catalyst Tuning for Highly Enantioselective Reactions of Ethylene. **Craig R. Smith** and T.V. RajanBabu, The Ohio State University

11:55 **264** Methylene-Bridge Functionalized Calix[4]Arenes: Routes to "Click-Chemistry" Reactants and to Dicalixarenes. **Jordan L. Fantini**, Michael J. Hardman and Samantha A. Williams, Denison University

Thursday, June 12, 2008, 9:30 AM - 5:30 PM
General Physical Chemistry - Contributed Talks
Marion (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Annabel M. Edwards, Denison University

9:30 **265** Thermal and Photochemical Generation of Carcinogenic Nitrobenzo[a]Pyrenoxy Radicals from Nitrobenzo[a]Pyrenes: A Computational Investigation. **Shubham Vyas**, Prabir K. Dutta and Christopher M. Hadad, The Ohio State University

9:55 **266** Pka Prediction the SMARTS Way. **Adam C. Lee**, Jingyu Yu and G.M. Crippen, University of Michigan

10:20 **267** The Origin of Slow Solvation Dynamics in Protein Water Systems. **Ali A. Hassanali**, Tanping Li, Dongping Zhong and Sherwin Singer, The Ohio State University

10:45 Break.

11:05 **268** Excited States of CH_5^+ by Group Theoretical Methods. **Charlotte Hinkle** and Anne B McCoy, The Ohio State University

11:30 **269** Dynamics of Atomic and Small Molecule Scattering from Self-Assembled Monolayers. **William A. Alexander**, John R. Morris and Diego Troya, Virginia Tech

11:55 **270** Surface Plasmon-Enhanced Infrared Spectroscopy of Thin Liquid and Solid Films on Nickel Mesh. **Joseph M. Heer**, Hong Tian, Katherine E. Cilwa, Kenneth R. Rodriguez and James V. Coe, Ohio State University

12:20 Lunch.

1:30 **271** Cyclobutane Pyrimidine Dimer Formation in Oligonucleotides: Effects of Base Stacking and Base Pairing. **Yu Kay Law**, Marc P. Coons, Javad Azadi and Bern Kohler, The Ohio State University

1:55 **272** Comparison of Thermodynamic Properties for a Series of Cycloalkanes. **Mike L. Renier**, Chemmeds

2:20 **273** Statistical Theory of Asteroid Escape Rates. **Charles Jaffé**[1], Shane D. Ross[2], Martin W. Lo[3], Jerrold Marsden[2], David Farrelly[4] and Turgay Uzer[5], (1)West Virginia University, (2)California Institute of Technology, (3)Jet Propulsion Laboratory, (4)Utah State University, (5)Georgia Institute of Technology

2:45 **274** Acid - Base Chemistry of Clay Nanoparticles for Supporting Myoglobin Electroactivity and Multi Conformation Continuum Electrostatics (MCCE). **Foster A. Amoako**, PLC Inc.

3:10 **275** Constant Energy DFT Molecular Dynamics Simulations of Solvated Carbohydrates at the B3LYP/6-31+G* Level of Theory. **Frank Momany**, Udo Schnupf and J. L. Willett, National Center for Agricultural Utilization Research

3:35 Break.

3:55 **276** Monte Carlo Modeling of Solution Structures with Small Organic Solutes in Pure and Mixed Solvents. **Peter I. Nagy**[1], Paul W. Erhardt[1], Gergely Völgyi[2] and Krisztina Takács-Novák[2], (1)University of Toledo, (2)Semmelweis University

4:20 **277** Theory and Simulation of Multidimensional Optical Spectra. **Porscha L. McRobbie** and Eitan Geva, University of Michigan

4:45 **278** Complex Time Velocity Autocorrelation Functions for Lennard-Jones Fluids with Quantum Pair-Product Propagators. **Jeb S. Kegerreis**[1], Akira Nakayama[2] and Nancy Makri[1], (1)University of Illinois at Urbana-Champaign, (2)Hokkaido University

Thursday, June 12, 2008, 9:30 AM - 12:30 PM
High School Teachers Education Program I
Sponsor: Battelle and ACS Division of Chemical Education
Grant/Harding (Hyatt Regency Columbus)

Organizers: Ted Klupinski, Battelle, Jodie Harper, Battelle

Session Overview: This program is designed to provide high school chemistry teachers with "real-world chemistry" content to use in the classroom. Lectures and laboratory workshops will be presented by scientists and by high school science teachers who have taught the subject matter to their students.

9:30 Introductory Remarks.

9:35 **279** Simply Science: A Research and Service Group. **Claire Baker**, Brebeuf Preparatory School

9:55 **280** Basic Education-Higher Education Science Partnerships. **Don Mitchell**, Juniata College

10:40 Break.

10:50 **281** The Real CSI. **Jami St. Clair**, Columbus Police Crime Laboratory

11:20 **282** Production and Properties of Biodiesel in a Classroom Setting. **Elizabeth Golowenski**, Olentangy Liberty High School

11:50 **283** Nanotechnology in the High School Classroom. **J. Aaron Frim**, The Wellington School

12:10 **284** Arsenic in the Water!. **Marie Wenzke**, South-Western Career Academy and Angela Paolucci, Battelle

Thursday, June 12, 2008, 9:30 AM - 12:40 PM
Undergraduate Education and the REEL Program I
Franklin D (Hyatt Regency Columbus)

Organizers: Ted M. Clark, The Ohio State University, Patrick M. Woodward, The Ohio State University

9:30 **285** Improving Student Learning in the Organic Laboratory. **David Baker**, Delta College

9:55 **286** Teaching Quantitative Analysis: The Old, the New, and the Bold. **Doris Zimmerman**, Penn Ohio Border Section

10:20 **287** Analysis of the Enantiomeric Composition of Linalool in a Variety of Essential Oils Using Proton NMR and GC-MS. **Michael A. Nichols**, John Carroll University

10:45 Break.

11:00 **288** Prebiotic Chemistry of Nucleic Acid Sugars? Acetal Formation of D-Ribose and D-2-Deoxyribose Characterized by NMR. Lauren A. Parker and **Thomas A. Evans**, Denison University

11:25 **289** The Use of Camtasia Studio® and a Graphics Tablet in Recording Organic Chemistry Lectures and Their Dissemination as a Form of Asynchronous Learning. **Michael A. Nichols**, John Carroll University

11:50 **290** Molecular Drawing a Method for Developing Student Learning. **David Baker**, Delta College

12:15 **291** Project REEL in AP Chemistry. **Brian M. Urig**[1], Christopher Stabler[1], Tony Ruggear[1] and Ted M. Clark[2], (1)Oxford High School, Oxford, PA, (2)the Ohio State University

Thursday, June 12, 2008, 12:30 PM - 2:15 PM
High School Teachers Lunch
Sponsor: Battelle
Chemistry (The Ohio State University)

Organizer: Jodie Harper, Battelle

Thursday, June 12, 2008, 12:00 PM - 1:30 PM
Steering Committee Luncheon
Peppercorn (Hyatt Regency Columbus)

Organizer: James A. Cowan, Ohio State University

Thursday, June 12, 2008, 1:30 PM - 4:00 PM
Chemistry of Supramolecular Assemblies I
Franklin A (Hyatt Regency Columbus)

Organizer: Jovica D. Badjic, The Ohio State University

Session Overview: This session will involve discussions about advances in physical organic chemistry of medium-sized and large molecular assemblies. The focus is on characterization and dynamic behavior of supramolecular structures as it applies to function.

1:30 **292** Supramolecular Chemistry in Polymeric Systems. **Stuart J. Rowan**, Aryavarta Kumar, Justin Fox, Lauren Buerkle and Roger E. Marchant, Case Western Reserve University

2:00 **293** Cuproamphiphiles as Precursors for Responsive Films. **Claudio N. Verani**, Wayne State University

2:30 **294** Molding the Energy Landscapes of Thermal Reactions with Light. **Roman Boulatov**, University of Illinois

3:00 **295** The Photophysical Properties of Dendritic Porphyrin-Containing Triads. **David A. Modarelli**[1], Tuan Nguyen[1], Jonathan R. Parquette[2] and Dian He[3], (1)The University of Akron, (2)The Ohio-State University, (3)Ohio State University

3:30 **296** Photoinduced Electron Transfer in Hydrogen-Bonded Donor-Acceptor Systems. **Ksenija D. Glusac**[1], Pavel Kucheryavy[1], Guifeng Li[1], Christopher M. Hadad[2] and Shubham Vyas[2], (1)Bowling Green State University, (2)The Ohio State University

Thursday, June 12, 2008, 1:30 PM - 5:30 PM
General Analytical Chemistry II - Contributed Talks
Grant/Harding (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: William J. Clark, Capital University

1:30 **297** High-Throughput Analytical System for Secondary Screening of Heterogeneous Catalysts. **Stacey Beyer**, Billy Bardin, Larry Wright, Mark Dittenhafer, Jeff Larson, Eric Schmidt and Chris Brady, The Dow Chemical Company

1:55 **298** Chemical Safety Awareness for Campus Security Personnel. **John T. Wood** and Roberta M. Eddy, Indiana University of Pennsylvania

2:20 **299** Qualification of New Chlorine Suppliers by Field Portable FTIR. **Wendy C. Flory**, Lamar Dewald, Gary Gellise, Mark Bingham, Todd Beebe and Joseph Bonadies Jr., The Dow Chemical Company Analytical Sciences - Process Analytical

2:45 **300** Nonaqueous Synthesis and Reduction of Diazonium Ions (without Isolation) to Modify Glassy Carbon Electrodes and the Effect on Electron Transfer. **Kristin K. Cline**, Dawn Lockwood and Alison Stalzer, Wittenberg University

3:10 Break.

3:30 **301** Oxygen-Sensing Paramagnetic Properties of Lithium Naphthalocyanine-Based Radical Probes for Biological Oximetry. **Ramasamy P. Pandian**, Michelle Dolgos, Patrick. M. Woodward and Periannan Kuppusamy, Ohio State University

3:55 **302** Ambient Ionization of Amphiphilic Conetworks: A Compartitive Study. **Sara E. Whitson**[1], Gabor Erdodi[1], Joseph P. Kennedy[1], Robert P. Lattimer[2] and Chrys Wesdemiotis[1], (1)The University of Akron, (2)Lubrizol Advanced Materials

4:20 **303** Electrochemical Studies of Horse Heart Cytochrome C on Boron-Doped Diamond Electrodes. **Yingrui Dai**, Denise A. Mills, Denis A. Proshlyakov and Greg M. Swain, Michigan State University

Thursday, June 12, 2008, 1:30 PM - 5:30 PM
General Biological Chemistry I - Contributed Talks
Garfield (Hyatt Regency Columbus)

Organizers: Claudia Turro, The Ohio State University, Thomas J. Magliery, The Ohio State University
Presider: Zhengrong (Justin) Wu, The Ohio State University

1:30 **304** Combinatorial Biophysics: Library Approaches to Hydrophobic Core Repacking of the Four-Helix Bundle Protein Rop. **Jason J. Lavinder**, Sanjay B. Hari and Thomas J. Magliery, The Ohio State University

1:55 **305** Computational Design of STAT3 Inhibitors for Targeted Anti-Cancer Therapy. **Katryna K. Cisek** and Chenglong Li, The Ohio State University

2:20 **306** Development of An Intra-Operative Probe for near-IR Detection of Occult Tissue. **R. Bryan Sears**, Claudia Turro, Joseph Heremans, Duxin Sun and Edward Martin Jr., The Ohio State University

2:45 **307** Nucleic Acid Chaperone Activity of the Feline Immunodeficiency Virus Nucleocapsid Protein. **Dominic F. Qualley** and Karin Musier-Forsyth, The Ohio State University

3:10 Break.

3:30 **308** Protein Engineering from Bioinformatics: The Design and Characterization of a Consensus Triosephosphate Isomerase. **Brandon J. Sullivan** and Thomas J. Magliery, The Ohio State University

3:55 **309** Mechanism of Posttransfer Editing of Mis-Charged Cys-$tRNA^{Pro}$ by Bacterial YbaK. **Byung Ran So**, Meredith Qualley and Karin Musier-Forsyth, Ohio State University

4:20 **310** Novel Ligand-Induced-Fit Simulation of Survivin Via Replica Exchange Molecular Dynamics (REMD) and Receptor-Based Reverse Virtual Screening (VS). **In-Hee Park** and Chenglong Li, The Ohio State University

4:45 **311** Oxygen's Reservoir. **Marvin DeTar**, Molecular Technologies, LTD

Thursday, June 12, 2008, 1:30 PM - 5:30 PM
General Inorganic Chemistry II - Contributed Talks
Franklin D (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Sibrina Collins, College of Wooster

1:30 **312** Syntheses and Photophysical Properties of Thiophenes Incorporating Quadruply Bonded Metal-Metal Complexes. Gotard Burdzinski[1], M. H. Chisholm[1], Pi-Tai Chou[2], **Yi-Hsuan Chou**[1], Yagnaseni Ghosh[1], Terry L. Gustafson[1], Mei-Lin Ho[2], Yao Liu[1], Ramkrishna Ramnauth[1] and Claudia Turro[1], (1)The Ohio State University, (2)National Taiwan University

1:55 **313** The Electrochemical Properties of 100 and 500 Nm Diameter Boron-Doped Diamond Powder Studied Using a Pipette Electrode. **Ayten Ay**, V. Matt Swope and Greg M. Swain, Michigan State University

2:20 **314** Dual Emission from a Ru(II) Complex with a DNA Intercalating Ligand. **Yujie Sun** and Claudia Turro, The Ohio State University

2:45 **315** Heterogeneous Reppé Catalysis of 2-Butyene-1,4-Diol Is a Kinetically Controlled Process with a Strong Dependence on pH. **Alex F. Polley**[1], Dawn M. Makely[2], William E. Schoster[1], Lisa Olson[1], Robert T. Hart Jr.[1] and Richard J. Mullins[3], (1)The Shepherd Chemical Company, (2)Vanderbilt University, (3)Xavier University

3:10 Break.

3:30 **316** Photoinduced Ligand Loss and Photoisomerization of *Cis*-$M(bpy)_2(CN)_2$ (M = Fe, Ru). **David B. Turner**, Yao Liu and Claudia Turro, The Ohio State University

3:55 **317** Synthetic, Electronic and Spectroscopic Studies of Molecular Assemblies with Quadruply Bonded Molybdenum Units. M. H. Chisholm, Nathan Patmore and **Namrata Singh**, Ohio State University

4:20 **318** Lewis and Bronsted Acid-Base Chemistry of [PCl2N]3, the Precursor of Chlorophosphazene Polymers. **Zin-Min Tun**, Amy J. Heston, Matthew J. Panzner, Doug A. Medvetz, Deepa Savant, Peter L. Rinaldi, Wiley J. Youngs and Claire A. Tessier, The University of Akron

4:45 **319** Synthesis and Photophysical Properties of Triply Bonded Dirhenium(II,II) Complexes. **Carly Reed**, Malcolm H. Chisholm and Claudia Turro, The Ohio State University

Thursday, June 12, 2008, 1:30 PM - 4:00 PM
General Organic Chemistry III - Contributed Talks
Franklin B (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Siva Muthukrishnan, The Ohio State Unversity

1:30 **320** GST Inhibiting Natural Products from Medicinal Plants. **Athar Ata**, The University of Winnipeg

1:55 **321** Acetylcholinesterase Inhibition Directed Phytochemical Studies on Various Buxus Species. **Athar Ata**, The University of Winnipeg

2:20 **322** The Cooperative Self-Assembly of Peptide-Dendron Hybrids. **Hui Shao** and Jon R. Parquette, The Ohio State University

Thursday, June 12, 2008, 1:30 PM - 5:35 PM
Nanoscale Materials Chemistry I
Sponsor: ACS Division of Inorganic Chemistry
Franklin C (Hyatt Regency Columbus)

Organizer: Yiying Wu, Ohio State University

1:30 Introductory Remarks.

1:35 **323** Optimization of the Power Factor by Directing the Crystallite Shape of in Situ Grown Nanostructured Thermoelectric Films. **Clemens Burda**, Case Western Reserve University

2:10 **324** Synthesis of Bismuth Nanowires for the Development of Nanostructured Bulk Materials for Use in Thermoelectric Devices. **Alexis Abramson** and Ananth Lyengar, Case Western Reserve University

2:45 **325** Dispersion of Single-Walled Carbon Nanotubes and Their Application in Electrochemistry. Dan Wang and **Liwei Chen**, Ohio University

3:20 Intermission.

3:35 **326** Metal Oxide Nanomaterials: Tuning Band Edges for Dye-Sensitized Solar Cells (DSSC). **Mario Alpuche-Aviles**[1], Gayatri Natu[1] and Yiying Wu[2], (1)The Ohio State University, (2)Ohio State University

4:00 **327** Fluorescence Voltage Sensors Based on Nanoscale Electron Transfer. **Liang-shi Li** and Binsong Li, Indiana University

4:35 **328** Synthesis and Applications of Uniform Arrays of Nanoparticles. Hongzhou Yang, Sachin Kumar and **Shouzhong Zou**, Miami University

5:10 **329** Polymer Supported Gold Nanoparticle Biosensors. **Kathleen Vermeersch**, Craig Buckley and Dr. Jessica O. Winter, The Ohio State University

Thursday, June 12, 2008, 2:15 PM - 5:00 PM
High School Teachers Education Program - Workshop I
Sponsor: Battelle and ACS Division of Chemical Education
Chemistry (The Ohio State University)

Organizers: Ted Klupinski, Battelle, Jodie Harper, Battelle

Session Overview: This program is designed to provide high school chemistry teachers with "real-world chemistry" content to use in the classroom. Lectures and laboratory workshops will be presented by scientists and by high school science teachers who have taught the subject matter to their students.

2:15 Workshop: Nanotechnology in the High School Classroom.

3:45 Break.

4:00 Workshop: Production and Properties of Biodiesel in a Classroom Setting.

Thursday, June 12, 2008, 2:15 PM - 5:00 PM
High School Teachers Education Program - Workshop II
Sponsor: Battelle and ACS Division of Chemical Education
Chemistry (The Ohio State University)

Organizers: Ted Klupinski, Battelle, Jodie Harper, Battelle

2:15 Workshop: Arsenic in the Water!.

3:45 Break.

4:00 Workshop: The Real CSI.

Thursday, June 12, 2008, 5:30 PM - 7:30 PM
General Poster Session II
McKinley/Hayes (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University

330 Optical Properties of Thermal Control Coatings after Weathering, Simulated Ascent Heating, and Simulated Space Radiation Exposure. **Donald A. Jaworske**[1], George C. Tuan[2], David T. Westheimer[2], Wanda C. Peters[3] and Lonny R. Kauder[3], (1)NASA Glenn Research Center, (2)NASA Johnson Space Center, (3)NASA Goddard Space Flight Center

331 Formal Total Synthesis of (+/-)-Isolaurepinnacin. **Jason H. Stengel** and Mark C. McMills, Ohio University

332 Hexacyclo[7.1.0.0^{1,3}.0^{3,5}.0^{5,7}.0^{7,9}]Decane, or Pentagramane: High-Level Computational Studies on a Novel Hydrocarbon. **David W. Ball**, Cleveland State University

333 Asymmetric Reactions Driven by Folded Dendrimer. **Siyu Tu** and Jon R. Parquette, The Ohio State University

334 Organocopper-Mediated Cascade Approach towards N-Fused Heterocycles. **Dmitrijs Cernaks** and Vladimir Gevorgyan, University of Illinois at Chicago

335 Chemistry in Antique "Receipts" for Soaps, Cosmetics and Perfumes. **A. L. Wilson**, Oolong Informatics

336 Preparations of PCP and NCN ^{19}F Reporter Pincer Complexes. Green Enough?. Man Lung (Desmond) Kwan[1], **Paul M. Schroder**[1], Wilson Luu[1], Adam Jenkins[1], Laura Gruber[1], Norris W. Hoffman[2], Rachel Traylor[2], Benjamin Wicker[2], Alan G. Marshall[3] and Gregory A. Khitrov[3], (1)John Carroll University, (2)University of South Alabama, (3)Ion Cyclotron Resonance Program

337 Exclusive 5-Exo-Dig Hydroarylation of O-Alkynyl Biaryls Proceeding Via C-H Activation Pathway. **Natalia Chernyak** and Vladimir Gevorgyan, University of Illinois at Chicago

338 A Solvent-Free Approach to Acid/Base Chemistry and the Tishchenko Reaction. **Daniel C. Waddell** and James Mack, University of Cincinnati

339 Thermo-Optical Properties and Characterization of Heat Generation of Single Gold Nanoparticles Embedded in Ice. **Alyssa C. Thomas**, Hugh H. Richardson, Michael C. Carlson and Alexander O. Govorov, Ohio University

340 Optimization of the Preparation of Flash Paper in the Lab. Benjamin Sunkel[1], Evan Buchanan[2] and **Ian H. Krouse**[1], (1)Denison University, (2)Purdue University

341 A One-Step, One-Pot Gewald Reaction for Alkyl-Aryl Ketones Via Mechanochemistry. **William C. Shearouse** and James Mack, University of Cincinnati

342 Bifunctional Silica-Based Mesoporous Materials for Mercury Ions Adsorption. **Rafal M. Grudzien**, Bogna E. Grabicka, Stacy M. Morris and Mietek Jaroniec, Kent State University

343 Catalytic Studies on Electrochemical Production of Hydrogen Peroxide. **Kevin D. Cassidy**, Joseph C. Obirai and Prabir K. Dutta, The Ohio State University

344 Local ACS Section Sponsored Summer Workshops in Crime Scene Investigation. **Larry Kolopajlo**, Eastern Michigan University

345 Synthesis of Polypyrrole-Based Ordered Mesoporous Carbons by Using Channel-Like and Cage-Like Silica Templates. **Pasquale F. Fulvio**, Joanna Gorka and Mietek Jaroniec, Kent State University

346 Thermal Effects of Electromagnetic Stimulation of Nanoparticles. **Michael T. Carlson**, Hugh H. Richardson and Martin E. Kordesch, Ohio University

347 Solventless Sampling of Phthalate Esters in Water. **Heather L. Distel** and James K. Hardy, University of Akron

348 Novel Functionalized Core/shell Nanocapsules for Imaging and Drug Delivery. **Duangruthai Sridaeng**, Tejal Deodhar, Jacob J. Weingart and Jun J. Hu, University of Akron

349 Investigating the Role of Vibrational Excitation on the Dynamics of the F(^{2}P) + HCl --> FH + Cl(^{2}P) Hydrogen-Transfer. **Sara E. Ray**, Ge W.M. Vissers and Anne B. McCoy, The Ohio State University

350 Developing New Types of Counter Electrodes for Dye-Sensitized Solar Cells. **Panitat Hasin**[1], Mario Alpuche-Aviles[1] and Yiying Wu[2], (1)The Ohio State University, (2)Ohio State University

351 Results of Line Shape Analysis of Dynamic Light Scattering by Microgel NANOPARTICLES: Effect of Polymer Concentration and Cross-Linking Density on Microgel Size and Shrinking Capacity. **Imaan Benmerzouga**, John T. McKenna and Kiril A. Streletzky, Cleveland State University

352 Integration of Structurally and Compositionally Diverse Metal Oxide Semiconductor Nanomaterials for Photovoltaic Applications. **Gayatri Natu**, Yanguang Li, Mario Alpuche-Aviles and Yiying Wu, The Ohio State University

353 The Identification of Antibiotics in Water Via HPLC-ICP-MS. **Brittany Catron**, Scott E. Afton and Joseph Caruso, University of Cincinnati

354 High Temperature Internal Reference Oxygen Sensors Using a Conducting Metal Oxide Electrode. **Julia Rabe**, Prabir K. Dutta and John Spirig, The Ohio State University

355 Permeation Sampling of Gasoline in Groundwater. **Alesia C. Salberg** and James K. Hardy, University of Akron

356 Occupational Monitoring of Carbonaceous Nanomaterials. **Toni Ruda-Eberenz**, M. Eileen Birch, Douglas E. Evans and Bon-Ki Ku, National Institute for Occupational Safety and Health

357 Wilson Coefficients from the Excess Gibbs Free Energy and the Activity Coefficient of One Component in a Binary Solution. **S. Alex Studniarz**, Penn State University

358 Synthesis of Colloidal Ag Nanocrystals and Their 2D Superlattices. **Ravi Shankar** and Terry P. Bigioni, University of Toledo

359 Computation of through-Space NMR Shielding Effects of Aromatic Hydrocarbons. **Ned H. Martin**, Brian W. Caldwell, Katie P. Carlson and Matthew R. Teague, UNCW

360 Two-Dimensional Crystallization of Colloidal Particles by Drop Drying. **Lindsay M. Sanzenbacher** and Terry P. Bigioni, University of Toledo

361 Reduction of O2 at a Glassy Carbon Electrode Coated with a Cobalt(II)/platinum(II) Porphyrin in Alkaline Solution. **David W. Johnson**[1], Jessica Knoll[2], Kalyan Gadamsetti[2] and Shawn Swavey[2], (1)Universiy of Dayton, (2)University of Dayton

362 Use of ATR-FT-IR Spectroscopy in the Characterization of Studio Paints. Chris Bowers and **David Stoker**, Ohio Northern University

363 Temperature and Pressure Effects on Tunable Selectivity for Gas Chromatography. **James Grinias**, Eastern Michigan University

364 An Integrated Laboratory Experiment: Synthesis and Characterization of Transition Metal Maleonitriledithiolate Complexes. **Paul Szalay**, Ray Rataiczak and Lois Zook-Gerdau, Muskingum College

365 Synthesis of Bis(2,2,2-trifluorethyl) β-Keto Phosphonates. **Kevin M. White** and John A. Jackson, Youngstown State University

366 A Density Functional Study of the Relative Stability of Intermediates in a McMurry Coupling Reaction. **Andrew J. Livingston** and M. C. Milletti, Eastern Michigan University

367 Excited State Properties and Electron Transfer Reactions of a Zeolite-Bound Ru Polypyridine Complex. **Cheruvallil S. Rajesh**, Haoyu Zhang and Prabir K. Dutta, The Ohio State University

368 The Relationship Between the Physical Structure and Magnetic Structure in the Substituted Double Perovskite $Ca_{(2-x)}Sr_{(x)}MnRuO_6$. **Rebecca A. Ricciardo**, Patrick M. Woodward, Adam Hauser and Fengyuan Yang, The Ohio State University

369 Vanadate Salts as Potential Pigments: Synthesis, Structure, and Band Gaps. **Derek Decker**, Graham King, Matthew W. Stoltzfus and Patrick Woodward, The Ohio State University

370 Synthesis and Purification of HLVEALYLV, An Insulin-Based Inhibitor for Human Islet Amyloid Polypeptide (hIAPP). **Balakrishna Kurva** and Deborah L. Heyl, Eastern Michigan University

371 Rhodium(II)-Catalyzed Decomposition of Furanose-Derived Diazoesters. **Jennie Patton**, Ashley Malich, Calvin Austin, Matthias Zeller and Peter Norris, Youngstown State University

372 In Situ Alkyl and Acyl Azide Synthesis Using P-ABSA/DBU. **Tracy Vadjinia**, Brooke Katzman, Patrick Anderson, Tareq Kayyali and Peter Norris, Youngstown State University

373 Synthesis of N-2-Modified Analogs of N-Acetyl-L-Fucosamine. **David McCutcheon**, Abdul-Basit Alhassan, Matthias Zeller and Peter Norris, Youngstown State University

374 Structure and Preliminary Biological Evaluation of N-Glycosides. **Erin Schuler**, Steve Knapp, Matthias Zeller, Peter Norris and Nina Stourman, Youngstown State University

375 Detailed NMR and X-Ray Structures of Synthetic N-Glycosides. **Lucas Beagle**, Matthias Zeller, Allen Hunter and Peter Norris, Youngstown State University

376 Cyanide Bridged Alkaline Earth Transition Metal Complexes: Structures and Application. **Matthew R. Sturgeon**, Sheldon G. Shore and Errun Ding, The Ohio State University

377 Crystallinity and Thermal Stability of Melt Pressed, Molded, and Drawn Poly-L-Lactic Acid. **Reza Gay S. Milallos**, Kenneth S. Alexander and Alan T. Riga, University of Toledo

378 Crystallization Kinetics of Sulfapyridine, Fluoxetine Hydrochloride and Lidocaine Hydrochloride. **Xiaojian Li**[1], Kenneth S. Alexander[2] and Alan T. Riga[2], (1)The University of Toledo, (2)University of Toledo

379 Evaluation of Pharmaceutical Dispersions by Volumetric Variation to Monitor Powder Porosity and Void Space. **Zhouyuan Liu**[1], Kenneth S. Alexander[2] and Alan T. Riga[2], (1)The University of Toledo, (2)University of Toledo

380 Development of a Skills Exercise for Organic Literature Reading and Analysis. **Katherine W. Stickney** and Lindsey G. Fischer, University of Indianapolis

381 Extended Structures with Isocarbonyl Linkages: M(sol)X[CoRu3(CO)13]. **Christopher M. Potratz**, Xuenian Chen, Edward A. Meyers and Sheldon G. Shore, The Ohio State University

382 Modification of An Immunohistochemical Method for Enhanced Antigen Reactivity of Polycystin 1. **Timothy T. Dick**, Jonathan L. Blandford, Rachel L. Cary, Derek W. Morgan and John Krzton-Presson, Owensboro Community College

383 Activation of Mitogen Activated Protein Kinase MAPK and Ikb/nf-Kb Pathways by Analogs of Cyclovirobuxine D. Imaan Benmerzouga, **Ameer Lotfi-fard**, Salaam Saleh and Aimin Zhou, Cleveland State University

384 Improving Drug-Like Properties of Paraoxonase-1. **Vivekanand Shete**, The Ohio State Unversity and Thomas J. Magliery, The Ohio State University

385 Precision of the DSC Melting and Crystallization Properties of Polyethylene Glycol Polymers and the Effect of Humidity and Molecular Weight. **Ranajoy Majumdar**, K.S. Alexander and Alan T Riga, The University of Toledo

386 Antileishmanial Activity of Some Naturally Occuring Phenolics. **Joshua N. Fletcher**, Young-Won Chin, Mark Bahar, Karl A. Werbovetz and A. Douglas Kinghorn, Ohio State University

387 4-Aryl-1,3,2-Oxathiazolylium-5-Olates as pH-Controlled NO-Donors: The Next Generation of S-Nitrosothiols. **Dongning Lu**, Janos Nadas, Jay Zweier, Frederick Villamena and Peng George Wang, the Ohio State University

388 The Investigation of Selenium Metabolites in Kale (Brassica oleracea acephala) Utilizing HPLC with ICPMS Detection. **Qilin Chan**, Scott E. Afton and Joseph Caruso, University of Cincinnati

389 Band Gap Manipulation of Ternary AVO_4 Oxides. **Michelle Dolgos**, Samantha Yarnell, Maggie Seitz and Patrick Woodward, Ohio State University

390 Synthesis and Structure of Metallocene and Lanthanide Compounds Containing Amidotrihydroborate: A Study of Amidotrihydroborate Coordination Modes. **Duane C. Wilson**, Jason M. Hoy, Christopher M. Potratz and Sheldon G. Shore, The Ohio State University

391 Dewetting of Polystyrene Thin Films on Poly(ethylene glycol) Modified Surfaces as a Simple Approach for Patterning Proteins. **Yangjun Cai** and Bi-min Zhang Newby, The University of Akron

392 Synthesis of 2,7-Di-T-Butyl-4-Methyl-9-(2,2,2-triphenylethylidene)-Fluorene. **Shannon L. Smuck**, Dino R. Phillippi and Daniel J. Phillips, Bethany College

393 Near-Infrared Emitting Ytterbium, Phenylene Based Metal Organic Frameworks. **Demetra A. Chengelis Czegan**, Kiley A. White, Nathaniel L. Rosi and Stephane Petoud, University of Pittsburgh

394 Asymmetric Hydrogenation Over Folding Dendrimer Rhodium(I) Complexes. **Jianfeng Yu**, T.V. RajanBabu and Jon Parquette, The Ohio State University

395 A Comparison of Approaches to the Synthesis of Falcarindiol. **Michael R. Shepard Jr.**, Nathan A. Furr and Robert E. Minto, IUPUI

396 Photomodulated Chiral Induction in Helical Azobenzene Oligomers. **Eric D. King**, The Ohio State University

397 Preparation and Characterization of Reversibly Photochromic Polydiacetylenes. **Nathan A. Furr**, Robert E. Minto and Michael Akers, IUPUI

398 Liquid Chromatography Coupled with Inductively Coupled Plasma Mass Spectrometry and Electrospray Ionization Mass Spectrometry Studies on Hydrolysis Products of Sulfur Mustards. **Karolin K. Kroening**, Douglas D. Richardson and Joseph A. Caruso, University of Cincinnati

399 Determination Manganese, Nickel and Copper Concentrations in Tea. Inês R. Coelho[1], **Karolin K. Kroening**[2], Santha K.V. Yathavakilla[3] and Joseph A. Caruso[2], (1)Instituto Nacional de Saúde Dr. Ricardo Jorge, (2)University of Cincinnati, (3)U.S. Environmental Protection Agency

400 Unusual Face-to-Face π–π Stacking Interactions within An Indigo-Pillared M_3(tpt)-Based Triangular Metalloprism. **Kuang-Lieh Lu**, Academia Sinica

401 Progress towards a Long-Wavelength, Photolabile Procting Group Based on a Phenoxazine Chromophore. **Nicole R. Hume**, Erika A. Crane and Tevye C. Celius, Ohio Northern University

402 The Effects of Electron Donating Groups on the Solvatochromism of the Benzo[a]Fluorenone and Benzo[B]Fluorenone Chromophores. **Emily A. Middleton**, Lisa Meyers, Jeffrey T. Wilson and Tevye C. Celius, Ohio Northern University

403 Investigation of Volatile Organic Compounds in Mouse Cecal Contents Using Gas Chromatography with Flame Ionization Detection. **John R. Heemstra**, Heather L. S. Holmes and Brittany Napier, Eastern Michigan University

404 A Gated Guest Entrance in Command of the Encapsulation Thermodynamics. Molecular Baskets at Work. **Baoyu Wang**[1], Jovica Badjic[1], Zhiqing Yan[2], Xiaoguang Bao[1] and Christopher Baddeley[1], (1)The Ohio State University, (2)Eastern Illinois University

405 Switchable Encapsulation of Guest Molecules in Gated Molecular Baskets. **Stephen Rieth**, Baoyu Wang and Jovica D. Badjic, Ohio State University

406 Hemeproteins and Enzymes in Bilayer Structures Bathed in Ionic Liquids: The Role of WATER in Electron Transfer and Protein Function. **John J. Moran**, Noufissa Zanati, Jeremiah Bolden and Mekki Bayachou, Cleveland State University

407 Study of the Protein-Protein Interactions Between Human ISU and Human Ferredoxin. **Wenbin Qi** and James A. Cowan, The Ohio State University

408 Hannah Wooley and Iatrochemistry in Seventeenth Century Cookery Books. **A. L. Wilson**, Oolong Informatics

409 CD24 Glycoanalysis with MALDI-Tof MS. **Edwin M. Motari**, The Ohio State University

410 Comparison of Authentic Designer and Designer Imposter Scents by Gas Chromatography-Mass Spectrometry and Principle Component Analysis. **Michael A. Nichols** and Amy Betschart, John Carroll University

411 Toward the Total Synthesis of Cicutoxin. **Ann O. Omollo** and Benjamin W. Gung, Miami University

412 Investigating the Thermodynamics and Kinetics of the Galactosyltransferase-Catalyzed Reactions of UDP-Galactose and Lactose. **Kaarina Lokko** and Peng George Wang, The Ohio State University

413 Synthesis, Coordination, and Host/Guest Studies of New Supramolecular Baskets. Matthew Gardlik, **Yuning Chang**, Sandra Stojanović and Jovica Badjić, The Ohio State University

414 Peptide-Dendron Hybrids: Synthesis and Conformation Study. **Chenyang Tie**, The Ohio State University

415 Design and Synthesis of Porphyrin Molecules with Expanded Pi-System as Dyes for DSSCs. **Rohitkumar Deshpande**, Miami University

416 The Synthesis of Ru(II)-Polypyridyl Dyes for the Study of Linker Effects on Nanocrystal ZnO Surfaces. **Aaron G. Nash**, Miami University

417 Carbazole-Fluorene-Based Emitting Compounds: Optical Switching with Substitution and Formation of Nanoparticles. **Alexey E. Leontyev**, Ravi M. Adhikari and Douglas C. Neckers, Center for Photochemical Sciences, Bowling Green State University

418 Investigation of Non-Enzymatic Browning in a Glycine-Lactose Model System: A Characterization Study. **Arpana Acharya**[1], K.S. Alexander[1], Alan Riga[2] and Koustuv Chatterjee[3], (1)The University of Toledo, (2)Cleveland State University, (3)Amgen Co.

419 Duel Responsive Poly(N-isopropylacrylamide) Hydrogels Having Spironaphthoxazines as Pendent Groups. **Erandimala U. Kulawardana**, Thilini Kuruwita-Mudiyanselage and Douglas C. Neckers, Bowling Green State University

420 Synthesis of Meridianins Via An Ionic Liquid Catalyzed Coupling Using An Indole Precursor. **Jeanne L. Kuhler**, Robey T. Brooks, Monica Hodge, Krystal D. Holley and Brandi L. Inman, Auburn University

421 Towards the Synthesis of Higher Acenes; Octacene and Nonacene. **Dmitriy Khon**, Yuewei Zhao, Rajib Mondal and Douglas C. Neckers, Bowling Green State University

Thursday, June 12, 2008, 6:30 PM - 8:30 PM
Banquet and Awards Presentation
Franklin A/B (Hyatt Regency Columbus)

Organizers: Jodie Harper, Battelle, Steven Rosenthal, Chemical Abstracts Service

Friday, June 13, 2008

Friday, June 13, 2008, 8:30 AM - 9:15 AM
Plenary Lecture by ACS President Prof. Bruce E. Bursten
Morrow (Hyatt Regency Columbus)

Organizer: Claudia Turro, The Ohio State University
Presider: Anne B. McCoy, The Ohio State University

8:30 **422** The Centrality of Chemistry. **Bruce E. Bursten**, University of Tennessee

Friday, June 13, 2008, 9:30 AM - 12:30 PM
Alternative Energy Technologies I: Chemistry, Chemical Engineering, and Environment
Morrow (Hyatt Regency Columbus)

Organizer: Robert D. Litt, Velocys Inc.

9:30 Welcoming Remarks.

9:40 **423** Artificial Photosynthetic Assemblies Based on Zeolite Membrane Architecture. **Jeremy C. White** and Prabir K. Dutta, The Ohio State University

10:05 **424** Hydrogen Production through Water-Gas Shift Reaction from Coal-Derived Synthesis Gas. **Lingzhi Zhang**, Preshit Gawade, Bing Tan and Umit S. Ozkan, the Ohio State University

10:30 **425** Sulfur and Coke Resistant Anode Catalysts for Solid Oxide Fuel Cells. **Nandita Lakshminarayanan**, Hyunkyu Choi and Umit S Ozkan, The Ohio State University

10:55 Break.

11:10 **426** O_2 Reduction on Uniform Pt Nanoparticle Arrays: Effects of Particle Size and Interparticle Distance. **Hongzhou Yang** and Shouzhong Zou, Miami University

11:35 **427** The Electrochemical Properties of Glassy Carbon Powder Coated with Boron-Doped Nanocrystalline Diamond. **Doo Young Kim** and Greg Swain, Michigan State University

12:00 **428** PEM Fuel Cells. **James H. Saunders**, Battelle

12:25 Concluding Remarks.

Friday, June 13, 2008, 9:30 AM - 12:30 PM
Chemistry of Supramolecular Assemblies II
Knox (Hyatt Regency Columbus)

Organizer: Jovica D. Badjic, The Ohio State University

9:30 **429** Contact: Symmetry and Weak Bonds. **Dongwhan Lee**, Indiana University

10:00 **430** Organic Building Blocks for Anion-Binding Triazolophanes. **Amar H. Flood**, Yongjun Li, Yuran Hua and Esther Uduehi, Indiana University

10:30 **431** The Structure and Function of Folded Molecules. **Jonathan R. Parquette**, The Ohio-State University

11:00 Break.

11:20 **432** Synthetic Eumelanin. **Jason M. Belitsky**, Oberlin College

11:50 **433** Responsive Amphiphilic Molecules: Conformational Control and Applications in Molecular Sensing and Catalysis. **Yan Zhao**, Iowa State University

Friday, June 13, 2008, 9:30 AM - 5:30 PM
General Biological Chemistry II - Contributed Talks
Marion (Hyatt Regency Columbus)

Organizers: Claudia Turro, The Ohio State University, Thomas J. Magliery, The Ohio State University
Presider: John Hofferberth, Kenyon College

9:30 **434** Molecular Dynamics Simulation of Beta-2 Adrenergic Receptor. **Vandana Kumari** and Chenglong Li, The Ohio State University

9:55 **435** Modeling Nicotinic Acetylcholine Receptors for Computational Drug Design. **Ryan Pavlovicz** and Chenglong Li, Ohio State University

10:20 **436** VEGF Peptidomimetics: An Alternative Approach for Angiogenesis Targeted Therapy. **Daniele Vicari**, Sharad V. Rawale and Pravin Kaumaya, OSU

10:45 Morning Break.

11:05 **437** Comparative Modeling of Human Protein Arginine Methyltransferase 5 (PRMT5) and Substrate Binding Site Characterization through Molecular Docking for Target Specific Inhibitor Design. **Kiran V. Mahasenan** and Chenglong Li, The Ohio State University

11:30 **438** Effect of Amino Acid Side Chain Size on Peptide Formation by Decarboxylative Condensation. Aditya K. Sanki, **Rommel S. Talan** and Steven J. Sucheck, University of Toledo

11:55 **439** Targeted Membrane Recognition Driven by Designed Hydrogen Bonding Between Synthetic Phospholipids. **Mingming Ma** and Dennis Bong, The Ohio State University

12:20 Lunch.

1:30 **440** Biological Activities Study on the Glycolipids Derivatives. **Wenpeng Zhang**, The Ohio State Universtiy

1:55 **441** Structure of the Nitrosomonas Europaea Rh Protein. **Xin Li**[1], Sanjay Jayachandran[2], Hiep-Hoa Nguyen[2] and Micahel K. Chan[1], (1)The Ohio State University, (2)TransMembrane Biosciences

2:20 **442** Retrovirus-Specific Differences in Protein-Nucleic Acid Interactions: Implications for Genomic RNA Packaging. **Meng Sun**[1], Louis M. Mansky[2], Robert J. Gerolick[3] and Karin Musier-Forsyth[1], (1)The Ohio State University, (2)University of Minnesota, (3)SAIC-Frederick, Inc.

2:45 Afternoon Break.

3:10 **443** Inositol Phosphates Modulate the Nucleic Acid Chaperone Activty of HIV-1 Gag. **Christopher P. Jones**[1], Siddhartha A. K. Datta[2], Alan Rein[2] and Karin Musier-Forsyth[1], (1)The Ohio State University, (2)HIV Drug Resistance Program, National Cancer Institute-Frederick

3:35 **444** Structure Property Correlations for a Series of Collagen Mimetic Peptides. **Mike L. Renier**, Chemmeds

Friday, June 13, 2008, 9:30 AM - 11:00 AM
High School Teachers Education Program II
Sponsor: Battelle and ACS Division of Chemical Education
Grant/Harding (Hyatt Regency Columbus)

Organizers: Ted Klupinski, Battelle, Jodie Harper, Battelle

Session Overview: This program is designed to provide high school chemistry teachers with "real-world chemistry" content to use in the classroom. Lectures and laboratory workshops will be presented by scientists and by high school science teachers who have taught the subject matter to their students.

9:30 Demonstration of Lessons from Science in Motion.

Friday, June 13, 2008, 9:30 AM - 5:30 PM
Nanoscale Materials Chemistry II
Sponsor: ACS Division of Inorganic Chemistry
Garfield (Hyatt Regency Columbus)

Organizer: Yiying Wu, Ohio State University

9:30 Introductory Remarks.

9:35 **445** Solution Chemistry Toolkit for the Synthesis of Complex Metal and Multi-Metal Nanostructures. **Raymond E. Schaak**, Pennsylvania State University

10:10 **446** Electrochemical Fabrication and Characterization of Group II-VI Nanowires. **Terry P. Bigioni** and Matthias Hanauer, University of Toledo

10:35 **447** Design and Synthesis of Mesoporous Carbons by Using Colloidal Silica Templates. **Mietek Jaroniec**, Kent State University

11:10 Intermission.

11:25 **448** Mass Transport Mechanism and Chemical Gating of Aligned Carbon Nanotube Membrane. **Bruce Hinds**, Univ. of KY

12:00 Lunch.

1:30 **449** Liquid Crystals: From Photodisplays to Organic Photovoltaics. Lisa Green, Xiaoli Zhou and **Quan Li**, Liquid Crystal Institute, Kent State University

2:05 **450** Development and Synthesis of Corannulene-Based Organic Materials. James Mack and **Derek Jones**, University of Cincinnati

2:30 Break.

2:50 **451** Conductive Diamond Powder: A New Electrocatalyst Support Material for the Polymer Electrolyte Membrane Fuel Cell. **V. Matt Swope**, Ayten Ay, Isao Sasaki, Doo Young Kim and Greg M. Swain, Michigan State University

3:15 **452** Length-Dependent Dielectric Response of Single-Wall Carbon Nanotubes in Electrostatic Force Microscopy. **Wei Lu**, Yao Xiong and Liwei Chen, Ohio University

3:40 Concluding Remarks.

Friday, June 13, 2008, 9:30 AM - 5:30 PM
Theoretical Modeling of Solvation: Methods and Applications
Sponsor: ACS Division of Physical Chemistry
Madison (Hyatt Regency Columbus)

Organizer: John Herbert, The Ohio State University

Session Overview: This session will present recent developments in the statistical-mechanical and electronic structure description of solvation and environment effects, broadly defined.

9:30 Welcoming Remarks.

9:40 **453** Simulating the Dynamics of Quantum Fluids. **Nancy Makri**, University of Illinois at Urbana-Champaign

10:15 **454** Applications of the Quantum Monte Carlo Method to Challenging. **Kenneth D. Jordan**, Wendy Lampart and Jiawei Xu, University of Pittsburgh

10:50 Break.

11:05 **455** Association Constant and Solution Structure of High Temperature Aqueous Sodium Chloride in a Model with Ab Initio Interactions. **Doug Doren** and Robert Wood, University of Delaware

11:40 **456** Proton-Coupled Electron Transfer Reactions in Solution and at Electrochemical Interfaces. **Sharon Hammes-Schiffer**, Pennsylvania State University

12:15 **457** Oil Drop Hydration and Aggregation: The Hydrophobic Effect on Various Length Scales. **Robin Underwood**, Jill Tomlinson-Philips and Dor Ben-Amotz, Purdue University

12:35 Intermission.

1:30 **458** Solvation in Room-Temperature Ionic Liquids. **Claudio J. Margulis**, University of Iowa

2:05 **459** QM/QM Electronic Embedding Models for Solvation Studies. **Krishnan Raghavachari**, Hrant P. Hratchian and Priya V. Parandekar, Indiana University

2:40 **460** Unraveling Water's Entropic Mysteries: A Unified View of Non-Polar, Polar and Ionic Hydration. **Dor Ben-Amotz**, Robin Underwood and Jill Tomlinson-Phillips, Purdue University

3:15 Discussion.

3:30 **461** Dielectric Model of Solvation for Use in Electronic Structure Calculations. **Daniel M. Chipman**, University of Notre Dame

4:05 **462** The Signature of Solvation on Vibrational Energy Relaxation Processes and Multi-Dimensional Infrared Spectra. **Eitan Geva**, University of Michigan

4:40 **463** Solvation Dynamics at Aqueous DNA Interfaces. **Steven A. Corcelli**, University of Notre Dame

5:15 **464** Spectral Signatures of Large Amplitude Vibrational Motions in Ion-Water Complexes. Anne B. McCoy, **Samantha Horvath** and Andrew T. Petit, The Ohio State University

Friday, June 13, 2008, 9:30 AM - 5:30 PM
Undergraduate Education and the REEL Program II
Harrison (Hyatt Regency Columbus)

Organizers: Patrick M. Woodward, The Ohio State University, Ted M. Clark, the Ohio State University, Prabir K. Dutta, The Ohio State University

9:30 **465** Application of Coulomb's Law in Explaining Sizes of Atoms and Ions. **Parinbam (RAJ) K. Thamburaj**, Ohio University- Zanesville

9:55 **466** Reflections on Implementing a Pigment Research Module in General Chemistry. **Patrick M. Woodward** and Matthew W. Stoltzfus, The Ohio State University

10:20 **467** DIVINE Chemistry and the OCUR-REEL Program: Student Experiences with DIgital Video Inquiry NarrativE Projects. **Richard Spinney**, James Treadway and Ted Clark, The Ohio State University

10:45 **468** Issues Concerning the Assessment of Student Experiences with DIgital Video Inquiry NarrativE (DIVINE) Projects in Chemistry Courses. **Ted M. Clark**, The Ohio State University and Caroline T. Clark, Ohio State University

11:10 **469** Research in the Teaching Lab: A Microwave Accelerated Synthesis of Oxazolidin-2-Ones. **Steven J. Sucheck**, University of Toledo

11:35 **470** POGIL at Xavier University. **Roy J. Cohen**, Xavier University

12:00 Break.

2:00 **471** Training Undergraduate Peer Mentors for a Research-Based General Chemistry Laboratory Course. **Matthew W. Stoltzfus** and Ted M. Clark, The Ohio State University

2:25 **472** The REEL Evaluation: Year 2007-2008. **Yue Li** and Jane Butler Kahle, Miami University

2:50 **473** Developing Assessment Synergy for Chemistry Programs & Courses. **David Baker** and Deb Temperly, Delta College

3:15 **474** The Challenge of *Searching Scientific Literature*. **Janet S. Rogers**, Edinboro University of Pennsylvania

3:40 **475** Insights and Observations of Student Searching Techniques with Print Resources and STN Databases in a Literature of Science Course. **Eleanor P. Randall**, Edinboro Universtiy of Pennsylvania

4:05 **476** Embedding Technology for Learning Enhancement on a Shoestring Budget. **Mark D. McClain**, Jeffrey W. Whitacre, Dara E. Fraley, Philip J. Schanely and Donald S. Humphreys, Cedarville University

4:30 **477** Making Chemistry Click: Use of An Electronic Response System to Encourage Active Learning. **Sarah S. Preston**, Ursuline College

Friday, June 13, 2008, 12:00 PM - 2:00 PM
Undergraduate and REEL Poster Session
McKinley (Hyatt Regency Columbus)

Organizers: Ted M. Clark, The Ohio State University, Claudia Turro, The Ohio State University

478 Determination of Nitrate Concentrations on the Olentangy River in Columbus OH. **Parevi Majmudar**, Mazen Roshdy, Joshua Illencik, Joel Ronoh and Ted Clark, Ohio State University

479 Fluorous Solvents for Slow Reaction of Thionyl Chloride and Alcohols. **Elisabeth R. Goei** and Richard T. Taylor, Miami University

480 The Influence of the OSU Wetlands on Nitrate Concentration and pH. **Kurt Farrell**, Jonathan Bonchak, Peter Davis, Joe Hipp and Ted Clark, Ohio State University

481 The Affect of the OSU Wetlands on Buffer Capacity, Nitrate Concentration, and pH. **Jacob Brenner**, Brad Rarick, Keith Lamping, Amenze Osa, Pam Ehule and Ted Clark, Ohio State University

482 Sonogel Carbon Zirconium Dioxide (ZrO2) Electrode Sensor to Detect 1,2-Dihydroxybenzenes. **Suzanne K. Lunsford**, Rachel Kingdom, Lindsey Hogle and Vincent Nguyen, Wright State University

483 Bioinformatics across the Undergraduate Chemistry Curriculum. **Regina Stevens-Truss**, Kalamazoo College

484 Fruits and Nutrition: Undergraduate Research Experiences Developing Experimental Protocols. **Faith J. Wyzgoski**[1], Kathryn F. Nebergall[1], Joshua R. Post[1], Jeffrey J. Hardesty[1], Molly L. Fraizer[1], Jonathan Reed[1], Joseph C. Scheerens[2], Ann M. Chanon[2] and R. Neil Reese[3], (1)The Ohio State University, (2)Ohio State University, Ohio Agricultural Research & Development Center, (3)South Dakota State University

485 Efficient Gallotannin Synthesis. Klaus B. Himmeldirk[1], **Jessica C. Ziepfel**[2] and Robert C. Binkley[2], (1)Ohio University, (2)Ohio University, Athens, OH

486 Intramolecular Click Chemistry. **Diana M. Kroll**, Travis M. Gilbert, Kurt S. Kadon, Heather R. Mandrell and Richard T. Taylor, Miami University

487 Flow Chemistry in the Kinetic Resolution of Naproxen. **Brittany M. Staarman**, Lauren C. Wene and Richard T. Taylor, Miami University

488 Lactobacillus RNA Secondary Structures. **Olivia Ringo**, University of Kentucky

489 To Nuke or Not to Nuke: The Joys and Pitfalls of Microwaves. Jonathan W. Crowe, Mallory P. Ladd, **Shannon C. McCann**, Derek L. Mull, Virginie Casarotto, Cora Lind and Steven J. Sucheck, University of Toledo

490 Synthesis of 1,4-Disubstituted 1,2,3-Triazole-Oxazolidin-2-Ones Via a Three-Component Reaction. **Jeffrey A. Demaray**, Jason E. Thuener, Matthew N. Dawson and Steven J. Sucheck, University of Toledo

491 Ammonia Borane - Reductions of Organic Functional Groups, Studies in Diastereoselectivity, and Solvent Effects. **Michael Woodruff**, Jennifer Scherer and Christopher Callam, The Ohio State University

492 Fluorous Carbohydrate Synthesis - Preparation of Fluorous Tagged Acceptors and Donors for Application to Glycoside Bond Synthesis. **Michael DiBartola**, Andrew Aten and Christopher Callam, The Ohio State University

493 Diastereoselective Reductions of Benzoin Using Ammonia Borane. Amy Amholt[1], Lisa Tubbs[1], Ahmad Saqr[2], Christopher Callam[2] and **Adam I. Keller**[1], (1)Columbus State Community College, (2)The Ohio State University

494 The Determination of Selenium in Broccoli Using ICP-AES. **Erica C. Goetz** and William C. Wetzel, Thomas More College

495 Inhibition of Luminol Chemiluminescence in Hypochlorite Solutions. **Brad Bellamy**, University of Cincinnati Clermont and Matt A., Widanski, University of Cincinnati Clermont College

496 Synthesis of Nanometer-Sized Microporous Aluminosilicates. **Mike Severance**[1], Kyle Nesbitt[1] and Prabir K. Dutta[2], (1)the Ohio State University, (2)The Ohio State University

497 Determination of Polycyclic Aromatic Hydrocarbons in Parking Lot Seal Coat. **Timothy Gauntner**, Sarah Horvath, Alethea Kypriotakis, Kerri Smith and Anne O'Connor, Cleveland State University

498 Degradation of Polychlorinated Biphenyls (PCB) by a Pleurotus Ostreatus. **Jermann Ashley**, Casandra Solis, Kerri Smith and Anne O'Connor, Cleveland State University

499 Effects of Microorganisms on the Breakdown of Polycyclic Aromatic Hydrocarbons in Motor Oil. **Klaire Freeman**, Kyle Sochacki, Kerri Smith, Robert Wei and Anne O'Connor, Cleveland State University

500 Development of BioMedical Devices and Sensors Based on Dielectrics and Electrochemistry. **John Bambakidis**[1], Alan Riga[1], Michael Ellen Matthews[1], Vadim Lvovich[2] and Michael Kaufman[2], (1)Cleveland State Univesity, (2)Buckeye Pharmaceuticals

501 Ring and Conical Nanoelectrodes for Scanning Electrochemical Microscopy. **Nathan M. Kidwell** and John E. Baur, Illinois State University

502 Measurements of Short-Term Toxicity of Six Polycyclic Aromatic Hydrocarbons by Vibrio Fischeri. **Nida Degesys**, Beth Apanasewicz, Zach Stiles and Robert Wei, Cleveland State University

503 Designing Magnesium Complexes Utilizing a Combination of N- and O- Donor Ligands. **Jessie Monegan** and Scott D Bunge, Kent State University

504 Quantitation of Plant Metallothioneins 2 by Three Methods. **Katie Baxter**, Cleveland State University

505 Kinetics of UV Photodegradation of a DNA Model System in a Room-Temperature Glass. **Marc P. Coons**, Yu Kay Law and Bern Kohler, The Ohio State University

506 Examination of Excited State Ordering in 1,4-Diphenylbutadiene Derivatives and Analogs. **Jessica E. Donehue**, Nicole M. Dickson, Dr. Christopher Callam and Dr. Terry L. Gustafson, The Ohio State University

507 Synthesis and Characterization of a Novel Series of Hetero-Ligated Lanthanide Compounds for the Ring Opening Polymerization of ε-Caprolactone. **Jesus A. Ocana** and Scott D. Bunge, Kent State University

508 Spectroscopic Analysis of the Reaction of Xanthine Oxidase with Benzotriazole-1-Methanol and Benzotriazole-1-Acetonitrile. Tarek Mahfouz, **Dana Koch**, Brad Petersen, Rajvi Patel and Amy Stockert, Ohio Northern University

509 Synthesis and Characterization of Lanthanide-3,6-Bis[({2-[bis(2-{[(2-hydroxyphenyl)Methyl]Amino}Ethyl)Amino]Ethyl}Amino)Methyl]Naphthalene-2,7-Diol Complexes. **Brian J. Domanski** and Peter M. Smith, Westminster College

510 Role of Oxidative Stress in HEK 293 Cells Induced by Arsenic Compounds. **Jamie Rhodes** and Yuh-Cherng Chai, John Carroll University

511 Purification and Molecular Weight Determination of Metallothionein Class II (MT-2) Isolated from Dwarf Sunflower (Helianthus annuus),. LeeAnn M. Westfall, Erin D. Huber and **Robert Wei**, Cleveland State University

512 Cholesterol Levels and Activity of Membrane Bound Proteins: Characterization by Thermal and Electrochemcial Methods. **Noufissa Zanati**, Michael Ellen Matthews, John J. Moran, Mekki Bayachou and Alan T. Riga, Cleveland State University

513 Analysis of DEET in Water Samples by Solid Phase Microextraction and Gas Chromatography-Mass Spectrometry. **Jillian Hutson**, Nicholas A. Pierson and Kristin K. Cline, Wittenberg University

514 A Family of 1,1,3,3-Tetraalkylguanidine (H-TAG) Stabilized Zinc Aryloxide Catalysts for the Ring-Opening Polymerization of Lactide. **Julia J. Ng** and Scott D. Bunge, Kent State University

515 The Synthesis, Structure and Characterization of Lanthanide Complexes Stabilized with 1,1,3,3-Tetramethylguanidine and 2,2,6,6,-Tetramethylpiperidiol. **Robert Rakosi III** and Scott D. Bunge, Kent State University

516 Computer Modeling of Glutamate Racemase. **Danny Krall**, Amy Stockert and Tarek Mahfouz, Ohio Northern University

517 Nitrate Levels in Central Ohio Waterways: A REEL Undergraduate Laboratory. **Jamie J. Schwefel**, Jillien H. Whiteside, Regan Rutherford, Megan Thiery, Ruta Berhanemeskel and Margaret E. Ginn-Pease, Capital University

518 Investigation of Chromium (VI) in Soil Surrounding Pressure Treated Wood. **Holly Baaklini**, Krista Freeman, Daniela Dogaru and Anne O'Connor, Cleveland State University

519 Software Development for Spinel Structure Prediction. **Daniel C. Hannah**, Ohio State University and Patrick M. Woodward, The Ohio State University

520 Analysis of Water from Alum Creek Combined Sewer Overflow for NO_3^-, Cl^-, and Pb^{2+}: A REEL Undergraduate Laboratory. **Chaunda N. Brooks**, Patricia Buck and Jens M. Hemmingsen, Capital University

521 MOLECULAR MODELING USING RAPID PROTOTYPE TECHNOLOGY – An Interdisciplinary Undergraduate Research Experience. **Jacquelyn Pohl**, Sam Antoline, Muthar Al-Ubaidi and Rajiv S. Soman, University of Cincinnati

522 Polymerization of Monomers Used in Denistry Catalyzed by Synthetic Phosphine Oxides and Measured by DSC. **Ibrahim Awawdeh**, Lauren

Primiano, Althea Pallom, Hany Sobhi, John Masnovi and Alan Riga, Cleveland State University

523 AA Determination of Lead in Areas Surrounding Brownfield Sites in Cleveland. **Katrina Johnson**, Erin Nemeth, Daniela Dogaru and Anne O'Connor, Cleveland State University

524 Development of a Dental Transoral Patch Including Lidocaine and a Water Soluble Polymer Based on Thermal Analysis. **Ibrahim Awawdeh**, Vipin Misra, Michael Ellen Matthews, Nicole Scholtz, Amer Najjar, Samer Almisehal and Alan Riga, Cleveland State University

525 Recent Developments of Malarial Resistance and Genomics. **Amina F. Basha**, Massachusetts Institute of Technology and Teresa McNally, Abbott Laboratories

526 Calculation of the Rotational Barriers of Urea. **Jeremy S. Hardinger**, Charles Jaffé and Xiaojian Mao, West Virginia University

Friday, June 13, 2008, 12:30 PM - 1:30 PM
Meet ACS President Bruce Bursten (Reception-style lunch)
Peppercorn (Hyatt Regency Columbus)

Organizers: Claudia Turro, The Ohio State University, James A. Cowan, Ohio State University

Friday, June 13, 2008, 1:00 PM - 3:45 PM
High School Teachers Education Program - Workshop III
Sponsor: Battelle and ACS Division of Chemical Education
Chemistry (The Ohio State University)

Organizers: Ted Klupinski, Battelle, Jodie Harper, Battelle

Session Overview: This program is designed to provide high school chemistry teachers with "real-world chemistry" content to use in the classroom. Lectures and laboratory workshops will be presented by scientists and by high school science teachers who have taught the subject matter to their students.

1:00 Workshop: The Real CSI.

2:00 Break.

2:15 Workshop: Arsenic in the Water!.

Friday, June 13, 2008, 1:00 PM - 3:45 PM
High School Teachers Education Program - Workshop IV
Sponsor: Battelle and ACS Division of Chemical Education
Chemistry (The Ohio State University)

Organizers: Ted Klupinski, Battelle, Jodie Harper, Battelle

1:00 Workshop: Production and Properties of Biodiesel in a Classroom Setting.

2:00 Break.

2:15 Workshop: Nanotechnology in the High School Classroom.

Friday, June 13, 2008, 1:00 PM - 2:30 PM
Tours - Ohio Department of Agriculture
Ohio Department of Agriculture - Consumer Analytical Lab (CAL), 8995 E. Main St., Reynoldsburg, OH 43068

Organizer: Claudia Turro, The Ohio State University
Presider: Cathy Williams, Ohio Department of Agriculture

1:00 Tour of Consumer Analytical Labs (30 min).

1:30 Break.

1:45 Tour of The Division of Animal Industry (30 min).

Friday, June 13, 2008, 1:30 PM - 5:30 PM
Alternative Energy Technologies II: Chemistry, Chemical Engineering, and Environment
Morrow (Hyatt Regency Columbus)

Organizer: Robert D. Litt, Velocys Inc.

1:30 Welcoming Remarks.

1:40 **527** Corn Ethanol as An Alternative Energy Source. Dwayne Siekman and **Tadd Nicholson**, Ohio Corn Growers Association

2:05 **528** Utilization of Chemical Looping Strategy for Liquid Fuel Synthesis from Coal. **Fanxing Li**, Deepak Sridhar, Fuchen Yu and L.S. Fan, Ohio State University

2:30 **529** Characterizing Biofuel/Petroleum Mixtures with Comprehensive Two-Dimensional Gas Chromatography. **Stacy K. Seeley**, Kettering University, James D. McCurry, Agilent Technologies, Inc. and John V. Seeley, Oakland University

2:55 Break.

3:10 **530** Fischer Tropsch Synthesis in Micro-Channel Reactors. **Kai Jarosch**, Bin Yang, Sean Fitzgerald, Rachid Taha, Soumitra Deshmukh, Terry Mazanec and Anna Lee Tonkovich, Velocys, Inc.

3:35 **531** Synthetic Jet Fuels with Additives - Seal Swell and Thermal Properties. **Robert J. Gormley**[1], Dirk D. Link[1], John P. Baltrus[1], Deborah C. Hreha[2] and Robert A. Ference[2], (1)U.S. Department of Energy, National Energy Technology Laboratory, (2)RDS-Parsons

4:00 Concluding Remarks.

Friday, June 13, 2008, 1:45 PM - 5:00 PM
SCHB Entrepreneurial Workshop
Sponsor: ACS Division of Small Chemical Business (SCHB)
Knox (Hyatt Regency Columbus)

Organizer: Joseph E. Sabol, CHEMICAL CONSULTANTS

Session Overview: If you have an idea for a product or service and would like to take it to market and profitability, come to this free workshop and panel discussion where you will hear sage advice from experts on starting and building a business, intellectual property, financing, technology transfer, and assistance. This workshop is open to anybody: students, faculty, and nonacademics. Even if you currently do not have an idea that you want to convert into an opportunity, you might become inspired! Bring your questions and get answers that will help you as an entrepreneur and improve your position.

Friday, June 13, 2008, 2:00 PM - 4:00 PM
Forum on Minority Participation In Science
Grant/Harding (Hyatt Regency Columbus)

Organizer: Robert Garner, The Ohio State University

Friday, June 13, 2008, 5:30 PM - 7:30 PM
OSU Alumni Reception
Sponsor: The Ohio State University College of Mathematical and Physical Sciences
Hayes (Hyatt Regency Columbus)

Organizers: Claudia Turro, The Ohio State University, James A. Cowan, Ohio State University

Saturday, June 14, 2008

Saturday, June 14, 2008, 8:00 AM - 12:00 PM
ACS Leadership Workshop: Involving Volunteers
Grant/Harding (Hyatt Regency Columbus)

Organizers: Priscilla Ratliff, ACS Columbus Section, Ronald K. Mitchum, DAT Laboratories, Inc.

Session Overview: This course is designed for emerging leaders in the Society. Involving Volunteers is for those members who are new to leadership roles and need additional guidance in making early leadership

assignments successful. We encourage those who are currently leading or who are planning to lead a new project and need assistance in gaining volunteer support to participate in this course. You'll gain skills that are highly transferable in managing projects and leading teams in your professional role.

Saturday, June 14, 2008, 8:00 AM - 12:00 PM
Laboratory Safety Workshop
Sponsor: The Laboratory Safety Institute (LSI) and ACS Division of Chemical Health and Safety
Garfield (Hyatt Regency Columbus)

Organizer: Mary Bailey, The Ohio State University

Session Overview: This classic presentation on laboratory safety by the Laboratory Safety Institute (LSI) has been attended by thousands of safety professions. With experience in both industrial and academic labs, the workshop leaders give a real-world approach to safety issues. Their stories are both interesting and pertinent. Interactive demonstrations help you deal with everything from creative wiring in the lab to administrators without a vision of what it means to have safe workplace. This workshop will be an excellent forum to speak openly about safety problems in your workplace. Registration to the workshop can be made on the registration form for the meeting.

Saturday, June 14, 2008, 8:30 AM - 5:30 PM
Symposium in Honor of Prof. Ming-Daw Tsai
Harrison (Hyatt Regency Columbus)

Organizer: Robert J. Hondal, University of Vermont, College of Medicine

8:30 Welcoming Remarks.

8:35 **532** A Glance at Professor Ming-Daw Tsai's Distinguished Career at OSU. **Dehua Pei**, The Ohio State University

9:05 **533** AMPK Functionally Phosphorylates eNOS Ser-633/635. **John Y.-J. Shyy**, University of California

9:25 **534** Leveraging Natural and Bio-Derived Feedstocks for Laundry Applications. **Dongyan Qin**, Jeff Scheibel, Nasser Fredj and Elizabeth Piocos, The Procter & Gamble Company

9:45 **535** Ultrafast Enzyme Dynamics: DNA Photolyase. **Dongping Zhong**, The Ohio State University

10:05 **536** The Interface of NMR, Membranes, Protein Folding, and Enzymology: Results from a Career Inspired by Ming-Daw Tsai. **Charles R. Sanders**, Vanderbilt University

10:25 Break.

10:45 **537** Phosphorothioates as Probes of Phosphoryl Transfer Mechanisms: The Past and Present. **KarolS Bruzik**, University of Illinois at Chicago

11:05 **538** Structure, Dynamics, and Catalytic Mechanism of Folate Biosynthetic Enzymes. **Honggao Yan**[1], Yue Li[1] and Xinhua Ji[2], (1)Michigan State University, (2)National Cancer Institute at Frederick

11:25 **539** Quantitative Structure Activity Relationships and Stereochemistry for Inhibitions of Serine Hydrolases and Phospholipase A2 by Carbamates. **Gialih Lin**, National Chung-Hsing University

11:45 **540** Negative Cooperativity in Transition State Binding Enhances Rate of Product Release in Phosphagen Kinases. **Mark J. Snider**, The College of Wooster

12:05 **541** Role of Transcription Factors in Cisplatin Mediated Apoptosis and Transport. **Rathindra N. Bose**, Northern Illinois University and Leila Maurmann, Kansas State University

12:25 Lunch Break.

1:30 **542** Quantitative Exploration of the Catalytic Landscape Separating Divergent Plant Sesquiterpene Synthases. **Joseph Noel** and Paul E. O'maille, The Salk Institute/Howard Hughes Medical Institute

1:50 **543** From Lipids to DNA and Back: Adventures in Phosphate Biochemistry. **Cynthia Dupureur**, Univ. Missouri St. Louis

2:10 **544** Insight into the Differential Interaction of iASPP/p53 and ASPP2/p53. **Jinwoo Ahn**, Byeon In-Ja L., Byeon Chang-Hyeock and Gronenborn Angela M., University of Pittsburgh

2:30 **545** Structural Basis for the Regulation of ASPP-Mediated Apoptosis of p53. **In-Ja L. Byeon**, Jinwoo Ahn, Chang-Hyeock Byeon and Angela M. Gronenborn, University of Pittsburgh

2:50 Afternoon Break.

3:10 **546** Research Involving Vitamin B-6. **Karen L. Ericson**, Indiana University-Purdue University Fort Wayne

3:30 **547** Mismatched dNTP Incorporation by DNA Polymerase β Does Not Proceed Via Globally Different Conformational Pathways. **Kuo-Hsiang Tang**[1], Ming-Daw Tsai[2], Marc Niebuhr[3], Chang-Shung Tung[4], Hsiu-chien Chan[5] and Chia-Cheng Chou[5], (1)the Ohio State University, (2)Ohio State University, Columbus, Ohio 43210, and Academia Sinica, Taipei, Taiwan, (3)Stanford Synchrotron Radiation Laboratory, MS99, SLAC,, (4)Theoretical Biology and Biophysics, Los Alamos National Laboratory,, (5)Genomics Research Center, Academia Sinica

3:50 **548** Formulating Microbial Agents for Pest Control Applications. **Christopher A. Dunlap**, National Center for Agricultural Utilization Research

4:10 **549** From Sulfur Substrates to Selenium in Enzymes. **Robert J. Hondal**, University of Vermont, College of Medicine

4:30 **550** From the End to the Beginning. **Ming-Daw Tsai**, Ohio State University, Columbus and Academia Sinica

Saturday, June 14, 2008, 1:00 PM - 5:00 PM
ACS Leadership Workshop: Innovation
Grant/Harding (Hyatt Regency Columbus)

Organizers: Priscilla Ratliff, ACS Columbus Section, Ronald K. Mitchum, DAT Laboratories, Inc.

Session Overview: This workshop is designed for leaders in the Society who need to rely on innovative thinking, ideas, and approaches to move a group of volunteers in a new direction or a project forward. Those leaders who are responsible for making significant changes to current processes, or are asked to create new ideas and approaches for addressing key issues, or who need to make a significant impact, will benefit greatly from this course.