

# Wednesday General Info

**Get your badge** - starting at 7 am at the Event Office in the upper level of the Convention Center

**Beverage Services** - water stations will be available outside the meeting rooms. Complimentary coffee and tea and other beverages will be available daily from 8 am - 5 pm in the WCC upper atrium. Official Coffee breaks from 10-10:30 am and 3-3:30 pm.

**Networking Space** - Networking space sponsored by Baylor University can be found in the WCC upper atrium.

## FOOD and Drink

### In the Convention Center

Upper Atrium  
Daily 11 am - 2 pm

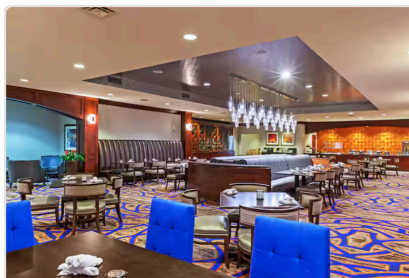
#### **Brown Bag Special**

Pulled Pork Sandwiches  
Brisket Sandwiches  
Sausage Sandwiches  
Chips  
Sodas/water  
BBQ Frito pie  
BBQ Nachos



### In the Hilton

Breakfast, lunch, and dinner daily



#### **Brazos Grille**

Brazos Grille at the Hilton Waco hotel offers a variety of regional Italian inspired dishes to meet everyone's tastes at an affordable price. Offering a casual, yet festive atmosphere with a wide variety of menu selections, it provides the perfect place to enjoy the panoramic views of Indian Hills Park & the Brazos River. Brazos Grille is open daily for breakfast, lunch and dinner serving fresh indigenous local products.

### Across the Street



WiFi Network Name: ccpublic Password: wacocc17

# Wednesday Events

**Senior Chemists Breakfast** - (7-8 am) meet Pat Farmer in the Hilton Brazos Grille (Patrick\_Farmer@baylor.edu)

**Board Meeting** 7:30 am - noon; Waco Room

**Coffee Breaks** 10-10:30 am, 3-3:30 pm Upper Atrium

**Award Luncheon** 12-1:30 pm; Hilton Hotel Brazos Room (ticketed)

# Wednesday Morning Technical Program

## ***Inorganic Chemistry (General)***

M. Akram, *Organizer, Presiding* Texas 113

## ***Emerging Topics in Environmental Chemistry***

G. P. Cobb, C. M. Sayes, *Organizers, Presiding* Lone Star 103

## ***Experimental and Computational Studies of Protein Structure and Dynamics***

J. Clinger, *Organizer, Presiding* Texas 117

## ***Materials for Energy and Environment***

J. Larson, *Organizer, Presiding* Texas 118

## ***Medicinal Chemistry***

K. G. Pinney, *Organizer, Presiding* Texas 115

## ***Organic Chemistry (General)***

N. Matsumoto, *Organizer, Presiding* Texas 114

## ***Physical Chemistry (General)***

K. L. Shuford, *Organizer*; U. De Alwis, *Presiding* Texas 116

## ***Analytical Chemistry (General)***

E. S. Gallagher, *Organizer*; T. Solouki *Presiding* Lone Star 104

## ***Advances in Polymer Chemistry***

J. A. Irvin, *Organizer*; M. Sheokand, *Presiding* Ranger 106/107

# Wednesday Afternoon Technical Program

## *Advances in Polymer Chemistry*

J. A. Irvin, *Organizer*; T. Betancourt, *Presiding* Ranger 106/107

## *Environmental Chemistry and Toxicology*

G. P. Cobb, C. M. Sayes, *Organizers, Presiding* Lone Star 103

## *Inorganic Chemistry (General)*

M. Akram, *Organizer, Presiding* Texas 113

## *Metalloenzyme Design*

I. V. Korendovych, *Organizer, Presiding*; L. R. Marshall, *Presiding*  
Texas 117

## *Organic Chemistry (General)*

N. Matsumoto, *Organizer, Presiding* Texas 114

## WEDNESDAY MORNING

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### *Inorganic Chemistry (General)*

M. Akram, *Organizer, Presiding*

Texas 113

7:55 Introductory Remarks.

8:00 749. Guest inclusion into novel pillared hydrogen-bonded metal-organic frameworks. **G.A. Hogan**

8:20 750. Development of earth-abundant Cu(I)-photosensitizers using *N*-heterocyclic carbenes with variable anionic chelating ligands. **S. Chakraborty**, T.S. Teets

8:40 751. Synthesis and reactivity of base-supported organopnictogen Lewis acids. **N.H. Hunter**, F.P. Gabbai

9:00 752. Effect of metal, coligand, and number of thiophenes on the ground and excited state redox potentials of complexes of the type  $[M(L)_2(IP-nT)]^{2+}$ . **A. Vali**, A. Talgatov, H. Cole, G. Kaur, G. Shi, C. Cameron, S.A. McFarland

9:20 753. Development of non-classical photoprecursors for Rh<sub>2</sub> Nitrenes. **A. Paikar**

9:40 754. Dinuclear late-transition metal complexes of polyaromatic heterocycles. **U. Ekanayaka Arachchige**

10:00 Coffee Break.

10:20 755. Synthesis, characterization, and binding studies of new 1,3 benzotellurazoles containing a central pyridine units: Incorporation of chalcogen bond donors into a NNN pincer ligand.. **A. Amaya**, L. Delgado Cordoba, M. Abbaschaleshtori, H. Arman, A.F. Cozzolino, Z.J. Tonzetich

10:40 756. Applications of Photoactivated Metallodrugs for Cancer Therapy. **A. Talgatov**, D. Lucas, G. Shi, G. Kaur, J. Rahmon, D. Sunday, A. Vali, C. Cameron, S.A. McFarland

11:00 757. Bonding analysis of tetramethylguanidinyll arms supporting copper(I) catalytic sites. **J. Adebajo**, Z. Lu, T.R. Cundari, P. Stavropoulos, M.A. Omary

11:20 758. Resonance-assisted hydrogen bonded fluorescent probe for relay recognition. **R. Mia**, B. Maillet, J. Weeks, M. Zepeta-Rodriguez

11:40 759. Photoreductive elimination of chlorine from a phosphine/oxaborine gold(III) complex. **P. Castro**, W. Liu, F.P. Gabbai

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### *Emerging Topics in Environmental Chemistry*

G. P. Cobb, C. M. Sayes, *Organizers, Presiding*

Lone Star 103

8:00 Opening Remarks.

8:05 760. Current status of micropollutants in aquatic environment. **V.K. Sharma**

8:30 761. Effect of the presence of emerging contaminants upon the compositional and functional dynamics of WWTPs sludge in Mexico. **L.G. Garcia Murillo**

8:55 762. New approaches to organofluorine sum parameter analysis. **C.P. Shelor**, C. Warren, C.V. Odina

9:20 763. Emerging tools for non-targeted analysis: Towards environmental decision making. **E.M. Ulrich**

9:45 Intermission.

- 10:00 764.** Marine microplastic analysis: A case study of Matagorda Bay. **M.A. Azadah**
- 10:25 765.** Mesoporous silica-based nanocarrier system as a strategy to deliver agrochemicals to plant crops. **X. Gao, S. Ghoshal**
- 10:50 766.** Natural organic matter, from molecules to Earth. **C. Zhang, M. Yan, G. Korshin**
- 11:15 767.** Insights into phosphate functionalization, kinetics, and mechanism of phosphorylated sporopollenin as a sustainable catalyst for selective 5-hydroxymethylfurfural formation in water. **R. Sharma, T. Selvaraj, V. Gowri, J. Varghese, J. Govindasamy**

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## ***Experimental and Computational Studies of Protein Structure and Dynamics***

J. Clinger, *Organizer, Presiding*

Texas 117

- 8:00 768.** Protein Bikram Yoga. **M. Fischer**
- 8:30 769.** Interrogating proteins as molecular machines aided by machine learning. **P. Tao**
- 9:00 770.** Active site electrostatics can gate enzyme dynamics during catalysis. **M.A. Wilson**
- 9:30 771.** Molecular-dynamics simulations of protein crystals and diffraction data. **M. Wall**
- 10:00 772.** Using deep learning and partial structure attention to solve the phase problem in crystallography. T. Pan, E. Dramko, M.D. Miller, A. Kyrillidis, **G.N. Phillips**
- 10:30 773.** Lipid regulation of GPCR dynamics and ligand-receptor association. **B. Wylie, E. van Aalst, J. Jang, S. Bannister**
- 10:50 774.** Quantum-mechanical molecular dynamics simulations of chemical reactions to investigate enzyme mechanisms. **R.A. Grove, M.A. Wilson, A.M. Niklasson, C.F. Negre, M.E. Wall**

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## ***Materials for Energy and Environment***

Cosponsored by ENFL

J. Larson, *Organizer, Presiding*

Texas 118

- 8:00 775.** Novel hydrocarbon derived carbon nanomaterials for wearable and flexible printed micro-supercapacitors. **R. Banavath, Y. Zhang, S. Deshpande, S. Dasari, M. Green**
- 8:20 776.** Covalent organic frameworks for rapid removal of perfluorooctanoic acid. **H. Vardhan, R. Verduzco**
- 8:40 777.** Green-emitting  $\text{Mn}^{2+}:\text{Cs}_3\text{CdBr}_5$  perovskite for WLEDs. **W. Yu**
- 9:00 778.** Improved the photoelectrochemical stability and performance of  $\text{BiVO}_4$  photoanode using  $\text{In}_2\text{Se}_3$  as a protective layer in a harsh environment. **N.B. Belachew**
- 9:20 779.** Metal quaterpyridine molecular complexes for photocatalytic  $\text{CO}_2$  reduction on a crystalline carbon nitride scaffold. **S. McGuigan, S.J. Tereniak, A. Smith, C.L. Donley, F. Zhao, S. Jeon, M. Pauly, L. Keller, L. Collins, S. Jana, S. Suhr, Y. Xu, N. Ghorai, H. Margavio, P.L. Holland, G. Parsons, T. Lian, E. Stach, P.A. Maggard**
- 9:40 780.** Unveiling the influence of cation mixing on photoelectrochemical water oxidation in  $\text{Mg}_{1-x}\text{Cu}_x\text{V}_2\text{O}_6$  solid solutions. **A. Rawat, R. Krishnan**

10:00 Coffee Break.

10:30 **781.** Structuring V<sub>2</sub>O<sub>5</sub> Positive Electrodes for Applications in Battery Cathodes and Direct Lithium Extraction. **J.L. Carrillo**

10:45 **782.** Fine-tuning microporosity of crystalline mixed-metal oxide frameworks for selective adsorptive separation of Kr from Xe. **S. Akter**, Y. Li, M. Kim, M. Faruque, Z. Peng, P.K. Thallapally, M. Momenitaheri

11:00 **783.** Effect of aluminum substitution ratio within nickel hydroxide cathodes for high performance alkaline nickel-zinc batteries. **J.A. Manley**, S.W. Kimmel, C.P. Rhodes

11:15 **784.** Lighting the path: Design principles for halide-ion solid electrolytes through spectroscopy and simulation. **J. Cheng**, S. Banerjee

11:30 **785.** *Withdrawn*

11:45 **786.** Low-temperature structural battery electrolytes produced by polymerization-induced phase separation. **S. Deshpande**, V. Vidyaprakash, S. Oka, S. Dasari, K. Liu, C. Wang, J. Lutkenhaus, M. Green

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## ***Medicinal Chemistry***

K. G. Pinney, *Organizer, Presiding*

Texas 115

8:00 **787.** Potent and selective small molecule PKCE inhibitors for non-opioid pain applications: Enantioselective synthesis, structure-activity relationship and *in vivo* efficacy studies. **S.F. McHardy**, H. De Kraker, C.N. Fleischer, A. Gregory-Flores, I. Magayewski Bonet, L. Barrera, H. Arman, R.N. Renteria, J. Levine, P. Parker, S. Kjaer, M. Marinelli, R.O. Messing

8:30 **788.** Evaluation of the cytotoxic properties of macrocyclic diterpenoids against triple negative breast cancer. J. Robles, **C.S. Fermaintt**

8:50 **789.** Design, synthesis, and biological evaluation of OXi8006 analogues bearing aryl ring bridge modifications as inhibitors of tubulin polymerization. **Y. Wong**, W.K. Rathnayake, C. Tamminga, Y. Deng, M.L. Trawick, R. Bai, E. Hamel, K.G. Pinney

9:10 **790.** Design, synthesis, and antimicrobial evaluation of some new thiopyrimidin-benzenesulfonamide compounds.. **S.H. Abdelwahed**

9:30 **791.** Site-selectively radiolabeled syndecan-1 antibody as a targeted radionuclide theranostics approach suitable for pancreatic cancer. **A. Yamaguchi**, R. Coll, Z. Yang, R. Ta, W. Yao, H.C. Manning

9:50 **792.** Strategies for selective delivery of vascular disrupting agents in the tumor microenvironment. **C. Pavlich**, W. Ren, Z. Shi, M.L. Trawick, K.G. Pinney

10:10 Coffee Break.

10:30 **793.** Synthesis of tripeptide drug-linker constructs cleavable by enzymes present in the tumor microenvironment. **K. Hamal**, Y. Wong, C. Pavlich, C. Borchardt, P. Tankoano, M.L. Trawick, K.G. Pinney

10:50 **794.** Unexpected directionality in thioamide hydrogen bonds stabilizes  $\beta$ -strands. **H. Zheng**, R.W. Newberry

11:10 **795.** Polygonum multiflorum: Recent updates on newly isolated compounds, potential hepatotoxic compounds and their mechanisms. **T.T. Teklehaimanot**, L. Wang, J. Gao, J. Mou, G. Pan, H. Yu, X. Gao, L. Han

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## ***Organic Chemistry (General)***

N. Matsumoto, *Organizer, Presiding*

Texas 114

**8:00 796.** Cyclic and acyclic acetals as effective methylene sources for the synthesis of pillararenes. **B. Machireddy**, M. He

**8:20 797.** Asymmetric ruthenium-catalyzed carbonyl allylation and *tert*-prenylation via hydrogen transfer to  $\pi$ -unsaturated hydrocarbon feedstocks. **C. Saludares**

**8:40 798.** Dynamically generated carbenium species via photoisomerization of cyclic alkenes: Mild Friedel-Crafts alkylation. **O. Alkhamayseh**, T. Schoch, N. Herndon, E. Lantz, T. Fleske, J.D. Weaver

**9:00 799.**  $\beta$ -phenethylamine synthesis: *N*-pyridinium aziridines as latent dual electrophiles. **S. Samanta**, P. Biswas, B. O'Bannon, D. Powers

**9:20 800.** Development of a universal SuFEx reagent for deaminative C–C cross-couplings. **D. Chattapadhyay**, A. Aydogan, M. Diaz, Q. Michaudel

**9:40 801.** Triphenylborane Catalyzed [2+3]-Cycloaddition of Bestmann's Ylide, Ph<sub>3</sub>PCCO, with Chiral Epoxides. **K. Nadella**, c. liu, C. Krempner

**10:00** Coffee Break.

**10:20 802.** Synthesis of novel chemosensors: Bridged Calix[4]arenes and photoswitchable spyropyrans. **F.W. Foss**, R. Madigan, R.L. Miller

**10:40 803.** Reliable macrocycle molecular frameworks: Capitalizing on conserved conformations in triazine macrocycles. **C. Patterson-Gardner**, E. Simanek

**11:00 804.** Synthesis of prodrugs of AER-270 with controlled release kinetics. **A. Sarkar**, M. Nicosia, A. Valujskikh, R.R. Kane

**11:20 805.** Progress towards to total synthesis of (+)-pedrolide. **H. Shen**, J.L. Wood

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## ***Physical Chemistry (General)***

K. L. Shuford, *Organizer*

U. De Alwis, *Presiding*

Texas 116

**8:20 806.** *Moved to 11:40 am in this session*

**8:40 807.** Molecules in oriented external electric field. **D. Lai**, D. Matthews

**9:00 808.** Generalizing electronic-vibrational couplings in the adaptive Hierarchy of Pure States (adHOPS). **J.K. Lynd**, D.I. Raccah

**9:20 809.** DFT study on the catalytic mechanism of N<sub>2</sub> reduction by a borylene complex. **S. Yu**, M.B. Hall

**9:40 810.** Computationally assessing electron-withdrawing chalcogen bond donors in N<sub>2</sub> activation chemistry. **K.A. French**, V. Choutipalli, K.L. Shuford

**10:00** Coffee Break.

**10:20 811.** Ligand characterization and DNA intercalation of Ru(II) polypyridyl complexes: A local vibrational mode study. **H. La Force**, M. Freindorf, E. Kraka

**10:40 812.** Astrochemical modeling of acetonitrile chemistry in the interstellar medium: A computational study. **K. Fleming**, E. Kraka

**11:00 813.** Automated atomic grids in least-squares tensor hypercontraction. **C. Yin**, J.H. Thorpe, D.A. Matthews

**11:20 814.** Uranium-ligand bonding in uranyl-peroxide dimers and uranyl-hydroxo dimers: A local vibrational mode pilot study. **D. Gamage**

**11:40 806.** Organization of mixed self-assembled monolayers: Case studies in adsorption and aggregation of biomolecules, inorganic catalysts, and petroleum mimics. **R.S. Thompson**, O. Guzman, I. Guzman, J. Godino, E. El-Shaer, L. Garcia, A. Havens, R. Escobedo, L. Payne, A. Nesheiwat, G. Caswell, L. Kandil

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## ***Analytical Chemistry (General)***

E. S. Gallagher, *Organizer*; T. Solouki *Presiding*

Lone Star 104

**8:30 815.** Characterization of volatiles emitted from 3D printed polymers: Implications for ghost gun manufacturing. **H. Browning**, J. Carrell, P. Tiedemann

**8:50 816.** Chemical analysis of electronic nicotine delivery systems. **j. mata**

**9:05 817.** Surrogate optimization for supercritical fluid extraction-supercritical fluid chromatography hyphenated mass spectrometry. **N. Bhakta**

**9:25 818.** Acoustofluidics for separation and purification of heavy metal adsorbed MPs in the aquatic environment. **N.A. DeSilva**, M.E. Piyasena, N. Perera

**9:45 819.** Analysis of eggshell health of East Texas landfowl and waterfowl. **C. Davis**, A.S. Frantzen, F. Majis

**10:00** Coffee Break.

**10:30 820.** Effect of the substituent groups of Tyr<sub>5</sub> and His<sub>6</sub> on the gas phase zinc affinities of acetyl-His<sub>1</sub>-Cys<sub>2</sub>-Gly<sub>3</sub>-Pro<sub>4</sub>-X<sub>5</sub>-X<sub>6</sub>-Cys<sub>7</sub> heptapeptides. **M.B. Owusu**, R.A. Adomako, P. Asare, K.N. Senyah, R. Oberdick, L.A. Angel

**10:50 821.** Retention-time alignment and imputation algorithms affect statistical comparisons when multiple samples are searched together in proteomics database searching software.. **J.M. Conforti**, C.C. Breus, C.S. Worth, J. Taube, E.S. Gallagher

**11:10 822.** Application of binomial distribution statistics for quantitative proteomic analysis. **S. Momin**, T. Solouki

**11:25 823.** Urinary fatty acid biomarkers for prostate cancer detection and prognosis. **E. Noriega Landa**, G. Quaye, W. Lee, X. Su

**11:45 824.** Variations in intracellular organometallic reaction frequency captured by single-molecule fluorescence microscopy. **G. Yan**, D. Nguyen, T. Chen, L. Do

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## ***Advances in Polymer Chemistry***

J. A. Irvin, *Organizer*

M. Sheokand, *Presiding*

Ranger 106/107

**8:55** Welcome.

**9:00 825.** On-demand drug delivery via photothermal stimulation of dynamic covalent poly(ethylene glycol)/PEDOT hydrogels. K. Thapa, M. Otakpor, A. Strait, E. Rodriguez, S. Bhuiyan, Y. Kinfe, T. FitzSimons, N. Conrad, A. Crowell, A. Rosales, **T. Betancourt**

**9:20 826.** Synthesis and application of electrochemically-active sequence-defined oligourethanes towards long-term data storage. **B. Pandey**, B. Muralidharan, E.V. Anslyn

**9:40 827.** Accessing sustainable polysulfamates through sulfur(VI) fluoride exchange (SuFEx) polymerization. **S. Das**, K. Doktor, Q. Michaudel

**10:00 828.** Leveraging steric effects in monomer design to access precise pyridine-containing polymers via ROMP. **A. Tran**, Q. Michaudel

**10:20** Intermission.

**10:40 829.** Mechanistically-informed stereoselective ring-opening metathesis polymerization for precise synthesis of poly(*p*-phenylene vinylene)s. **J. Nicholson**, S. Kempel, Q. Michaudel

**11:00 830.** Continuous flow synthesis of polar polyethylene block copolymers. **S. Sarkar**, H. Dau, E. Harth

**11:20 831.** Closing the loop for Polyacylhydrazone(PAcHy) soft materials. **M.B. Minus**, C. Ufodike, A. Rahman, E. McHenry, M. Giles, G. Nzebuka

## WEDNESDAY AFTERNOON

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### *Advances in Polymer Chemistry*

J. A. Irvin, *Organizer*

T. Betancourt, *Presiding*

Ranger 106/107

**1:00 832.** Vapor phase deposition of electroactive polymers onto electrospun commodity polymer nanofibers. **S. Brahma**, N.R. Lontkowski, J. ur Rehman, T. Betancourt, J.A. Irvin

**1:20 833.** Tensile behavior of electroactive polymer coated polyacrylonitrile nanofibers. **A. Gustafson**, J.A. Irvin, K. Bay, S. Brahma, A. Libonati

**1:40 834.** Bio-sourced adhesive with fire protection. **D.L. Smith**, D. Rodriguez-Melendez, M.O. Convento, M. Montemayor, J.C. Grunlan

**2:00 835.** Fully biobased and biodegradable oxygen barrier coating for poly(lactic acid). **S. Fisher**, E. Iverson, E. Chang, J.C. Grunlan

**2:20 836.** Effects of alkyl polyglucoside tail length on surfactant foaming properties. **G.R. Overholt**

**2:40 837.** Solvent-Induced Mobility of Polymer Chains and Metallocene Migration into LDPE: A HRMAS NMR Study. **M.R. Kimball**, J.C. Hoefler, J. Bluemel

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### *Environmental Chemistry and Toxicology*

G. P. Cobb, C. M. Sayes, *Organizers, Presiding*

Lone Star 103

**1:00** Open Discussion.

**1:05 838.** Inductively coupled plasma-mass spectrometry (ICP-MS) preparation techniques for solid-state sample analysis. **M. Stevens**, C.M. Sayes

**1:30 839.** Moved to Monday poster session #P005

**1:55 840.** Study of microplastics in wastewater treatment plants in deep east Texas. **J. Swallow**, K.K. Onchoke, R. Friedfeld

**2:20 841.** Determining the degradation rate of polystyrene microplastics after reacting with Amano lipase, manganese peroxidase, and Fenton oxidation.. **J. Lugo**, T. AYORINDE, A. Charlton-Sevcik, C. Sayes

**2:45 842.** Quantification of microplastics in soil and mulch. **C. Hyppolite**, T. Phan, A. Bastidas, K. Miller, I. Simon, V. Tran

**3:10 843.** **Withdrawn**

**3:35 844.** Biodiesel vs conventional diesel: An analysis of particulate matter formation. **C.C. Watkins**

**4:00** Introductory Remarks.

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## ***Inorganic Chemistry (General)***

M. Akram, *Organizer, Presiding*

Texas 113

- 1:00 845.** Extraction and synthesis of the active components of inorganic sunscreen. **C.C. Watkins**
- 1:20 846.** Designing Metal Halides for Fast Neutron Imaging: Chain-Head Engineering in Hybrid  $A_2MnCl_4$  Emitters. D. Banerjee, E.J. Brand, **K. McCall**
- 1:40 847.** Efforts to improve crystallization protocols of an unknown plutonium compound to allow for its full structural characterization. **R.A. Zehnder**
- 2:00 848.** Design Principles for Cooperativity in Redox Processes. A. Henderson, H. Watts, A. Telford, M. Garcia Dalmases, C. Young, E. Ah Leong, L. Kimble, S. Shipman, B.M. Barngrover, **J.B. Gary**
- 2:20 849.** Structure, activity and stability of ruthenium-chromium oxide aerogel oxygen evolution electrocatalysts. **J. Adame Solorio**, S.W. Kimmel, C.P. Rhodes
- 2:40 850.** Antimony(V)/crown ether conjugates as cation-anion symporters. **A. Kim**
- 3:00** Coffee Break.
- 3:20 851.** Creating solid solutions of ferrocene, cobaltocene, and nickelocene: A paramagnetic solid-state NMR study. **G. Harmon**, V. Bakmutov, J. Bluemel
- 3:40 852.** Low temperature synthesis, crystal and electronic structures of Osmium & Ruthenium Chalcobromides :  $Os_2S_4Se_2Br_{10}$ ,  $Os_2Se_6Br_{12}$  &  $Ru_2Se_6Br_{10}$ . **T. Kandabadge**, S. Baranets
- 4:00 853.** Joule heating as a high-temperature out-of-oven manufacturing technique for nanocarbon/inorganic composites. **S.T. Upama**, A. Mikhalchan, L. Arévalo, A. Pendashteh, J. Vilatela, M. Green
- 4:20 854.** Aerobic oxidation of hydrocarbons using site isolated vanadyl in Metal Organic Frameworks. **T. Ericson**, M. Ghartemani, J. Emanuele, S. Khatib, A.F. Cozzolino
- 4:40 855.** Structure and performance of high-energy ball milled iridium-titanium oxide oxygen evolution electrocatalysts. **K.R. Bailey**, J. Adame Solorio, C.P. Rhodes

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## ***Metalloenzyme Design***

I. V. Korendovych, *Organizer, Presiding*

L. R. Marshall, *Presiding*

Texas 117

- 1:00 856.** Peroxidase behaviors of heme-amyloid species. **L.R. Marshall**, O. Zozulia, I. Kim, E.M. Kohn, I.V. Korendovych
- 1:30 857.** Uno Ferro, a de novo designed protein, binds transition metals with high affinity and stabilizes semiquinone radical anion. **O. Makhlynets**
- 2:00 858.** *De novo* design of protease-activated antimicrobial proteins. **S. Bhattacharya**, W.F. Degrado
- 2:30 859.** Catalytic nanoassemblies formed by short peptides promote highly enantioselective transfer hydrogenation. **I.V. Korendovych**

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## ***Organic Chemistry (General)***

N. Matsumoto, *Organizer, Presiding*

Texas 114

**1:00 860.** Concise total synthesis of the psammalydin alkaloids. **A. Morrow**

**1:20 861.** *Withdrawn*

**1:40 862.** Vitamin B<sub>12</sub>-catalyzed cyclopropanation reactions. **J. Teye-Kau**, S. Pitre

**2:00 863.** Molecular motors driven by electrons and protons. **Y. Feng**

**2:20 864.** Halogen-bonding photocatalyzed radical perfluoroalkylation reactions. **T. Tasnim**, S. Pitre

**2:40 865.** Bioorthogonal engineering of trehalose-modified glycolipids in mycobacterium: Unraveling molecular interactions via click chemistry. **D. Czapski**

**3:00** Coffee Break.

**3:20 866.** Electronically mismatched Diels-Alder reaction via Lewis Acids catalyst. **M. Qureshi**, S.R. Hussaini

**3:40 867.** Phthalimide addition to styrene oxide or glycidyl phenyl ether using ammonium salts as catalysts. **C.J. Neef**, E. Hammeke, C. Wheeler, H. Humes

**4:00 868.** *Withdrawn*

**4:20 869.** Co-catalytic coupling of alkyl bromides and chlorides: The curious role of Lutidine. **P. Sharma**, R. Hanumanthu, A. Ethridge, J.D. Weaver

**4:40 870.** Cu-catalyzed strain-release-driven radical difunctionalization reactions of unsaturated compounds. **A. Popov**, V. Viviani, P. Skumial, T.L. Jefferson, S.G. Salman, H.H. Baxter, K. Hull

**5:00 871.** Mechanochemical synthesis of enamino carbonyl compounds.. **M. Ndlovu**, S.R. Hussaini