

# 41st Northeast Regional Meeting

**Binghamton, NY**

**October 5-8, 2016**

Christof Grewer and Nikolay Dimitrov

*Program Chairs*

## **THURSDAY MORNING**

DoubleTree by Hilton Hotel Binghamton  
North Riverside Room

### **Analytical Chemistry**

M. R. Hepel, *Organizer*  
F. V. Bright, *Presiding*

**8:00** Introductory Remarks.

**8:05 1.** Mapping complex interfaces and surfaces across length scales. **F.V. Bright**

**8:35 2.** Recent advances in forensic analysis. **J. Halamek**, E. Brunelle, J. Agudelo, C. Huynh, L. McGoldrick, L. Halámková

**8:55 3.** Raman markers used for monitoring of targeted delivery and controlled release of anti-cancer drugs. **T. Santiago**, M. Smith, M.R. Hepel

**9:15** Intermission.

**9:45 4.** Electroanalytical evaluation of engineered nanoparticles: Studies of surface reactivity, functionalization and catalysis. A. Karimi, K. Kirk, **S. Andreescu**

**10:15 5.** Examination of copper speciation in electrolyte solutions using electron spin resonance spectroscopy at room temperature: A tool for evaluating the fitness of organic molecules as ligands sequestration agents and as precursors for templated synthesis. **C. Bender**

**10:35 6.** Study of oxidative degradation in monoethanolamine by LC-TOF mass spectrometry. **S. Bhatnagar**, J. Thompson, K. Liu

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Endicott Room

## Biochemistry

*Cosponsored by BIOL*

A. Shekhtman, *Organizer*

J. Sheng, *Organizer, Presiding*

**8:00 7.** DNA nanotechnology for ultrasensitive detection. **M.V. Yigit**, M. Rana, M. Balcioglu

**8:20 8.** Selenium in proteins and RNA: A chemical and biological rationale. **R. Hondal**

**8:40 9.** Computational study of nucleic acid adsorption on graphene. **S. Ranganathan**, K. Halvorsen, A.A. Chen, M.V. Yigit, C. Myers, N. Robertson

**9:00 10.** Bright, photostable new probe to detect biomolecule carbonylation in live cells. **S. Ghosh**, S.L. Bane

**9:15** Intermission.

**9:35 11.** Direct observation of structural evolution of expanded CAG trinucleotide RNA repeats. **P. Li**

**9:55 12.** Directed evolution for the design of new catalysts. **T. Dunston**, Y. Moroz, O. Makhlynets, O. Moroz, Y. Wu, J. Yoon, A. Olsen, J. McLaughlin, K.L. Mack, P. Gosavi, N. van Nuland, I.V. Korendovych

**10:10 13.** Development of LC/MS-based direct RNA sequencing with concomitant base-calling and modification analysis capability. **S. Zhang**

**10:30 14.** Structural studies of C-terminal binding protein (CtBP): Working towards an understanding of oligomeric state to design small-molecule inhibitors. **A.G. Bellesis**

**10:45 15.** Towards the chemo-enzymatic synthesis of the heptapeptide antibiotic complestatin: Investigating the role of the P450 oxygenases ComI and ComJ in aryl linkage formation. **A. Mollo**

DoubleTree by Hilton Hotel Binghamton  
Carlton Room A

## Chemical Hazard Mitigation

*Cosponsored by CATL*

N. Pomerantz, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 16.** Self-decontaminating systems for environmental and military applications. **D. Dwyer**, G.S. McGrady, W.E. Jones

**8:25 17.** Fabrication and characterization of plasmonic nanocomposites for use in obscuration and catalysis. **D.L. McCarthy**, Z.B. Zander, B.G. DeLacy

**8:45 18.** Reactions of metal oxides and hydroxides with hazardous gases, vapors and liquids: Detection and decomposition. **J.E. Whitten**, Y. Wang, S. Kim, R.S. Somaratne, O. Grimm, S.K. Sengupta

**9:05 19.** Sulfur mustard breakthrough behavior on various metal-organic frameworks. **B.J. Schindler**, E.J. Bruni, W. Gordon, M. McEntee, J.B. DeCoste, A.M. Ploskonka, G.W. Peterson

**9:25** Intermission.

**9:55 20.** Functionalized fabrics as a threat agent barrier. **B.J. Johnson**, B.J. Melde

**10:15 21.** Multifunctional polymer supported polyoxometalates. **M. Laskoski**, K.P. Sullivan, H.L. Ricks-Laskoski, C.L. Hill

**10:35 22.** Sequestration coating for decontamination of chemical agent contaminated surfaces. **L.F. Hancock**

**10:55 23.** High-capacity chloramine surface treatments for self-decontaminating textiles. **C. Howland**

**11:15 24.** Iron Oxyhydroxide deposited on cotton cloths as protection media against chemical warfare agent surrogate (2-chloroethyl ethyl sulfide). **R. Wallace**, D.A. Giannakoudakis, M. Florent, C.J. Karwacki, T. Bandosz

DoubleTree by Hilton Hotel Binghamton  
Carlton Room B

## **Inorganic Chemistry**

J. Fang, *Organizer, Presiding*

**8:00 312.** Ru<sub>3</sub>60: Investigating the chemistry of a dinuclear MCU-inhibitor. **S.R. Nathan**

**8:25 313.** Investigation of conjugated polyelectrolytes as fluorescent chemosensors. **W. Wu**, A. Chen, Z. Qing, W. Bernier, W.E. Jones

**8:50 26.** Mechanochemical synthesis of [L<sub>n</sub>CuX<sub>2</sub>] (L = 3-cyanopyridine, 2-amino-3-cyanopyridine, 2-amino-5-cyanopyridine; n = 1, 2; X = Cl, Br) via drop-solvent grinding. **J.E. Chellali**, P.C. Farris, C.P. Landee, M.M. Turnbull

**9:15 27.** Structural variations involving s-block metal pyrazolates. **J.J. Woods**, A.G. Goos, C.M. Lavin, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

**9:40** Intermission.

**10:00 28.** Electrochemical rectification of molecular multilayered films towards redox mediators for dye-sensitized solar cells. **M.R. Civic**, S. Donovan, J. Edgington, P.H. Dinolfo

**10:25 29.** Structural, magnetic susceptibility, and EPR results for a family of weakly interacting copper(II) halide compounds with 1,4'-bipyridinium. **J.C. Monroe**, C.P. Landee, M. Rademeyer, F.T. Greenaway, M.M. Turnbull

**10:50 30.** Mechanochemical synthesis of copper(II) halide complexes: Synthesis, structure and magnetic properties of 2-amino-5-bromo- and 2-amino-5-chloropyridine complexes. P.C. Farris, C.P. Landee, **M.M. Turnbull**, A.D. Wall, J.L. Wikaira

DoubleTree by Hilton Hotel Binghamton  
Johnson Room

### **Nanotechnology: From Fundamentals to Applications**

J. Luo, *Organizer*

C. Zhong, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 331.** Understanding surface properties and reactivity of metal oxide nanoparticles for diagnostics and therapeutic applications. **S. Andreescu**

**9:05 332.** Programmable release with photo-disruptable layer-by-layer polyelectrolyte multilayers incorporating quadruple photocleavable chromophores. **X. Hu**, S.W. Thomas

**9:25 333.** A general strategy for the synthesis of metal sulfide quantum dot nanoparticles. **L. Bian**, K. Ring, J. Ritz, P. Goulet

**9:45 334.** Hairy nanoparticles as soft templates to grow mesoporous oxides and carbons. B. Liu, **J. He**

**10:05 335.** Nanoparticle-based biomolecule detection using SPR and SERS: Understanding the role of the interparticle interactions. **Z. Skeete**, C. Salazar, W. Sun, F. Vides, J. Luo, C. Zhong

**10:25** Intermission.

**10:40 336.** Insights into the synthesis of alkanethiolate-protected metallic nanoparticles. **J. Ritz**, B.G. Root, P. Goulet

**11:00 337.** Toxicity evaluation of metal oxide particles and chemical additives used in the CMP industry. **E. Dumitrescu**, D. Karunaratne, K. Wallace, S. Andreescu

**11:20 338.** Nanocomposites from tunable dendrons and nanoparticles. **S. Yan**, X. Liu, C.L. Ghazvini, S. Bryant, N. He, W. Zhao, J. Lombardi, Z. Skeete, J. Luo, M.D. Poliks, I.G. Ivanov, C. Zhong

**11:40 339.** Ultra-thin layer growth of palladium on polycrystalline gold electrodes by surface limited redox replacement redox replacement. **I.O. Achari**, S. Ambrozik, N.G. Dimitrov

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Watson Room

### **Organic Chemistry**

M. J. Vetticatt, *Organizer, Presiding*

**8:00 40.** Revisiting the Witkop-Winterfeldt oxidation through organic photoredox catalysis. K. Wu, S. Kaur, **T. Wang**

**8:35 41.** From proton sponge analogues and N<sup>1</sup>-centered cations to Au(I) catalysis. **T. Dudding**

**9:10 42.** Enantiodivergent catalysis of the  $\alpha$ -amination reaction of aldehydes. **J.M. Macharia**

**9:35** Intermission.

**9:55 43.** Reversible covalent inhibition of isocitrate lyase by 3-nitropropionate. **A.S. Murkin**, S. Ray, M. Moynihan

**10:30 44.** Catalytic intermolecular anti-Markovnikov hydroamination via a visible-light photoredox protocol. **B.C. Lainhart**, A. Musacchio, X. Zhang, R.R. Knowles

**10:55 45.** Trichloroacetimidate substitution reactions in the synthesis of pyrroloindolines. **J.D. Chisholm**, A.A. Adhikari

Holiday Inn  
La Tasse Room

### **Smart Energy**

G. S. McGrady, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:10 46.** Process intensification in preparative chemistry: Developing and using new tools for energy efficient synthesis. **N.E. Leadbeater**

**8:55 47.** Rationally controlling bioluminescence resonance energy transfer through modification of quantum rod-luciferase nanoconjugates. **L.M. Karam**, M.M. Maye

**9:25 48.** Novel synthesis of oxynitride photocatalysts. J. Shaves, J. Miller, **N. Abrams**

**9:55 50.** Teaching freshman advanced smart energy concepts through research immersion. **J. Proper**, W.E. Jones, L. Piper, M.S. Whittingham, B. White, M. Fegley, N. Stamp, M.J. Wahila

**10:25** Intermission.

**10:45 49.** Effect of grain improvement on carrier lifetime in perovskite solar cells. **T.P. Dhakal**, D. Fisher, F. Saouma, J. Jang

**11:15 51.** Solid-state dye sensitized solar cells using vapor phase polymerized poly(3,4-ethylenedioxythiophene) as a hole transport layer. **S.M. Boyer**, F. Schreffler, W.E. Bernier, W.E. Jones

DoubleTree by Hilton Hotel Binghamton  
Link Room

## Theoretical & Computational Chemistry

R. A. Distasio, *Organizer*

J. Panetier, *Organizer, Presiding*

**8:55** Introductory Remarks.

**9:00 53.** Computational study of batteries utilizing chevrel phase cathodes for intercalating  $\text{Ca}^{2+}$  ions. **M. Smeu**

**9:20 54.** SiR/TiO<sub>2</sub> and GeR/TiO<sub>2</sub> (R = H, Me) heterostructures: Promising candidates for photocatalytic applications. **A. Nijamudheen, A.V. Akimov**

**9:40 55.** Density-functional study of the La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> low-index faces. **Y. Mantz, Y. Duan**

**10:00** Intermission.

**10:30 56.** When can the Landauer formalism reproduce time-dependent transport? **I. Franco**

**10:50 57.** The dipole polarizability of a condensed-phase water molecule. **K. Lao, J. Lunger, R. Maitra, R.A. Distasio**

**11:10 58.** Effective Hamiltonian theory treatment of multireference effects in dissociation reactions of water oxidation catalysts with multiple transition metal atoms: An efficient theoretical approach with practical applications. **J.R. Buchwald, V. Meunier, P.H. Dinolfo**

**11:30 59.** Study of the kinetics of hydrogenation of benzene using numerical methods. **R. Kyung, H. Lew, D. Hwang, K. Acquah**

DoubleTree by Hilton Hotel Binghamton  
Serling Room

## Chemical Education

*Cosponsored by CHED*

D. P. Brennan, B. Turnpenny, *Organizers*

A. M. Sheridan-Brennan, *Organizer, Presiding*

**9:00 60.** CHEM 150: Improving student interest from general chemistry to organic chemistry. **P. Tanui**

**9:20 61.** Keeping students engaged in large lecture format organic chemistry classes. **R.M. Kissling, P. Tanui**

**9:40 62.** Engaging students in bringing laughter to chemistry classrooms! **V.A. Jouraeva**

**10:00 63.** Inquiry based learning in an organic chemistry undergraduate curriculum. **V.C. Waghulde, U. Panse**

**10:20** Intermission.

**10:40 64.** To incorporate interdisciplinary approach and research-based learning in an undergraduate curriculum. **U. Panse**, V.C. Waghulde

**11:00 65.** Benefits of an introduction to college chemistry course to general chemistry students. **B. Turnpenny**, E.K. Mushibe, A.S. Silva

**11:20 66.** Blended vs. traditional offerings in forensics: An investigation into student outcomes. **D.P. Brennan**

**11:40 67.** Chemistry education collaborations across cultural and national borders: The Middle East. **M.Z. Hoffman**, Z.M. Lerman

## **THURSDAY AFTERNOON**

DoubleTree by Hilton Hotel Binghamton  
South Ballroom

### **Women Chemists Committee Luncheon**

A. Charlebois, *Organizer, Presiding*

**12:00** Introductory Remarks.

**12:10 68.** Balancing the equation of professorship, parenting, and personal satisfaction as a female chemistry professor. **M. Levine**

DoubleTree by Hilton Hotel Binghamton  
North Riverside Room

### **Analytical Chemistry**

M. R. Hepel, *Organizer*

J. Halamek, *Presiding*

**1:00 69.** Recognition of originator attributes from fingerprints using chemical assays. **E. Brunelle**, C. Huynh, A.M. Le, L. Halámková, J. Agudelo, L. McGoldrick, J. Halamek

**1:30 70.** Utilization of fingerprints for the determination of biological sex via bioaffinity-based cascades. **C. Huynh**, E. Brunelle, L. Halámková, J. Agudelo, L. McGoldrick, J. Halamek

**1:50 71.** Analyzing heavy metals in the soil samples of local farms in Oswego NY. **J. Calvert**, H. Posada, V. Niri

**2:10** Intermission.

**3:00 73.** Developments in application of multidimensional time model for probability cumulative function with Brownian motion on fractals to chemical reactions. **M. Fundator**

**3:20 74.** Qualitative and quantitative analysis the vapor of electronic cigarettes. **T. Jones**, G. Peterson, V. Niri

**3:40 75.** 50 Shades of the glucose and galactose binding protein. **L.A. Luck**, S.A. Asher, Z. Cai

**4:00** Concluding Remarks.

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Serling Room

### **Chemical Education**

*Cosponsored by CHED*

A. M. Sheridan-Brennan, *Organizer*

D. P. Brennan, B. Turnpenny, *Organizers, Presiding*

**1:00 76.** Models for integrating chemistry and biology laboratory instruction at the introductory level. **N. Abrams**

**1:20 77.** Development of an introductory biological chemistry lab with an undergraduate research component. **T. Curtis**, D.P. Brennan, A.S. Silva, S. Solmaz, B.P. Callahan

**1:40 78.** Teaching freshman advanced concepts in biomedical chemistry through a sequence of course-based research experiences. **S.C. Flynn**

**2:00 79.** Safety in the undergraduate laboratory: A mother's perspective. **A.M. Sheridan-Brennan**

**2:20** Intermission.

**2:40 80.** Implementation of a peer mentor program in the general chemistry labs. **K.I. Gublo**

**3:00 81.** A study of olivine cathode materials for lithium ion batteries: A material science laboratory exercise for chemistry majors. **D. Ji**, F. Omenya, A.S. Silva, Y. Sun

**3:20 82.** A research based chemistry lab: Synthesis and characterization of fluorescent conjugated polymer. **W. Wu**, **D. Ji**, A.S. Silva, A. Chen, Y. Sun

**3:40 83.** ChemDetectives: A stoichiometry case study for general chemistry. **A.K. Sharma**

**4:00 84.** Maximizing effectiveness of chemistry presentations for elementary and middle school aged students: Applications in chemical education. **A. Zhang**, **S. Nadkarni**, **A. Shayya**, M. Levy

DoubleTree by Hilton Hotel Binghamton  
Arlington Room A

### **Computer Aided Drug Discovery**



A. Schlessinger, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 85.** Design of heterochiral peptides to target protein-protein interactions in Influenza. **V. Nanda**

**1:30 86.** Computational detection of steric and electrostatic influences on protein binding specificity. **B.Y. Chen**

**1:55 87.** Structural characterization of substrate transport selectivity of the SLC13 Family of Na<sup>+</sup>/dicarboxylate cotransporters. **C. Colas**, A.M. Pajor, A. Schlessinger

**2:20** Intermission.

**2:35 88.** Permeation, gating, and modulation of a TRP channel. **H. Koldsø**

**3:00 89.** DFGmodel: Predicting protein kinase structures in inactive states and application in structure-based discovery of type-II inhibitors. **P. Ung**, A. Schlessinger

**3:25 90.** Computational understanding of drug resistance of HCV NS3/4A protease: The curious R155K\_D168A variant. **Z. Guo**

Holiday Inn  
Southern Tier Room

### **Electrochemical Energy Conversion & Storage**

G. Wu, *Organizer, Presiding*  
W. Sheng, J. Suntivich, *Presiding*

**1:00 91.** Electrocatalysis on single-crystal transition-metal oxides. **J. Suntivich**, D. Kuo

**1:30 92.** Hydrogen electrocatalysis: Finding the reaction descriptor and developing advanced materials. **W. Sheng**

**2:00 93.** Structural and mechanistic basis for the activity of iron-nitrogen-carbon electrocatalysts toward oxygen reduction in acid. **Q. Jia**, J. Li, S. Ghoshal, S. Mukerjee, F. Jaouen, M. Sougrati

**2:30** Intermission.

**3:00 94.** Precious metal-free catalyst technology for polymer electrolyte fuel cells. **G. Wu**

**3:30 95.** Biomimetic electrocatalysts for renewable energy storage applications. **P.H. Dinolfo**, J.R. Buchwald, S. Kal, T.R. LeBlond

**3:48 96.** Intrinsic challenges in creating a reversible copper(II) fluoride cathode for lithium-ion batteries. **N.J. Zagarella**, F. Omenya, Y. Chung, M.S. Whittingham

**4:06 97.** Application of bifunctional nanoalloy catalysts in rechargeable lithium-oxygen battery and its synergistic properties. **N. Kang**, J. Kim, W. Zhao, J. Yin, S. Shan, J. Luo, C. Zhong

**4:24 98.** Synthesis, characterization and optimization of vanadium phosphates as cathode material for lithium-ion batteries. **Y. Shi**, H. Zhou, F. Xin, Y. Huang, N. Chernova, F. Omenya, M.S. Whittingham

**4:42 99.** Corning's lithium ion capacitor technology. **R.S. Kadam**, K.P. Gadkaree

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Endicott Room

### **General Papers**

C. Grewer, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:10 100.** Influence of metal ions on the mode of action of tunicate antimicrobial peptides. **A.M. Angeles Boza**, S. Juliano

**1:30 101.** Reductive mobilization of iron from ferritin: Reality or artifact? **A. Melman**, E. Vane

**1:50 102.** Design of Co(III) complexes as theragnostic agents. **A.P. King**, J. Ahn, H. Gellineau, L. Feng, J. Wilson

**2:10** Intermission.

**2:40 103.** Unique roles of metals in biocatalytic systems. **Y. Zhang**

**3:00 104.** Self-assembly of short peptides in presence of copper to produce oxygen activation catalyst. **P. Gosavi**, O. Makhlynets, I.V. Korendovych

**3:20 105.** Structure-based peptide-modeling software for rational drug design. **A.S. Bayden**, J.T. Swanson, J.H. Audie, M.A. Jarosinski, D.J. Diller

**3:40 106.** Iron(II) induced linker cleavage in transferrin-doxorubicin conjugates. D. Folmsbee, A. Rudkouskaya, M. Barroso, **A. Melman**

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Carlton Room B

### **Inorganic Chemistry**

J. Fang, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 107.** Morphology control synthesis of Pt-Ni tetrahexahedron. **Y. Luan**, J. Fang

**1:45 108.** Oxidation resistant behavior of stainless Fe/FeCrNi core/alloy nanoparticles. **L. Pathade**, T.L. Doane, M.M. Maye

**2:10 109.** Investigating the mechanism of formation of metal-organic frameworks by small and wide angle X-ray scattering. **C.C. Webb Jr**, M. Kriechbaum, A. Torvisco, H. Amenitsch, K. Ruhlandt-Senge

**2:35 110.** Cathode materials for Li-ion batteries synthesized from  $\text{LiVOPO}_4 \times 2\text{H}_2\text{O}$ . **M.V. Hidalgo**, Y. Chung, F. Omenya, N.A. Chernova, M.S. Whittingham, L. Wangoh, L. Piper, Y. Lin, S. Ong

**3:00** Intermission.

**3:20 111.** Li diffusion and chemical transformations of  $\text{Li}_2\text{VO}_2\text{F}$ . **X. Wang**, F. Omenya, N. Chernova, M.S. Whittingham

**3:45 112.** Coordination chemistry of magnesium and bismuth compounds. **B. Wilson**, Y. Takahashi, A. Torvisco, A.Y. O'Brien, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

**4:10 113.** Synthesis and structures of heteroleptic alkaline earth metal tetraarylborate pyrazolates. **C.M. Lavin**, J.J. Woods, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

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Carlton Room A

### **Metals and Metalloproteins**

F. Bou-Abdallah, *Organizer, Presiding*

**1:00 114.** Iron and heme: Their exquisite relationship makes blood red. **P. Ponka**

**1:45 115.** Mechanisms of iron trafficking in the neurovascular unit: Capillary endothelial cells, astrocytes and neurons. **D. Kosman**

**2:30** Intermission.

**2:45 116.** Ferritin: Not just an intracellular iron storage protein. **J. Connor**

**3:30 117.** Mitochondrial iron and heme metabolism in red cells. **B. Paw**

DoubleTree by Hilton Hotel Binghamton  
Kilmer Room

### **New Investigator**

*Financially supported by Krackeler*

K. R. Kittilstved, S. Solmaz, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05 118.** Organometallic manganese for water splitting chemistry. **D.C. Lacy**

**1:30 119.** Electronic properties of colloidal ternary semiconductor nanocrystals. **K.E. Knowles**

**1:55 120.** Tunable optical properties of manganese doped quantum rods for green energy applications. **W. Zheng**

**2:20 121.** Enzymes, RNA and nanomaterials: Using biochemical approaches to control the targeting, release and biological activity of nanoparticle drug delivery systems. **J.L. Rouge**

**2:45** Intermission.

**3:15 122.** Sterols as covalent modifiers of protein function. **B.P. Callahan**

**3:40 123.** Receptor recognition by porcine circovirus 2. S. Feng, A. Schreyer, **R. Khayat**

**4:05 124.** Membrane disruption Induced by 40-residue beta-amyloid peptides in Alzheimer's Diseases. **W. Qiang**, K. Doherty, D. Delgado, Q. Cheng, H. Dong, C. Grewer

**4:30 125.** Nucleic acid-based nano tools for bioanalytical studies. **M. You**

**4:55** Concluding Remarks.

DoubleTree by Hilton Hotel Binghamton  
Johnson Room

### **Organometallic Catalytic Activation of Small Molecules**

A. Lees, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 126.** Pincer supported iron complexes for the reversible hydrogenation of CO<sub>2</sub> to formic acid and methanol. **N. Hazari**, W.H. Bernskoetter

**1:30 127.** Hybrid photocatalysts for solar energy conversion. **G. Li**

**1:55 128.** Differences in carbon isotope discrimination during the reduction of CO<sub>2</sub> by rhenium and ruthenium complexes. **A.M. Angeles Boza**, T. Schneider

**2:20** Intermission.

**2:50 129.** Solar hydrogen production using carbon nanomaterials in hybrid photocatalytic schemes. **C.A. Caputo**

**3:15 130.** Ionic liquid-enhanced electrocatalytic reduction of CO<sub>2</sub> with a homogeneous catalyst. **D.C. Grills**, Y. Matsubara, Y. Kuwahara

**3:40 131.** Tuning the catalytic active site of Mn(I) and Re(I) polypyridyl catalysts for CO<sub>2</sub> reduction. **J.J. Rochford**

**4:05 132.** Metal-templated synthesis of ammonia borane. **D. Wolstenholme**, J.L. Dobson, J.H. Lee, G.S. McGrady

**4:30 133.** Electrochemical reduction of CO<sub>2</sub> by homogeneous early transition metal catalysts. **K.A. Grice**, C. Saucedo, M. Sovereign, A. Cho

Holiday Inn  
La Tasse Room

### **Smart Energy**

G. S. McGrady, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 134.** Accelerating the development of hydrogen storage material development through national laboratory led collaborative research efforts. **N.T. Stetson**

**1:50 135.** Solution-based routes to ammine metal borohydrides: Unprecedented formation of ammonia borane. **G.S. McGrady**, M. Mostajeran, D. Wolstenholme, C. Frazee, R.T. Baker

**2:20 136.** Hydride-hydride bonding: The missing link in the evolution of hydrogen from main group hydrides. **D. Wolstenholme**, G.S. McGrady

**2:50** Intermission.

**3:10 137.** Novel carbon(C)-boron(B)-nitrogen(N)-containing H<sub>2</sub> storage materials. S.Y. Liu, **J.S. Ishibashi**

**3:40 138.** Freeze-dried ammonia borane-polyethylene oxide composites: Phase behaviour and hydrogen release. **A. Ploszajski**, M. Billing, A. Nathanson, M. Vickers, F. Tariq, N. Brandon, S. Bennington

**4:10 139.** Hydrogenation of polycyclic aromatic hydrocarbons for smart energy applications. **G.S. McGrady**, C. Allen, S. Brough, S. Riley

**4:40** Concluding Remarks.

DoubleTree by Hilton Hotel Binghamton  
Link Room

### **Theoretical & Computational Chemistry**

J. Panetier, *Organizer*

R. A. Distasio, *Organizer, Presiding*

**1:00 140.** Kohn-Sham DFT and TDDFT calculations of charge-transfer and 'charge-transfer-like' electronic excitations and other band gaps. **J. Autschbach**

**1:30 141.** Investigation of electron-hole interaction in nanoparticles using explicitly correlated wavefunction based methods. J. Scher, **A. Chakraborty**

**1:50 142.** Electron correlation in the two-electron atom with variable nuclear charge. **L. Tu**, P. Varga, R.A. Distasio

**2:10** Intermission.

**2:40 143.** Nonadiabatic dynamics with complete active space methods and graphical processing units. **E.G. Hohenstein**

**3:00 144.** Scaling relationships for nonadiabatic energy relaxation times in warm dense matter: Toward understanding the equation of state. E. Pradhan, R.J. Magyar, **A.V. Akimov**

**3:20 145.** Quantum dynamics and electronic structure in organic photovoltaics. **T.J. Hele**, E.G. Fuemmeler, S.N. Sanders, E. Kumarasamy, M. Sfeir, R. Hoffmann, L. Campos, N. Ananth

**3:40 146.** Non-adiabatic molecular dynamics with  $\Delta$ SCF excited states ( $\Delta$ SCF-NA-MD). **E. Pradhan, A.V. Akimov**

**4:00** Concluding Remarks.

DoubleTree by Hilton Hotel Binghamton  
South Ballroom

### **Keynote Address**

C. Grewer, *Organizer, Presiding*

**5:00 147.** Taxol, tubulin and tumors. **S. Horwitz**

## **THURSDAY EVENING**

DoubleTree by Hilton Hotel Binghamton  
North Ballroom

### **General Posters**

A. S. Silva, *Organizer*

**6:00 - 7:00**

**148.** Ab initio studies of magnesium hydroxide nanoparticles as potential catalysts for thermal decomposition of acetic acid. **D.C. Perera**, J.C. Rasaiah, J.W. Hewage

**149.** Using magnetic resonance force microscopy (MRFM) to probe triplet excitons in organic photovoltaic devices. **E.A. Curley**, J.A. Marohn

**150.** Activatable interpolymer complex – superparamagnetic iron oxide nanoparticles (IPC-SPIOs) as magnetic resonance (MR) contrast agents sensitive to oxidative stress. **E. Yoo**, H.A. Cheng, C.A. Nwasike, L.E. Nardacci, D.J. Beaman, O. Fisher, A.L. Doiron

- 151.** Carbohydrate-based inducers of cellular stress for targeting cancer. **F. Ndombera**
- 152.** Synthesis, properties and complexation study of novel fluorenone macrocycles. **I. Tamgho**, D. Jones, M. Levine
- 153.** The effects of hierarchical structure on out-of-plane charge transport in organic solar cell active layers. **J. Mehta**, S. Button, J.M. Mativetsky
- 154.** Computational analysis of the dynamics and energetics of secondary-active glutamate transport. **J. Wang**, C. Grewer
- 155.** Multifunctional nanoprobe for biological applications. **J. Li**, S. Shan, Z. Skeete, J. Luo, M.R. Hepel, C. Zhong
- 156.** Novel electrochemical biosensors for assessing food safety. **J. Zhang**, O.A. Sadik
- 157.** TiO<sub>2</sub> nanotubes sensitized with CdS QDs photoanodes for hydrogen generation by solar energy. **J. Gonzalez Moya**, Y. Garcia Basabe, D. Maia Oliveira, G. Machado
- 158.** Homogeneous catalysis of the electrochemical reduction of CO<sub>2</sub> by Re(I) complexes: Role of the pyridine ligands. **J. Nganga**
- 159.** Kinetic isotope effects and theoretical models help probe long-standing mechanistic debate for diphenylprolinol silyl ether catalyzed Michael Reaction between aldehydes and nitroolefins. **J.A. Izzo**, S.C. Marker, M.J. Veticatt
- 160.** Crime scene simultaneous estimation of the time since deposition and the age of the originator from a blood spot. **J. Agudelo**, L. Halámková, R. Rodrigues, C. Huynh, E. Brunelle, J. Halamek
- 161.** Computational investigations of nickel based electrocatalysts for CO<sub>2</sub>RR. **K. McCardle**, J. Panetier
- 162.** Electrochemical evaluation of nanoparticles by nano-impact methodology. **K. Kirk**, A. Karimi, N.P. Sardesai
- 163.** Understanding the oxidation behavior of stainless transition metal core/alloy nanoparticles. **L. Pathade**, T.L. Doane, M.M. Maye
- 164.** Identification by body fluids using single analyte bioaffinity-based assays. **L. McGoldrick**, J. Agudelo, E. Brunelle, C. Huynh, L. Halámková, J. Halamek
- 165.** Understanding the role of defects in high energy transfer efficiency between firefly luciferase and semiconductive quantum rods. **L.M. Karam**, M.M. Maye
- 166.** Vapor-phase polymerized poly(3,4-ethylenedioxythiophene) (PEDOT) on TiO<sub>2</sub> fibers for supercapacitor electrodes. M.T. Fox, **L. Tong**, J. Liu, S.M. Boyer, L.A. Sonnenberg, W. Bernier, W.E. Jones
- 167.** Investigation of energy transfer in perylene diimide based multilayer light harvesting arrays. **L. Ayensu-Mensah**, Z. Huang, P.H. Dinolfo
- 168.** Preparation of an Infrared light responsive layer-by-layer film on colloidal substrates. **M. Feeney**, S.W. Thomas

- 169.** Engineering the extracellular loops of Outermembrane protein G in creating a nanopore sensing platform. **M.A. Fahie**
- 170.** Unconventional hydrogen bonding in chemical hydrides: Supramolecular interactions and crystal engineering of borazine analogues. **N. Ding**, L.L. Tomasevich, J. Proper, G.S. McGrady
- 171.** Characterization of electrical properties of nanoparticle-nanofibrous membranes. **N. Kang**, J. Kim, F. Lin, W. Zhao, M. Almihdhar, J. Lombardi, S. Yan, J. Luo, B.S. Hsiao, M.D. Poliks, C. Zhong
- 172.** Progress towards the synthesis of pestalazine A. **N.S. Mahajani**, J.D. Chisholm
- 173.** Synthesis, base pairing and structural studies of DNA duplexes containing geranyl-2-thiothymidine derivatives. **P. Haruehanroengra**, R. Wang, J. Sheng
- 174.** High-resolution structures of the A $\beta$ <sub>40</sub> fibrils grown from the surface of phospholipid liposomes. **Q. Cheng**
- 175.** Brønsted acid catalysis of intermolecular cope-type hydroamination. **R. Karugu**, M.J. Vetticatt
- 176.** Structure elucidation of 2 novel 24,28-cyclopropyl sterols from a tropical orchid.. **R. Joseph**, J.P. Giner
- 177.** Single and few layer WS<sub>2</sub> as a chemical vapor sensor. **S. Matthews**, D.T. McCall, C. Zhao, H. Zeng, F.V. Bright
- 178.** Membrane location and protonation driven membrane insertion of pH-low insertion peptide (pHLIP) by solid state nuclear magnetic resonance. **S.A. Otieno**
- 179.** Functional nanocomposites towards advanced sensing interfaces. **S. Yan**, X. Liu, **C.L. Ghazvini**, S. Bryant, N. He, W. Zhao, J. Lombardi, Z. Skeete, J. Luo, M.D. Poliks, I.G. Ivanov, C. Zhong
- 180.** Calcium and titanium substitution effect on magnetic properties of Sr(Sn<sub>(1-x)</sub>Fe<sub>x</sub>)O<sub>3-d</sub>. **S. Suzuki**, K. Nomura, T. Mizunuma, A. Okazawa, Y. Koike
- 181.** Radioactive cesium in suspended matter collected at Tamagawa River basin. **S. Okumura**, K. Ochi, G. Ishihara, K. Fujii, K. Hagiwara, Y. Koike
- 182.** Multilateral chemical analysis of UV irradiated paraloid™ B-72. **S. Okamoto**
- 183.** Photophysical and biological properties of rhenium tricarbonyl complexes bearing water-soluble phosphine ligands. **S. Marker**, **J. Wilson**
- 184.** Illuminating the requirements for bioluminescence with the latent luciferase CG6178 and luciferin analogs. **S.T. Adams**, D. Sharma, M. Bohn, C.A. Schiffer, S.C. Miller
- 185.** Ab initio study of the electronic structure of copper-doped nickel tungstate. **S. Shepard**, M. Smeu
- 186.** Fluorophore disaggregation for thiol sensing. **T.I. Chio**, T.I. Radford, S.L. Bane
- 187.** Rearrangement of benzylic trichloroacetimidates to trichloroacetamides. **T. Suzuki**, A.A. Adhikari, J.D. Chisholm
- 188.** First-principles evaluation of the chevrel phase intercalated with Ca for battery cathodes. **T.R. Juran**, M. Smeu



- 189.** Factors influencing the performance of organic nanofiber array transistors. **T. Yang**, J. Mehta, J. Ortiz, E. Shehi, C. Cooper, J.M. Mativetsky
- 190.** 'Click' based functionalization of DNA nanostructures. **V. Valsangkar**, A.R. Chandrasekaran, R. Wang, P. Haruehanroengra, V.R. Pelliccia, O. Levchenko, K. Halvorsen, J. Sheng
- 191.** Kinetic isotope effects and mechanism for *N*-heterocyclic carbene catalyzed hydroacylation of unactivated olefins. **V. Wambua**
- 192.** Computational study for the CO<sub>2</sub> reduction reaction using rhenium-electron catalysts. **X. Li**, J. Panetier
- 193.** Nanoalloy catalysts: Structural characterization and electrocatalytic oxygen reduction reaction in fuel cells. **Y. Zhao**, S. Shan, H. Cronk, J.W. Donohue, J. Luo, C. Zhong
- 194.** Smart gel-like carbon dots material. **Y. Zhou**
- 195.** The impact of gold nanoparticle exposure on endothelial cells. **Y. Liu**, C.H. Maiorana, K. Harada, B. Lappies, N. Rogel, L. Jarett, G.K. German, G. Mahler, A.L. Doiron
- 196.** Improving DNA-mediated self-assembly of quantum rods onto DNA origami via zwitterionic coating. **Y. Chen**, T.L. Doane, M.M. Maye
- 197.** Isotope effect, mechanism and methodology development of the Michael addition of carbonyl to trans-*b*-nitrostyrene catalyzed by L-proline and its derivatives. **Y. Hong**, M.J. Vetticatt
- 198.** Femtosecond impulsive vibrational spectroscopy of rhodamine and rosamine sensitizers: Structural displacements in the excited-state. **Z. Piontkowski**, D. McCamant
- 199.** Smart Ni coating for corrosion protection of Mg alloy. **Z. Xie**, D. Li, C. Zhong
- 200.** Design and synthesis of fluorescent conjugated polymers as fluoride chemosensor. **Z. Qing**, A. Chen, W. Wu, W. Bernier, W.E. Jones
- 201.** Design of mononuclear non-heme enzyme for oxygen activation. **Z. Lengyel**, J.J. Rempillo, I.V. Korendovych, O. Makhlynets

DoubleTree by Hilton Hotel Binghamton  
North Ballroom

### General Posters

A. S. Silva, *Organizer*

**7:15 - 8:15**

**202.** Facilitating STEAM-based mentorships between high school students and elementary-middle school aged youth in their community, through the establishment of a 501(c)(3) not-for-profit organization: Applications in chemical education. **A. Zhang**, **S. Nadkarni**, **S. Vollero**

**203.** CMDscaffold: A virtual peptide library for *de novo* rational drug design. **A.S. Bayden**, D.J. Diller, J.H. Audie

- 204.** CoMBASA: A hydrophathy-based tool for mapping out receptor-based pharmacophores. **A.S. Bayden,** A. Tripathi, C. Da, G.E. Kellogg
- 205.** Derivatives of 5-(imidazo[2,1-b]thiazol-6-yl)-4-methylthiazol-2-amine new effective EGFR-kinase inhibitors. **A.S. Bunev**
- 206.** Investigating the background interferences of carpet substrates in accelerant identification. **A. Aldrich,** **G. Odugbesi,** S. Haddadi
- 207.** Effectiveness of pre-lab videos for sophomore an organic chemistry course. **A.J. Kiessling**
- 208.** Controlled fabrication of patterned calcium alginate hydrogels through reductive cation exchange. **A. Melman,** M. Bruchet
- 209.** Mechanistic organic chemistry with reactive oxygen speices (ROS): Air-water interface reactions. **B. Malek,** W. Fang, I. Abramova, A.A. Ghogare, A. Greer
- 210.** Determination of organochlorine pesticides and polychlorinated biphenyls using GC-MS/MS operated in the MRM mode. **B. Prakash,** T. Ogura, R. Kitano, W. Lipps
- 211.** Investigation on the accumulation and the effects of lead on invertebrate nervous system function and behavior. L. Lubecki, S. Amico-Ruvio, **D.T. Stewart**
- 212.** Get involved with the ACS Division of Chemical Education. **D.L. Zimmerman**
- 213.** Removal of heavy metal ions by a polymer matrix containing ditiocarbamate as a chelating group. **F. Damkaci,** **B. Ladd,** R. Scalzo
- 214.** Grafting acrylic acid to polystyrene surfaces modified with oxygen atoms. X. Li, F. Lu, J. On, R. Divens, M. Cocca, K. Vega, A. Bailey, T. Debies, M. Mehan, S. Gupta, **G.A. Takacs**
- 215.** Photoactive silica surface coated with (3-phenoxypropyl)silane: Studies of photosensitizer release and singlet oxygen production. **G. Ghosh,** M. Vignoni, N. Walalawela, A.A. Ghogare, S.A. McFarland, A.H. Thomas, A. Greer
- 216.** Mechanism for cell cycle-specific localization of CENP-F. **H. Cui,** K. Loftus, S. Solmaz
- 217.** Computed regioselectivity in ene reactions of singlet oxygen with the natural product hyperforin. **I. Abramova,** B. Rudshiteyn, J.F. Liebman, A. Greer
- 218.** Comparison of chemical structures of environmental hormones for cardiact and phototactic effects on daphnia magna. S. Moon, **J. Lee**
- 219.** Millisecond-resolved transient EQCM studies of monolayers of heavy metals and DNA on gold electrodes. **J. Peter,** G. Flechsig
- 220.** Antimicrobial activity of extracts of anacardium occidentale stem barck and isolation of phtochemicals. **J.K. Adesanwo,** I. Adewusi
- 221.** Extractives from root of *Morinda lucida*(Benth), their antimicrobial and antioxidant activities. **J.K. Adesanwo,** O.A. Igbeneghu

- 222.** Characterization of chromium substituted lithium vanadium phosphate. **K.J. Lee**, Y. Chung, N.A. Chernova, F. Omenya, M.S. Whittingham
- 223.** Specificity determinants of insulin-degrading enzyme. **L. Stefanidis**, J.E. Smith-Carpenter, B.J. Alper
- 224.** Manganese- and copper-doped ZnS quantum dots synthesis and characterization. **L. Ji**, M.R. Hepel
- 225.** Delivery of anti-cancer drug methotrexate and adjuvant leucovorin. **M. Palmer**, A. Ortiz, A. Marotta, M.R. Hepel
- 226.** Target-induced release of anti-leukemia drug azacitidine covalently attached to AuNP nanocarriers. **M. Smith**, M.R. Hepel
- 227.** Polymerization model study: Synthesis of an epoxyenone. **M. Blauvelt**
- 228.** Bio-catalyzed regioselective synthesis in undergraduate organic laboratories: Multi-step synthesis of 2-arachidonoylglycerol. **M.R. Johnston**
- 229.** Synthesis and evaluation of potential inhibitors of hedgehog cholesterololysis. **M.T. Jorgensen**, J.P. Giner, D. Ciulla, B.P. Callahan
- 230.** Fluorinated trisalkoxide bismuth species as potential MOCVD precursors. T.B. Ngo, M.E. Vonden Steinen, Y. Takahashi, B. Wilson, A. Torvisco, **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge
- 231.** Synthesis, characterization, and coordination studies of novel bismuth compounds. M.E. Vonden Steinen, T.B. Ngo, Y. Takahashi, B. Wilson, **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge
- 232.** Interfacial photosensitization reactions. **N. Walalawela**, A. Greer
- 233.** Synthesis and characterization of long chain pterin derivatives: O vs N substitution. M. Vignoni, **N. Walalawela**, S.M. Bonesi, A. Greer, A.H. Thomas
- 235.** Underpotential deposition and anodic stripping voltammetry of copper in water samples using heated screen-printed gold electrodes. **S. Colón-Rodríguez**, J. Abdulkhalek, M. Schönhoff, D. Arrigan, G. Flehsig
- 236.** Wavelength selective generation of aryl radicals and aryl cations from arylazosulfones. S. Crespi, **S. Protti**, M. Fagnoni
- 237.** Adsorption of Cr (VI) from aqueous solutions by amine functionalized cellulose pretreatment by microwave-H<sub>2</sub>O<sub>2</sub>. **S. Jingjing**
- 238.** HPLC-MS analyses of the photocatalytic degradation products of phenazopyridine. **T.A. Gray**, E. Obuya, F. Chen
- 239.** Supercritical CO<sub>2</sub> extraction of polyphenols from green tea: A new method of extraction. **T. Scott**, A.M. Fedor
- 240.** Copper catalyzed hydroxylation of aryl halides to generate phenols. F. Damkaci, **T. Sobiech**, X. Mahemuti, J. McGrath, G. Kerr
- 241.** Chemical assembly of a new ubiquitin-like post-translational modification. **T. Zheng**, T.P. Dao, J. Madison, C. Castaneda

242. Folate receptor-recognizing directed delivery of chemotherapeutic drug lenvatinib. **T. Santiago**, M.R. Hepel
243. Analysis of drugs used in facilitated criminal acts. **V. Niri**, K. Lagatta, K. Herard, S. Haddadi
244. Reductively-labile sulfonate protecting groups for live cell imaging. **A. Choi**, S.C. Miller
245. Sediments as an active source of PCB contamination to Onondaga Lake in Syracuse, New York. **A. Ingham**, J.P. Hassett
246. Template-controlled growth of organic semiconductor nanowires. **A.M. Haruk**, T. Yang, J.M. Mativetsky
247. Colorimetric assay for quantitative detection, screening and reactivity evaluation of ceria nanoparticles. **A. Othman**, S. Andreescu
248. Electrochemical investigation of surface adsorption of arsenic on metal oxide nanoparticle. **A. Karimi**, D. andreescu, S. Andreescu
249. Computational study on iron-based complexes for water oxidation. **A. Xu**, J. Panetier
250. Lewis acid catalyzed C3-alkylation of 2,3-disubstituted indoles using trichloroacetimidates. **A.A. Adhikari**, L. Radal, J.D. Chisholm
251. Synthesis and analysis of hydroxyl-modified HMBPP analogs on the stimulation and activation of Vgamma9Vdelta2 T cells. **A.M. Kilcollins**, R. Shippy, G.N. Shivers, N.A. Lentini, B.M. Zangari, C.C. Hsiao, D.F. Wiemer, A.J. Wiemer
252. Examination of nucleic acid multi-equilibriums using electrospray mass spectrometry. **B. Toro**, P. Li, D. Fabris
253. Vapor-phase polymerized crystalline PEDOT nano/micro ribbons array on patterned FeCl<sub>3</sub> formed by microcontact printing. **B. Li**, L. Tong, S.M. Boyer, J. Liu, W. Bernier, W.E. Jones
254. The essential role of ran binding domains in nuclear transport. **C. Noell**, S. Foreman, K. Loftus, A. Ceravolo, D. Pereiras, S. Solmaz
255. Determination of short-lived atmospheric radionuclides using gamma-ray disk sources prepared chemical reagents. **D. Fukuda**, K. Hagiwara, K. Fujii, Y. Koike
256. Rational design and development of polysialic acid-binding peptides. **D. Shastry**, P. Karande

## FRIDAY MORNING

DoubleTree by Hilton Hotel Binghamton  
Endicott Room

### Biochemistry

*Cosponsored by BIOL*

J. Sheng, *Organizer*

A. Shekhtman, *Organizer, Presiding*

**8:00 257.** Redefining the potential prenylome: Prenylation of non-canonical c-terminal sequences in peptides and proteins. **M.J. Blanden**, W. Schmidt, J. Houglund

**8:20 258.** Molecular mechanisms underlying eye-lens clouding and the maintenance of transparency. **J. Pande**

**8:40 259.** Biochemical and structural investigation of Ghrelin recognition and processing. **E. Cleverdon**, C.L. Cabrinha, C. Castaneda, J. Houglund

**8:55 260.** Investigation of a functionally essential domain within human ghrelin *O*-acyltransferase. **M. Campana**, J. Houglund

**9:10 261.** Antinociceptive agents targeting fatty acid binding proteins (FABP). **S. Tong**, M.W. Elmes, J. Sweeny, H. Hsu, M. Kaczocha, H. Li, R.C. Rizzo, D.G. Deutsch, I. Ojima

**9:25** Intermission.

**9:45 262.** Allosterity in bacterial environmental sensors: Understanding nature's switches to develop scientists' tools. **K.H. Gardner**, F. Correa, I. Dikiy, E. Orth, U. Edupuganti, Z. Jaber

**10:05 263.** Utility of alkylcobalamins for light-controlled biological applications. **A.C. McCue**, T.A. Shell

**10:15 264.** Kinetics of tau-hexapeptide promoted  $\beta$ -amyloid fibrillogenesis. **P.P. Rao**

**10:35 265.** Modeling a chaperone-client interaction: Mellitin binding to alpha crystallin. **L. Ramirez**, A. Pande, A. Shekhtman, J. Pande

**10:50 266.** Amplification effect of hexammine complexes upon potential pulse-induced frequency transients of DNA on an electrochemical quartz crystal microbalance. J. Peter, **G. Flechsig**

**11:10 267.** tRNA<sup>Arg</sup> and tRNA<sup>Lys</sup> - a "modified" story. **S. Vangaveti**, K. Sarachan, W. Cantara, S. Ranganathan, A.A. Chen, J. Sheng, P.F. Agris

DoubleTree by Hilton Hotel Binghamton

Watson Room

### **Biological Nuclear Magnetic Resonance Spectroscopy**

W. Qiang, *Organizer*

C. Castaneda, C. DeMott, C. Isaac, H. Nguyen, M. Tang, C. Wang, D. P. Weliky, *Presiding*

**8:00** Introductory Remarks.

**8:05 268.** Solid-state NMR of viral fusion proteins. **D.P. Weliky**

**8:35 269.** Applications of paramagnetic effects and NMR on structural studies of membrane systems. **M. Tang**

**9:05 270.** Implementing dynamic nuclear polarization in a magnetic resonance force microscope experiment for nanoscale imaging. **C. Isaac**, C. Gleave, P. Nasr, H. Nguyen, E.A. Curley, E. Afshari, J.A. Marohn

**9:30** Intermission.

**10:00 271.** A single aspartate coordinates two catalytic steps in hedgehog autoprocessing. J. Xie, T. Owen, B.P. Callahan, **C. Wang**

**10:30 272.** Effects of ALS mutations on structure, dynamics, and function of ubiquilin-2. T.P. Dao, **C. Castaneda**

**11:00 273.** Using in-cell NMR to identify potent inhibitors of *M. tuberculosis*. **C. DeMott**, R. Girardin, J. Cobbert, S. Reverdatto, D.S. Burz, K.A. McDonough, A. Shekhtman

**11:25 274.** Nanoscale magnetic resonance imaging with electron spin labeling. **H. Nguyen**, J.A. Marohn

DoubleTree by Hilton Hotel Binghamton  
Kilmer Room

### **Biosensors**

S. Andreescu, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 275.** Can your smartphone check if your food is safe? Nanosensors for rapid detection of food pathogens. **O.A. Sadik**

**8:25 276.** Low cost point-of-care protein-based cancer diagnostics. **J. Rusling**

**8:45 277.** Nanoscale optosensor. S. Matthews, J.F. Destino, D.T. McCall, **F.V. Bright**

**9:05 278.** "Phage-bots" for the rapid separation and detection of bacterial pathogens. J. Chen, T. Hinkley, Z. Wang, **S.R. Nugen**

**9:25** Intermission.

**9:40 279.** Peptide-conjugated gold nanoprobe: Intrinsic nanozyme-linked immunsorbant assay of integrin expression level on cell membrane. **X. Gao**

**10:00 280.** Colorimetric detection of *Escherichia coli* using freeze-dried engineered bacteriophage. **J. Chen**, D. Wang, V.M. Rotello, S.R. Nugen

**10:20 281.** Printable paper based biosensors. **S. Andreescu**

DoubleTree by Hilton Hotel Binghamton  
Link Room

### **Computational Chemistry**

A. Kolmogorov, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 282.** Computational prediction of hydrides of the main group elements under pressure. **E. Zurek**

**8:35 283.** Development of new density functionals and new methods for analysis of convergence of ab initio molecular dynamics simulations. **M. Fernandez-Serra, M. Fritz, J. Soler**

**9:05 284.** Screening of charge impurities and defects: Alternative mechanisms for the detection of gases on graphene and nanotubes. **J.O. Sofo**

**9:35 285.** First-principles prediction of the electrochemical stability of bimetallic catalysts for use as fuel cell electrodes. **I. Dabo**

**10:05** Intermission.

**10:35 286.** Stratified construction of neural network-based interatomic models for multicomponent materials. **S. Hajinazar, A. Kolmogorov**

**10:55 287.** Bond polarizability model of SFG reveals strong and weak H-bonds at the  $\text{Al}_2\text{O}_3(0001)\text{-H}_2\text{O}$  interface. **M. DelloStritto, J.O. Sofo**

**11:15** Concluding Remarks.

DoubleTree by Hilton Hotel Binghamton  
Serling Room

## **Education K1-12**

D. J. Simpson, *Organizer, Presiding*

**8:00 289.** Integrating sustainable practices and innovative technologies into the high school classroom. **V. O'Donnell, M. Clayton, K. Anderson**

**11:00** Intermission.

**11:15 290.** But how do I do that in *my* classroom?: Using a learning management system to increase the efficiency in your chemistry classroom. **R. Bray**

**12:15** Intermission.

**1:15 291.** Teacher center of Broome County to the rescue! **C. Panko**

**1:55** Intermission.

**2:10 292.** American association of chemistry teachers (AACT): Supporting K–12 teachers of chemistry. **A. Boyd**

**2:50 293.** Technology use in the flipped classroom. **D.J. Simpson**

DoubleTree by Hilton Hotel Binghamton  
Arlington Room B

### General Papers

C. Grewer, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:30 300.** Dual-color time-resolved methods yield significant enhancement of third-harmonic generation in air. **D.L. Weerawarne**, R.I. Grynko, B. Shim

**8:30 301.** Introduction of P-F bonds into phosphorus-containing biomolecules using aqueous fluoride ion and a water soluble carbodiimide. **M.F. Aldersley**, P.C. Joshi, S.A. McCallum, A.J. Kirby

**8:50 302.** Theory and measurement of sub-cycle photo-capacitance dynamics in polymer bulk heterojunction films. **R. Dwyer**, S.R. Nathan, J.A. Marohn

**9:10 303.** Nanostructured gauge sensors. **J. Luo**, W. Zhao, J. Lombardi, S. Shan, N. Kang, S. Yan, Z. Pan, M.D. Poliks, S. Lu, C. Zhong

**9:30** Intermission.

**10:00 304.** Fullerene and aluminum hydride complexes as hydrogen fuels. R. Hur, T.W. Yoon, C. Kim, **J. Lim**

**10:20 305.** Ta-based nano particles as an alternative metal oxide catalyst in the transformation of hydrocarbons into methanol. S. Park, H.J. Lim, J. Kim, **E. Kang**

**10:40 306.** Preparation of  $^{19}\text{F}$  NMR-reporter pincer ligand: Trying to be greener. **G.E. Hoffman**, M.L. Kwan, **G.S. Rey**, **E.E. Skerl**

DoubleTree by Hilton Hotel Binghamton  
Carlton Room B

### Inorganic Chemistry

J. Fang, *Organizer, Presiding*

**8:00 307.** Crystallography and functional properties of titanates. **B.I. Lee**

**8:40 308.** Rational design and synthesis of coordination-based sensors for metal ion determination: Iron detection. N.O. Laschuk, I.I. Ebralidze, **O.V. Zenkina**

**9:05 309.** Next frontier in MOCVD precursors: Synthesis of novel bismuth coordination compounds. **V. Lopez**, S. Reischauer, M.M. Gillett-Kunnath, K. Ruhlandt-Senge



9:30 Intermission.

9:50 **310.** Curious stability of binuclear alkyl hydrides of chromium and their reaction with hydrocarbons. **Y. Hung**, K.H. Theopold, G.P. Yap

10:15 **311.** Synthesis, properties and coordination chemistry of polytopic redox-active ligands. **N. Bonanno**, P.K. Poddutoori, A.J. Lough, M.T. Lemaire

10:40 **25.** Iron catalyzed cross-coupling with simple ferric salts. **M.L. Neidig**

Holiday Inn  
Southern Tier Room

### **Materials for Energy: New Trends & Challenges**

S. Wittingham, *Organizer*  
M. A. Petrukhina, *Organizer, Presiding*  
P. H. Dinolfo, *Presiding*

8:00 **314.** Nanostructured metal oxide and nanocup graphene nanosheets as supercapacitor materials. **M.R. Hepel**, M.A. Petrukhina, V. Samuilov

8:30 **315.** Corannulene: A curved and highly symmetric platform for synthesis of new organic materials. **C. Dubceac**, S.N. Spisak, Z. Zhou, M.A. Petrukhina

9:00 **316.** Examination of energy transfer in molecular multilayered donor-acceptor thin films. **P.H. Dinolfo**, L. Ayensu-Mensah, Z. Huang, M.R. Topka

9:30 Intermission.

10:00 **317.** New class of highly active and stable graphene tube catalysts via a template-free graphitization for bifunctional oxygen reduction and evolution. **G. Wu**

10:30 **318.** High-voltage graphene supercapacitors. **V. Samuilov**

11:00 **319.** Mapping electrical function in organic photovoltaic nanomaterials. **J.M. Mativetsky**

11:30 **320.** Solution-phase synthesis of silver-alloyed  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  for highly efficient solar cells. **P.D. Antunez**, T.S. Gershon, D.M. Bishop, R. Haight

Holiday Inn  
La Tasse Room

### **Microscopy & Spectroscopy of Surfaces**

L. Piper, *Organizer, Presiding*  
N. F. Quackenbush, *Presiding*

**8:15 321.** Thermodynamics of the interphase: Theoretical description and experimental observation of the concentration gradient at a solid/solution interface. **M.N. Kobrak**

**8:30 323.** Probing nonlinear rheology layerbylayer in interfacial hydration water. **W. Jhe**

**8:45** Discussion.

**8:50 324.** Experimental evidence against the bulk metal-insulator transition of vanadium dioxide extending to the surface. **N.F. Quackenbush**, J.T. Sadowski, M.J. Wahila, H. Paik, D. Schlom, L. Piper

**9:05 325.** Quasiparticle interference of heavy fermions in resonant X-ray scattering. **P. Aynajian**

**9:20 326.** Evidence of rhombohedral structure within hetero-epitaxially grown BiFeO<sub>3</sub> thin films. **I. Bae**

**9:35** Intermission.

**10:05 327.** Electron spectro-microscopy of 2D materials. **J.T. Sadowski**

**10:35 328.** Oxidation-driven surface dynamics on NiAl(100). H. Qin, X. Chen, J. Li, L. Li, P. Sutter, **G. Zhou**

**10:50** Discussion.

**10:55 329.** Chemistry at model catalyst surfaces: Spectro-microscopic investigations. **D. Grinter**

**11:25 330.** Importance of aluminum at the electrode-electrolyte interface for LiNi<sub>0.8</sub>Co<sub>0.15</sub>Al<sub>0.05</sub>O<sub>2</sub> electrodes. **Z. Lebens-Higgins**, S. Sallis, N. Pereira, N. Faenza, G. Amatucci, L. Piper

DoubleTree by Hilton Hotel Binghamton  
Johnson Room

### **Nanotechnology: From Fundamentals to Applications**

C. Zhong, *Organizer*

J. Luo, *Organizer, Presiding*

**8:30 31.** Self-assembly and characterization of two-color quantum rod-DNA origami conjugates. **Y. Chen**, T.L. Doane, M.M. Maye

**8:50 32.** Self-renewing carbon nanotube thick films under energetic ion bombardment. **G. Konesky**

**9:10 33.** Polymer nanocomposite foam materials for applications in sensors. **H. Kumar**

**9:30 34.** Design, synthesis and engineering of multifunctional nanoprobe for biological detection and targeting. **J. Li**, S. Shan, Z. Skeete, C. Hou, J. Luo, M.R. Hepel, C. Zhong

**9:50 35.** Charge properties of doped semiconductor nanocrystals. **A.R. Freyer**, T. Krauss

**10:10** Intermission.

**10:25 36.** Toward a <sup>19</sup>F MRI contrast agent based on mesoporous silica nanoparticles. **J.L. Steinbacher**

**10:45 37.** Clodronate control of the reticulo-endothelial system (circulating macrophages) to increase circulation time of theranostic Immunolabeled gold-coated nanoparticles. **B. Kogos**, N. Sobol, **P. Pevsner**

**11:05 38.** Sub-5nm  $\beta$ -NaGdF<sub>4</sub>:Yb 50%: A design of a theranostic nanoplatform for radiotherapy. **J. Damasco**, G. Chen, T. Ohulchansky, S. Mahajan, P. Prasad

**11:25 39.** Fundamental understanding of the synergy between electroactive poly (amic) acid membranes and their interaction with nanoparticles. **V. Kariuki**

DoubleTree by Hilton Hotel Binghamton  
Arlington Room A

## **Nucleic Acids**

E. Rozners, *Organizer, Presiding*

**8:45** Introductory Remarks.

**8:50 340.** Enhancing siRNA / RNA aptamer affinity and activity with backbone-modified nucleic acids. **M. Egli**

**9:30 341.** Transition metal-based paramagnetic probes to study RNA-protein interactions using NMR. **M. Royzen**, L. Seebald

**10:00** Intermission.

**10:20 342.** Synthesis of amide-modified RNA. **V. Kotikam**, E. Rozners

**10:40 343.** Synthesis and thermal stability of novel Watson-Crick base pair mimics. **I. Novosjolova**, S. Kennedy, E. Rozners

**11:00 344.** Modifying RNA to understand and improve it: NMR and modeling studies. **S. Kennedy**, R. Kierzek, D. Mutisya, P. Pallan, M. Egli, E. Rozners, D.H. Turner

## **FRIDAY AFTERNOON**

DoubleTree by Hilton Hotel Binghamton  
Endicott Room

## **Bioorthogonal Chemistry**

*Financially supported by Harpur College Dean's Office*  
S. L. Bane, *Organizer, Presiding*

**1:00 345.** Bio-orthogonal chemistry allows for local activation of systemically administered pro-drugs. **M. Royzen**

**1:25 346.** Selective derivatization of recombinant proteins using hexahistidine tag. V. Kadambar, X. Liu, **A. Melman**

**1:50 347.** Bioorthogonal chemistry: Impact on molecular imaging. **P. Adumeau**

**2:15 348.** Expedient synthesis of “clickable” sterols for bioconjugation by hedgehog proteins. **T. Owen**, B.P. Callahan

**2:35** Intermission.

**3:00 349.** Reactivity-based chemical tools for biomedical research. **Q. Lin**

**3:25 350.** Engineering and exploiting multispecific enzymes for bioorthogonal protein labeling. **J. Hougland**, S.A. Gangopadhyay, M.J. Blanden

**3:50 351.** Inhibition of the sonic hedgehog/patched 1 protein-protein interaction via evolved macrocyclic peptides. **A. Owens**, R. Fasan

**4:15 352.** Effect of substituents on the reactions of substituted hydrazides with 2-formylphenylboronic acid and the structures and stability of the products. **H. Gu**, J. Hirschi, S.L. Bane

DoubleTree by Hilton Hotel Binghamton  
Kilmer Room

## **Chemical Biology**

B. P. Callahan, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 353.** Fifty years of smelling sulfur: From the chemistry of garlic to the molecular basis for olfaction. **E. Block**

**1:50 354.** Lipid raft formation via a push-pull mechanism. **S.L. Regen**

**2:20** Intermission.

**2:40 355.** Deconvoluting mixed redox messages with precision redox targeting. **Y. Aye**

**3:00 356.** Small-molecule on/off switches for signaling enzymes: Target-specific inhibition and activation of protein tyrosine phosphatases. **A.C. Bishop**

**3:20 357.** Larval trail pheromones for species-specific control of an invasive insect. **F.M. Rossi**

**3:40 358.** Beyond D-luciferin: A bright future for bioluminescence. **S.C. Miller**

DoubleTree by Hilton Hotel Binghamton  
North Riverside Room

## Energy & Fuels

K. Litz, *Organizer, Presiding*

**1:00 359.** Heavy oil desulfonation catalyzed by coconut carbon. **S. Briggs**, K. Litz, J. Rankin

**1:30 360.** Vapor phase polymerized poly(3,4-ethylenedioxythiophene) (PEDOT) based composites as the electrode materials for supercapacitors. **L. Tong**, J. Liu, S.M. Boyer, L.A. Sonnenberg, M.T. Fox, J. Manning, W. Bernier, W.E. Jones

**2:00 361.** Supercritical water treatment of fractions of crude oil: Quantification of the products using GCxGC, NMR, FT-IR & Raman spectroscopy. **S. Gudiyella**, L. Lai, A. Lui, I. Borne, J. Cai, G. Tompsett, M.T. Timko, W.H. Green

**2:30** Intermission.

**2:40 362.**

Numerical simulation of sub-bituminous coal de-volatilization and gasification in a fluidized bed gasifier. **R. Ghandriz**, R. Sheikhi

**3:10 363.** Sulfur speciation of sulfoxidized oils by FT-IR. **J. Rankin**, K. Litz

**3:40 364.** Monitoring algae growth in marine water culture solutions using TOC/TN. **D. Davis**

**4:10 365.** Room temperature sulfur adsorption/desorption process for ultra-low sulfur diesel. **E. Shipley**, K. Litz, J. Rankin, T. McCaskill

DoubleTree by Hilton Hotel Binghamton  
Carlton Room B

## Environmental Chemistry & Impacts of Pollution in the Great Lakes Region & Beyond

D. S. Aga, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 294.** Chemical analysis of legacy and emerging contaminants in Great Lakes fish. **M. Milligan**, T. Holsen, B.S. Crimmins, P. Hopke, J.J. Pagano

**1:30 295.** A suspect screening for organic micropollutants in the Cayuga Lake region of the Great Lakes Basin. **D.E. Helbling**, A. Pochodylo

**1:55 296.** Field deployable bioassays for rapid and sensitive detection of emerging contaminants. G. Bulbul, A. Othman, **S. Andreescu**

**2:20** Intermission.

**2:35 297.** Comparative analysis of different water categories as sources of *N*-nitrosamine precursors. **T. Zeng**, C. Glover, E. Marti, W. Mitch, E. Dickenson

**3:00 298.** Mass spectrometry based method for measuring vitellogenin in fish as biomarker of exposure to endocrine disrupting chemicals. **P. He**, E. Matich, A. Friedman, G. Atilla-Gokcumen, D.S. Aga

**3:25 299.** Indoor air quality in the office environment and volatile emission fluxes from printers. **N.C. Eddingsaas**, D.C. Rodriguez Alberto, S. Gray

**3:50 373.** Using stable isotopes ( $\delta D$  and  $\delta^{13}C$ ) to determine spatial origin of PAH contaminants in soils throughout Connecticut, USA. **A. Oakes**, G.M. Harris, C.E. Fagan, M.T. Hren

DoubleTree by Hilton Hotel Binghamton  
Carlton Room A

### **Green/Environmental Chemistry**

G. W. Ruger, *Organizer*

N. O'Neil, L. J. Tucker, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:10 366.** Engaging high school teachers in green chemistry. **L.J. Tucker**, A. Klotz

**1:35 367.** Making the case for green chemistry in NY High Schools. **V. O'Donnell, M. Clayton, K. Anderson**

**2:00 368.** How can we make analytical labs greener? **M. Dilip**

**2:25 369.** Green Chemistry at New York State Pollution Prevention Institute (NYSP2I). **C.J. Ruffing, K. Winnebeck**

**2:50 370.** Network of early-career sustainable scientists & engineers. **N. O'Neil**

**3:15 371.** LOCNO (Low Cost No Cost) systems and technologies for use by global masses to treat their own water. **S. Shukla, A. Shukla**

**3:40 372.** Bio-inspired poly (amic) acid nanostructured membranes as smart food packaging materials. **I. Yazgan**

**4:05 374.** Photochemical synthesis and biological applications of anisotropic gold nanoparticles. **F.J. Osonga, I. Yazgan, O.A. Sadik**

**4:30 375.** Environmentally benign synthesis of vinyl ester resin (VER) and its fabrication for anti-flammable VER composites from glycerin bio-waste. P. Shah, N. Kim, **Y. Lee**

Holiday Inn  
Southern Tier Room

**Materials for Energy: New Trends & Challenges**

M. A. Petrukhina, S. Wittingham, *Organizers*  
E. Dikarev, V. Samuilov, *Presiding*

**1:00 376.** Li batteries: Future trends and challenges. **M.S. Whittingham**

**1:40 377.** Mixed-valent transition metal precursors for the synthesis of energy related materials. **E. Dikarev**, C.M. Lieberman, Z. Wei, A.M. Abakumov

**2:10 378.** FeSn<sub>2</sub> and FeSn<sub>5</sub> alloy with high and stable capacity as anodes in lithium-ion batteries. **F. Xin**, H. Zhou, D. Ji, X. Wang, J. Ding, F. Omenya, N. Chernova, M.S. Whittingham

**2:30** Intermission.

**3:00 379.** Realizing the full reversible capacity of layered oxide lithium ion battery cathodes: The role of phase transformations at Li<sub>1-x</sub>Ni<sub>0.8</sub>Co<sub>0.15</sub>Al<sub>0.5</sub>O<sub>2</sub> surfaces. **L. Piper**

**3:30 380.** Substituted epsilon-VOPO<sub>4</sub> as multi-electron cathode for Li-ion battery. **C. Siu**, Y. Chung, F. Omenya, N. Chernova, M.S. Whittingham, Y. Lin, S. Ong, L. Wangoh, L. Piper

**3:50 381.** Characterizing dendrite growth in lithium-ion batteries using *in situ* MRI. **A.J. Ilott**, M. Mohammadi, H. Chang, N. Trease, C. Grey, A. Jerschow

**4:10 382.** Germanium based anodes for lithium-ion batteries. **D. Ji**, N. Chernova, M.S. Whittingham

**4:30 383.** High light absorption and charge separation efficiency at low applied voltage from Sb doped SnO<sub>2</sub>/BiVO<sub>4</sub> core/shell nanorod array photoanodes. **L. Zhou**, P.M. Rao

**4:50 384.** SnWO<sub>4</sub> porous film photoanode with visible-light photoresponse at low voltage. **Z. Zhu**, P. Sarker, C. Zhao, L. Zhou, R.L. Grimm, M.N. Huda, P.M. Rao

DoubleTree by Hilton Hotel Binghamton  
Arlington Room B

## **Metals in Biochemistry**

R. Dempski, *Organizer, Presiding*

**1:00 385.** Design of metalloprotein catalysts. **I.V. Korendovych**

**1:30 386.** Engineered biocatalysts for hydrogen evolution. **K. Bren**, B. Kandemir, Y. Guo, S. Chakraborty, C. Dickerson

**2:00 387.** Photoinduced decarboxylation strategies for uncaging of biologically important Zn<sup>2+</sup> from photocaged zinc complexes. **P. Basa**, S. Burdette, R. Dempski, C.A. Barr

**2:30** Intermission.

**3:00 388.** Illuminating the pivotal role of ATP in cytosolic iron sulfur cluster assembly. **D. Perlstein**, J. Grossman, K. Gay

**3:30 389.** The role of a novel genetic factor (SLC30A10) in manganese-induced toxicity in *C. elegans*. **P. Chen**, A.B. Bowman, S. Mukhopadhyay, M. Aschner

**4:00 390.** Zinc inhibits hedgehog autoprocessing: Linking zinc deficiency with hedgehog activation. J. Xie, T. Owen, B.P. Callahan, **C. Wang**

DoubleTree by Hilton Hotel Binghamton  
Watson Room

## **Organic Chemistry**

M. J. Vetticatt, *Organizer, Presiding*

**1:00 391.** Total syntheses of nannocystins A and A0. J. Huang, **Z. Wang**

**1:35 392.** Mixed dioxygen relay and O-atom transfer mechanisms of nitrosamine photoreactions. A.A. Ghogare, C.J. Debaz, M. Silva Oliveira, E. Greer, F. Manso Prado, P. Di Mascio, **A. Greer**

**2:10 393.** Enantioselective brønsted acid catalysis with chiral cyclopentadienes. **C. Gheewala**, B. Collins, T.H. Lambert

**2:35** Intermission.

**2:55 394.** Shaping the future of polymer molecular weight distributions. **B.P. Fors**

**3:30 395.** Development of a green and sustainable commercial manufacturing process. **H. Ren**

**3:55 396.** Functionalization of amines via redox-neutral reaction cascades. **D. Seidel**

DoubleTree by Hilton Hotel Binghamton  
Johnson Room

## **Small Chemical Businesses**

*Cosponsored by SCHB*

J. L. Maclachlan, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 397.** SCHB member benefits: Discover the resources the ACS Division of Small Chemical Businesses offers. **J.L. Maclachlan**

**1:35 398.** The art of getting the buy. **A. Russo**

**2:05 399.** Building an effective technology transfer operation to support small business development. **P.K. Dorhout**, C. Brandt, K. Glasscock

**2:35 400.** Chemistry, money, & theft: How intellectual property rights enable you to monetize and protect your work. **M. Keenan**



**3:05** Intermission.

**3:20 401.** Marketing and advertising the small chemical business. **S. Mardigian**

**3:50 402.** Leveraging linked-In and other simple social media in your sector of the chemical enterprise. **J.L. Maclachlan**

**4:20 403.** Forensic chemistry: Dealing with a false positive in a drugs of abuse case. **D.M. Manuta**

Holiday Inn  
La Tasse Room

### **Smart Energy**

G. S. McGrady, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 404.** Coupling in-situ TEM and ex-situ analysis to understand heterogeneous sodiation of antimony. **D. Mitlin**

**1:50 405.** Enhanced adhesion of NPG on modified glassy carbon surfaces and de-alloying of  $\text{Cu}_x\text{Au}_{(1-x)}$  alloys at different length scales. **J. Xia**, I. Achari, S. Ambrozik, N.G. Dimitrov

**2:20 406.** Design and structural characterization of nanoalloys as catalysts for ethanol oxidation reaction. **Y. Zhao**, S. Shan, H. Cronk, Z. Skeete, J. Donohue, J. Luo, V. Petkov, C. Zhong

**2:50 407.** Structural characterization of nanoalloy catalysts for low-temperature hydrocarbon oxidation. **S. Shan**, H. Kareem, H. Cronk, Y. Zhao, J. Li, E. Kim, F. Chang, J. Luo, V. Petkov, C. Zhong

**3:20** Intermission.

**3:40 408.** Pre-lithiated  $\text{Li}_4\text{Ti}_5\text{O}_{12}$ /activated carbon hybrid battery for energy storage device. **J. Feng**, F. Omenya, N. Chernova, L. Tong, W.E. Jones, A. Rastogi, M.S. Whittingham

**4:10 409.** High-voltage behavior of layered oxides in Li-ion batteries: Insight from the magnetic properties. **N. Chernova**, F. Omenya, C. Siu, H. Liu, S. Meng, S. Wittingham

**4:40** Concluding Remarks.

DoubleTree by Hilton Hotel Binghamton  
Link Room

### **Spectroscopy**

B. Shim, *Organizer, Presiding*

**1:00 410.** Building practical applications for benchtop NMR: Case studies from real beans to fake weeds. **M. Lachenmann**, D. Williamson

**1:15 411.** Ultrafast laser studies of the primary photochemical events in artificial photosynthesis. **D.W. McCamant**, M. Mark, Z. Piontkowski

**1:40 412.** Measuring biopolymer elasticity with terahertz spectroscopy. **T.M. Korter**

**2:05 413.** Solitary wave propagation in condensed matter. **R.I. Grynko**, D.L. Weerawarne, X. Gao, H. Liang, H.J. Meyer, K. Hong, A.L. Gaeta, B. Shim

**2:20** Intermission.

**2:50 414.** A spectroscopic and computational analysis of anethole-water clusters. **J.J. Newby**, J. Nesheiwat

**3:05 415.** Water at surfaces with tunable surface chemistries and the DNA's chiral spine of hydration. **P.B. Petersen**

**3:30 416.** Stark control of electrons along nanojunctions. **I. Franco**

**3:55** Concluding remarks.

DoubleTree by Hilton Hotel Binghamton  
South Riverside Room

### **Surface Chemistry/Catalysis**

M. M. Maye, *Organizer, Presiding*

L. M. Karam, *Presiding*

**1:00 417.** Characterizing working catalysts with correlated electron and photon probes. **E. Stach**, Y. Li, S. Zhao, A. Gamalski, J. Chen, R.G. Nuzzo, A. Frenkel

**1:30 418.** Utilizing perovskite nanoparticles as both colorimetric assays of chemical reactions and halide reservoirs in catalysis. **T.L. Doane**, K.J. Cruz, L. Pathade, M.M. Maye

**2:00 419.** Carbon monoxide oxidation over Pd-based nanoalloy: Design & characterization. **H. Kareem**, S. Shan, Y. Zhao, Z. Skeete, J. Luo, C. Zhong, V. Petkov

**2:30** Intermission.

**3:00 420.** Synthesis and characterization of WO<sub>3</sub> nanowires. **K.J. Dietz**, A.T. Carroll, A. Mahdavi-Shakib, B.G. Frederick

**3:15 421.** Ultrafine and ligand-free noble metal nanoclusters on carbon supports through a "soft nitriding" method. B. Liu, H. Yao, L. Jin, S.L. Suib, **J. He**

**3:30 422.** CdSe/ $\beta$ -Pb<sub>x</sub>V<sub>2</sub>O<sub>5</sub> Heterostructures: Role of lone Pairs in achieving directional charge transfer. **L. Wangoh**, K.E. Pelcher, C.C. Milleville, S. Chauhan, M.L. Crawley, P.M. Marley, D. Watson, S. Banerjee, L. Piper

**3:45 423.** Tungsten oxide as a solid acid catalyst for the conversion of glucose to HMF and lactic acid. **A. Mahdavi-Shakib**, A. Crane, B.G. Frederick

DoubleTree by Hilton Hotel Binghamton  
Arlington Room A

## Nucleic Acids

E. Rozners, *Organizer, Presiding*

**1:30 424.** Folding RNA: From tetramers to Influenza. **D.H. Turner**

**2:10 425.** Structural and functional studies of 2'-5'-linked RNA. F. Sheng, R. Wang, O. Levchenko, P. Haruehanroengra, V. Valsangkar, **J. Sheng**

**2:40 426.** Designed RNA-targeted compounds for altering protein recoding in HIV. **B.L. Miller**

**3:10** Intermission.

**3:30 427.** *E. coli* tRNA arginine isoacceptors employ multiple post-transcriptional modification strategies to enable six-fold degenerate codon recognition. **K. Sarachan**, W. Cantara, S. Vangaveti, J. Spears, H. DeMirci, F.V. Murphy, S. Ranganathan, P.F. Agris

**4:00 428.** 2-Aminopyridine modified peptide nucleic acids and their peptide conjugates are promising tools for fast and sequence-selective recognition of double-stranded RNA in vitro and in live cells: Applications in molecular biology, biomedical research and biotechnology. **D. Hnedzko**, D. W. McGee, Y. A. Karamitas, E. Rozners

**4:20 429.** Probing nucleic acid grooves using fluorescent aminosugars. **D.P. Arya**

## FRIDAY EVENING

DoubleTree by Hilton Hotel Binghamton  
North Ballroom

### General Posters

A. S. Silva, *Organizer*

**5:00 - 6:30**

**430.** Effect of Zn<sup>2+</sup> and Mg<sup>2+</sup> on glutamate transporter efflux. **A. Wiss, C. Breed, S. Powell, L. Pak, C. Grewer, S.C. Flynn**

**431.** Identification and quantification of limonene in hard candies. **A. Hanse, C. Minogue**

**432.** Progress towards the synthesis of new benzofuran analogs targeting polyketide synthase 13 (Pks13) for inhibiting *mycobacterium tuberculosis (Mtb)*. **A. Gittens**, R.C. Dhakal, A. Aggarwal, M.K. Parai, R. Shrestha, J.C. Sacchettini

- 433.** Light-mediated control of drug activity for phototherapeutics. **A.C. McCue, C.I. Muldoon, E. Karic , T.A. Shell**
- 434.** Electrospun fibers of fluorescent conjugated polymer chemosensors in polymer blend matrix. **A. Niyongabo, A. Chen, W.E. Bernier, W.E. Jones**
- 435.** Ruthenium-based donor compounds as building blocks for proton-coupled electron transfer. **B. Plaman, N. Odewade, L.M. Aguirre Quintana, D. Villagran, E.R. Young**
- 436.** Iron oxidation and core formation in recombinant heteropolymer ferritins. **B. Smith, M. Mehlenbacher, F. Bou-Abdallah**
- 437.** Colours of chaos: An in-depth study of chemical oscillations. **C. Misiewicz, S. Glazier, D. Look**
- 438.** The electrochemical behavior of early metal metallocene Cp<sub>2</sub>MCl<sub>2</sub> complexes under CO<sub>2</sub>. **K.A. Grice, C. Saucedo, M. Sovereign, A. Cho**
- 439.** Development of a hand-portable chemosensor device to aid in combatting the trade of illegally caught fish through the cyanide fishing method. **C. Flynn, C. Sweet, C. Murphy**
- 440.** Developing a metalloporphyrin-based photo and electrochemical detector of thiocyanate ions in marine environments. **C. Sweet, C.P. Flynn, A.R. McCabe, C. Murphy**
- 441.** Optimization of a route to 2<sup>nd</sup> generation organosilicate systems. **D. Monk, L. Dake, M.A. Boucher**
- 442.** Synthetic sterol derivatives for bioconjugation by hedgehog proteins. **D. Moumin, T. Owen, B.P. Callahan**
- 443.** Characterization of the doxorubicinone-DNA complex formation. **E. Curtis, H. Anchukaitis, S. Tartakoff, S. Glazier**
- 444.** Supramolecular assembly of donor-acceptor energy transfer system. **E.B. Conklin, J. Rosenthal, E.R. Young**
- 445.** Isotope Effects and the weak CH-O and  $\delta^-$ H-H  $\delta^+$  hydrogen bond in the enantioselective cyclopropanation catalyzed by a cinchona alkaloid derivative. **G.T. Bedard, J. Izzo, M.J. Veticatt**
- 446.** Synthesis of doxorubicin analogs for DNA binding studies. **H. Anchukaitis, S. Glazier, S. Tartakoff**
- 447.** Conformational energetics of cyclohexane, tetrahydropyran, and dioxane. **I. Bogacz, Y.A. Abdo, S.P. Lee, H.B. Reed, T.L. Ellington, K.M. Dreux, G.S. Tschumper**
- 448.** Synthesis, characterization, and application of water soluble poly (pyromellitic dianhydride-p-phenylene diamine) to synthesize anisotropic silver nanoparticles. **J. Hoffmeier, V. Kariuki, O.A. Sadik**
- 449.** Voltage-induced reduction of graphene oxide. **J.N. Flournoy, A.C. Faucett, J. Mehta, J. Mativetsky**
- 450.** Changes in synthetic and calf thymus DNA in the presence of osmolytes. **J. Finan, S. Glazier**
- 451.** Nanofibrous polymer and metal organic framework composites for the degradation of simulated chemical warfare agents. **J. Troiano, D. Dwyer, W. Bernier, W.E. Jones**

452. Solvent dependent electron transfer in a BODIPY dyad series. **J.C. Strahan**, B. Popere, S. Thayumanavan, E.R. Young
453. Synthesis of stercobilin: A potential biomarker for Autism. **J. Coffey**, A. Charlebois, A. Vadas
454. Transition metal complexes of 2-amino-3,5-dihalopyridines: Synthesis, structures and magnetic properties of (3,5-diCAP)<sub>2</sub>Cu<sub>2</sub>X<sub>6</sub> and (3,5-diBAP)<sub>2</sub>Cu<sub>2</sub>X<sub>6</sub>. **J. Cipi**, C.P. Landee, M.M. Turnbull, J.L. Wikaira
455. High-resolution infrared spectroscopy of C<sub>5</sub>S. **J. Kozubal**, J.B. Dudek, S. Thorwirth, T. Salomon
456. Dye sensitized solar cells: A push towards lowering cost and improving efficiency. **K. Digan**, C. Sweet, C.J. Timpson
457. Identifying kinetically-stable proteins in peanut. **K. Fallows**, K. Xia, W. Colon
458. Use of native active oils to create naturally-derived antimicrobial surfaces. **K. Velez**, J.I. Rizzo
459. Freezing-induced gold nanoparticle aggregation and its effect on SERS. **K. Hoyt**, J. Heo
460. Introductory organic chemistry for the high school laboratory. **K.J. Cassidy**, M.A. Walker
461. Synthesis of a series of methyl-1-indanone derivatives. **K.S. Podolak**, D.R. Case, G. Abbot, C.R. Pulliam, M.A. Boucher
462. Adaptation of a rapid extraction method for lead analysis of community soil samples. **L.M. Nitti**, C.R. Pulliam, J. Crandall
463. Determination of inorganic anions and cations in potable and waste waters with capillary zone electrophoresis with indirect UV detection. **L. Varden**, B. Smith, F. Bou-Abdallah
464. Analysis and characterization of vapor phase polymerized poly(3,4-ethylenedioxythiophene) on carbon materials as supercapacitor electrodes. **L.A. Sonnenberg**, L. Tong, W.E. Bernier, W.E. Jones
465. Enzyme inhibition: Monitoring of enzymatic reactions using a pH scale. **M.R. Pierce**, D. Olschewske, C.S. Rossiter
466. A greener synthesis of vinyl sulfones. L.E. Johnson, **M.A. Walker**
467. Dye-sensitization of titanium dioxide nanofibers with photo-oxidizing and photo-reducing dyes for the photodegradation of environmental and biological pollutants. **M. Ehrlich**, S.M. Boyer, W.E. Jones, W. Bernier
468. Synthesis, structure, and magnetic behavior of nickel (II) and cobalt (II) halide complexes of isoquinoline. **M.T. Kebede**, C.P. Landee, M. Rademeyer, M.M. Turnbull
469. Synthesis of alkaline earth metal tetraarylborate pyrazolate compounds. K. La, J.J. Woods, C.M. Lavin, **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge
470. Application of thin film molecular assemblies as electrochromic devices. **M.J. Amdur**, P.H. Dinolfo
471. Study of chemical composition and prospecting anticholinesterase of volatile oils at *Corymbia citriodora* and *Vitex agnus castus*. **R. Brito Oliveira**, J. França Orlanda

- 472.** Biocompatible bone cements as an alternative to modern methods of bone fracture repair. **S. Medina, S. Qadiri**
- 473.** Synthesis and characterization of size- and shape-controlled PtNiCo nanoparticles for fuel cell catalysts. **S. Kim, H. Cronk, S. Negi, Z. Skeete, J. Luo, C. Zhong**
- 474.** Inhibitory effects of triterpenoids on human mitochondrial Lon protease. **S. Sakhamuri, C. Suzuki, A. Pandey**
- 475.** Investigating metal allosteric sites on glutamate transporters. **S. Chen , D. Fama , R. Jimenez , W. Kelmenson , M. Tarrash , I. Territo , C. Grewer, S.C. Flynn**
- 476.** Preparation of biocompatible magnetic nanoparticles by ligand exchange reaction of capping agents. **S. Negi, H. Cronk, S. Kim, Z. Skeete, J. Luo, C. Zhong**
- 477.** Chemistry in the aerosol interfacial region: A computational study. **T. Cropley**
- 478.** The study of amyloid protein formation by soil bacteria in presence of subinhibitory antibiotic concentrations. **V. Chilunda, N. Marano, L. Olendzenski**
- 479.** Extraction of green tea polyphenols by sonication and the inhibitory effects on digestive enzymes. **V.I. Bednar, A.M. Fedor**
- 480.** Behavior of chemically coupled oscillating gels. **Y. Kim, Z.A. Jimenez, I.R. Epstein**
- 481.** In a search of an enzymatic pH oscillator for the delivery of an anti-depressant. **Z. Wang, Z.A. Jimenez, V. Horvath, I.R. Epstein**

## **SATURDAY MORNING**

DoubleTree by Hilton Hotel Binghamton  
Arlington Room A

### **Drug Delivery**

*Cosponsored by ORGN*  
*M. An, Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 482.** Increasing effectiveness of tethered antimicrobial peptide chrysophin-1. **Z. Lipsky, T.E. Alexander, L.D. Lozeau, T.A. Camesano**

**8:25 483.** The pH low insertion peptide (pHLIP) as a drug carrier targeting acidic tumor microenvironments. **L. Klees, E. Lichter, C. Eng, X. Wang, C. Shi, A. Bodman, V. Nazarenko, M. Bell, I. Bandler, Y. Lan, J. Luo, M. An**

**8:45 484.** Di-substituted maleamic acid, an ultra-acid-sensitive, cleavable linker for releasing drugs in response to tumor acidosis. **A. Zhang, M. An**

**9:05 485.** Rational design of peptides for cancer targeting. **F. Barrera**

**9:35** Intermission.

**9:50 486.** Specific targeting and delivery of therapeutics to cancer cells based on the tumor microenvironment. **D. Thevenin**, K.E. Burns, T.P. McCleerey

**10:20 487.** Membrane insertion of the pH-low insertion peptides studied by the solid-state NMR spectroscopy. **W. Qiang**, N. Shu, S. Hanz, J. Qian, N. Christman, M. An, C. Grewer

**10:50 488.** Novel telodendrimer nanoplatform for therapeutic delivery. **J. Luo**

DoubleTree by Hilton Hotel Binghamton  
Kilmer Room

### **Membrane Biochemistry**

L. Niu, *Organizer, Presiding*

**8:00 489.** ATP synthase of bacteria: Distinct inhibitory states of subunit  $\epsilon$  may control opposite directions of rotary catalysis. **T.M. Duncan**

**8:30 490.** Metal-Citrate complex symport in radiation resistant kineococcus radiotolerans. **R. Doyle**

**9:00 491.** Functional roles of the edited isoform of GluA2 in GluA2-containing AMPA receptor channels. **L. Niu**

**9:30 492.** Structure, function and dynamics of glutamate receptors. **R. Oswald**, A.H. Ahmed, C.P. Ptak, L.M. Nowak

**10:00 493.** Action mechanisms of drugs targeting the ATP gated P2X7 receptor membrane channel. **T. Kawate**

**10:30 494.** Dynamics and mechanism of transmembrane glutamate transport. **C. Grewer**

DoubleTree by Hilton Hotel Binghamton  
Watson Room

### **Organic Chemistry**

M. J. Veticatt, *Organizer, Presiding*

**8:00 495.** Synthesis and characterization of polybenzimidazole based phosphonate esters and phosphonic acids.. **F.E. Johnson**, I. Cabasso

**8:30 496.** Studies toward the synthesis of oxa-adamantyl substituted cannabinoids. **J. Mullins**

**9:00 497.** Discoveries and developments toward a supported synthesis of  $\alpha$ -hydroxytropolones. **M. D'Erasmo**, R.P. Murelli

**9:20 498.**

Structure determination of alkali metal enolates and phenolates using the method of continuous variation.

**L.L. Tomasevich**, D.B. Collum

**9:40** Intermission.

**10:00 499.** Covalent organic frameworks as molecularly tunable materials for electrocatalytic CO<sub>2</sub> reduction.

**S. Lin**

**10:30 500.** Selective optical aqueous anion detection by 4-pyrrolylpyridine. **L. Schmitt**, A. Lees

**10:50 501.** Engineering optical behavior in donor- $\pi$ -acceptor phenylene ethynylene trimers with fluoroarene-arene side chain interaction. **S.A. Sharber**, R.N. Baral, S.W. Thomas

**11:10 502.** Photo-induced phase transfer of aromatic Pi-Pi complexes. C. Lin, **R.E. Partch**

DoubleTree by Hilton Hotel Binghamton

Johnson Room

### **Small Chemical Businesses**

*Cosponsored by SCHB*

J. L. Maclachlan, *Organizer, Presiding*

W. Bernier, *Presiding*

**8:00** Introductory Remarks.

**8:05 503.** Breakthrough performance from aligned sales, marketing and product development. **E. Host-Steen**

**8:35 504.** Ecoelectro Inc: Novel alkaline anion exchange membranes (AAEMs) with exceptional base stability. K.M. Hugar, **G. Rodriguez-Calero**

**9:05 505.** Thermally stabilized optical nanomaterial for plastics and inks. **B.P. Hughes**, K.H. Skorenko, F.D. Goroleski, B. Galusha, W. Bernier, W.E. Jones

**9:35** Intermission.

**9:50 506.** Sunthru: Fulfilling the promise of aerogel windows. **M.K. Carroll**

**10:20 507.** Hydrogen gas management for flooded lead acid batteries. **A. Chen**, G.S. McGrady, W. Bernier, W.E. Jones, B. Chan, M. Sweeney, C. Brower, E. Sidorenko, M. Pentaris

**10:50 508.** Ecodyst innovative ecochyll is revolutionizing the rotary evaporator. **G.M. Adjabeng**

DoubleTree by Hilton Hotel Binghamton

Carlton Room A

### **Younger Chemist Committee Workshop**



C. Rawlins, *Organizer, Presiding*

**8:00 509.** Navigating ACS and your career: A guide for young chemists. **C. Rawlins**, C.L. Mills

**8:10 510.** The (True) value of volunteering as a younger chemist. **J. Breffke**

**8:40 511.** ACS involvement for young chemists: A personal account. **G.D. Labenski**

**9:10** Intermission.

**9:25 512.** Active learning and engagement strategies for successful employment opportunities. **D.G. Sykes**

**9:55 513.** Personal branding in the digital age to advance your career in the chemical sciences. **J.L. Maclachlan**

**10:25 514.** Making ACS membership more valuable for younger chemists. **T.R. Gilbert**

**10:55** Concluding Remarks.

## **SATURDAY AFTERNOON**

DoubleTree by Hilton Hotel Binghamton  
North Ballroom

### **General Posters**

A. S. Silva, *Organizer*

**12:00 - 1:30**

**515.** TiO<sub>2</sub> nanofiber formation using microwave irradiation. **D. Dwyer**, G.S. McGrady, W.E. Jones

**516.** Discovery of an aqueous variant of the Wohl degradation. **T. Cheewawisuttichai**, A. Yu, M. Brichacek

**517.** Synthesis of X-shape molecules as electron acceptors in organic solar cells. **F. Caban**, Y. Jiang, S. Wei

**518.** Origin of diastereodivergence in an organocascade catalytic cycle. **F. Marrone**, J. Izzo, M.J. Veticatt

**519.** The refractive index of malonic acid measured by zoom-in method and extension method. **H. Kim**, J.H. Shin

**520.** Thermodynamic study of esterification of acetic acid with various alcohols using a microwave reactor. **H. Yun**, J.H. Shin

**521.** Cleaning and protecting the water we use via NYC's wastewater treatment system & DEP shoreline survey unit. **I. Sun**, J. Villacis, P. Meleties, P.D. Svoronos

522. The determination of pesticides in fruits, vegetables and grains via the Luke method. **I. Sun**, K. Williams, M. Iorsh, P.D. Svoronos
523. The detection of salmonella in foods via microbiological methods. **I. Sun**, A. Lara, P.D. Svoronos
524. Can two lithium ions be reversibly intercalated in  $\epsilon$ -Li<sub>x</sub>VOPO<sub>4</sub>? **J. Hwang**, L. Wangoh, L. Piper
525. Understanding the formation and size distribution of porous poly(*o*-toluidine) microspheres. **J. Hwang**, D.M. Sarno
526. Determining the total number of antioxidant quantities present in commercially available beverages via the folin ciocalteau microspectrophotometric analysis. **J. Leong**, M. de los Santos, S. Svoronos, P.D. Svoronos
527. Determining the total amount of oxygen consumption in effluent via carbonaceous biochemical oxygen demand (CBOD) and biochemical oxygen demand (BOD). **J. Leong**, F. Jacques, P. Meleties, P.D. Svoronos
528. The determination of gallic acid present in juice and tea beverages using high performance liquid chromatography. **M. de los Santos**, J. Leong, P.D. Svoronos
529. Impedimetric biosensors based on modularly designed synthetic peptides for recognition, detection and live/dead differentiation of pathogenic bacteria. **X. Liu**, M. Marrakchi, D. Xu, H. Dong, S. Andreescu
530. A redox-active aptaswitch for rapid and sensitive detection of mycotoxins. **G. Bulbul**, A. Hayat, S. Andreescu
531. Probing substrate specificity in hedgehog protein cholesterololysis. **D. Ciulla**, J.P. Giner, B.P. Callahan
532. Determination of the ionization constant of weak carboxylic acids using microscale freezing point depression measurements. **D. Kwun**, P. Irigoyen, P.D. Svoronos
533. Hydrothermal synthesis and characterization of lithium mixed-transition-metal phosphates. **K.J. Lee**, P. Sideris
534. Coinage metal nanocluster coalescence simulations: Two-temperature model molecular dynamics (MD) versus classical MD. **B.C. Sousa**, J. Lomba, Z. Bolduc, T.D. Morse
535. Detection of water pollutants using silver nanopartilcels-nanocellulose 3D SERS substrate. **M. Hossen**
536. Tungsten oxide as an electro-catalyst for the electrolysis of water and the reduction of carbon dioxide. **A.T. Carroll**, K.J. Dietz, A. Mahdavi-Shakib, B.G. Frederick
537. Synthesis, characterization and electrochemical investigation of ferrocenyl gold (I) thiolate complexes. **K.A. Veillette**, G.S. Garusinghe, A.E. Bruce, M.R. Bruce
538. Magnetic photocatalyst for removal of organic pollutants from drinking water. **S. Sultana**
539. Hydrogen purification and capture system for use in a *chlamydomonas reinhardtii* bioreactor. **A. Castonguay**, G.S. McGrady, L.L. Tomasevich, J.R. Amey, S. Ackermann
540. Dye-sensitized semiconductor systems for photocatalytic hydrogen production. **S. Wang**

**541.** Light weight metal hydrides as high capacity negative electrode for lithium based batteries. Y. Hua, G.S. McGrady, S. Beattie, **Y. Zhang**

**234.** Application of *in vivo* fast-scan cyclic voltammetry for electrochemical monitoring of salicylic acid, an active metabolite of aspirin, in the rat brain. **R. Bhimani**, J. Park

**288.** A mechanistic exploration in the formation of chiral C-S stereocenters from  $\alpha,\beta$  unsaturated aldehydes and *tert*-butyl mercaptans. **J.E. Anesini**, M.J. Veticatt

**72.** In-situ emission gas analysis in lithium ion battery using gas chromatography with electrolysis cell. **R. Takechi**, E. Kobayashi, D. Fukushima, M. Furukawa, T. Hiraoka, M. Taylor, **M. Janeczko**

**322.** Easy absolute specular reflectance and transmittance measurements of anti-reflective coatings used in alternative energy applications. **C.M. Talbott**