

NORM 2018

V. Glezakou and R. Devanathan, *Program Chairs*

SUNDAY MORNING

Discovery Hall
Horizon B

Pre-College Teachers Program: General Papers

Cosponsored by CHED
Financially supported by AACT
F. N. Smith, *Organizer*
J. A. Soltis, *Organizer, Presiding*

8:00 Welcome and program overview.

8:20 1. Workshop 1: Exploring dissolution and crystallization with a smartphone microscope. **G.J. Lumetta**

9:20 Intermission.

9:40 2. Workshop 2: Cameraphone colorimetry in the classroom. E. Kehoe, **J.A. Soltis**, R. Penn

10:40 Intermission.

11:00 3. Preparing students for the real world. **F.K. Wood-Black**

11:20 4. PROJECT SEED: Summer research experiences for economically disadvantaged high school students. **A.G. Cavinato**

11:40 5. Teacher research immersion opportunities at PNNL. **A. Wright-Mockler**

1:00 6. Workshop 3: Climate science concepts fit your classroom: a hands-on workshop. **J.A. Bell**, A. Crosby

SUNDAY EVENING

Discovery Hall
Horizon C/D/E

General Posters

R. Devanathan, V. Glezakou, *Organizers, Presiding*

6:00 - 8:00

7. Advancing infectious disease research through structural genomics: The Seattle Structural Genomics Center for Infectious Diseases (SSGCID). **G.W. Buchko**, T.E. Edwards, B. Staker, R. Stacy, D. Veessler, G. Varani, W.C. Van Voorhis, P.J. Myler
8. Tools for understanding molecular scale mechanisms in P2X receptors: Single molecule kinetics, super-resolution imaging, and hidden Markov walks. J.A. Brozik, **K. Lam**
9. ProDock: A 3D visualization enabled web modeling environment for rapid structure-based small molecule high-throughput virtual screening and protein-protein docking. **A. Tao**, Y. Shinohara, Y. Huang, M. Caylor, **D. Xu**
10. TargetSearch: An integrative cross-database molecular search engine for drug discovery, drug repurposing, and drug safety research. **Y. Huang**, M. Caylor, A. Tao, **D. Xu**
11. In silico analysis and predictive models of serotonin 2B receptor ligands and its implications in drug-induced cardiotoxicity. **S. Rahman**, Y. Huang, A. Tao, M. Caylor, **D. Xu**
12. Theoretical insights on solvent control of intramolecular and intermolecular proton transfer of 2-(2'-hydroxyphenyl)benzimidazole. **C. Prommin**, N. Kungwan
13. Bulk and surface electronic structure of hydrated actinide (IV) oxalates, $\text{An}(\text{C}_2\text{O}_4)_2 \cdot 6\text{H}_2\text{O}$ (An = U, Pu). **K. Garrett**, A. Ritzmann, F.N. Smith, S.H. Kessler, N. Henson, D. Abrecht
14. Understanding the mechanism of a self-sensitizing tellurium-containing chromophore for thiol oxidation: a DFT study. **H. Irving**
15. Predicting carboxylic acid pK_a 's using density functional theory with implicit and explicit solvents: Results for $\text{RCOOH}-(\text{H}_2\text{O})_n$ clusters containing 1-5 waters. **J.W. Keller**
16. Controlled gold nanoparticle (AuNP) aggregation: Aggregate toxicity in *D. Magna*. **C. Vandermeer**, S.E. Lohse
17. Synthesis and metallation of a novel stimulus responsive ligand. **G.L. Bourne**, M.L. Scheuermann
18. Stereoselective reduction of α -fluoro- β -ketoesters by NADH and NADPH-dependent ketoreductases. **T. Green**, M. Vanagel, A. Damarancha, S. Kolberg, B. Showalter, A. Thompson
19. Preparation of metal-decorated zirconium phosphate nanoplatelets. **X. Li**, Q. Zhang
20. Extraction kinetics of dysprosium ions with Cyanex 572 and HEH(EHP). **T. Babikian**, A. Bosch Font, M. Nilsson

21. NiO nanoparticle synthesis, characterization, and toxicology. **P.T. Gwin**, C.C. Pena, K. Cornell, J.E. Cowan, J.D. Harris
22. Synthesis and characterization of ZnO nanoparticles and their use as a photocatalyst. **J.D. Harris**, C.C. Pena, A.E. Harris, J.E. Cowan
23. Synthesis of a tantalum methyldene complex relevant to methane oligomerization. **E. Reeves**, S. Neufeldt
24. Preparation and characterization of vinylimidazole-base polymeric monolithic stationary phase for reversed-phase LC and hydrophilic interaction LC. **M. Fuh**, S. Lin
25. Synthesis of biologically relevant α -ketophosphonates. **L. Kruger**, D. Shen, T.T. Denton
26. Synthesis, *in vitro* and *in vivo* analysis of phosphonate analogues of lanthionine ketimine: development of small molecule treatments for neurological disorders. **D. Shen**, I. Bains, J. Gerstner, T.T. Denton
27. Effects of antifreeze proteins and their hyperactive mutants on calcite crystallization. **A. Kishishita**, **J.J. Lugo**, **J. Castellon**, **F. Rojas**, X. Wen
28. Investigation of *Pseudomonas aeruginosa* acyl-ACP substrate specificity in RhII quorum sensing signal synthesis. **A. Poppe**, S. Basu, E. Paz Munoz
29. Comparative toxicity of ZnO nanoparticles synthesized using different amines. **C.C. Pena**, K. Cornell, J.E. Cowan, J.D. Harris
30. Exploration of the dynamic cytochrome P450 metabolon: A single molecule approach. **E.L. Taylor**, C. Barnaba, M.J. Martinez, J.A. Brozik
31. A novel ditopic selective chemosensor for cadmium and fluoride and its application as a pH sensor. **A. Roy Chowdhury**, P. Banerjee
32. Reaction-based fluorescence approach for quantitative detection of sulfite. T. Ding, **H. Cao**
33. Native luminescence of cytochrome P450 3A4 within a endoplasmic reticulum biomimetic nanodiscs. **M.J. Martinez**, C. Barnaba, J.A. Brozik
34. Sorbent coated metal filters simultaneous collection and detection of ultratrace levels of vapor and particulate explosives. **W. Chouyyok**, R.S. Addleman, X.S. Li, R. Ewing, D. Atkinson, K. Kottapalli, I. Novosselov
35. As(III) detection on GUITAR(Graphenic carbon from University of Idaho Thermalized Asphalt Reaction) based electrode. **H. Zhu**, F. Cheng
36. Techniques to investigate apatite crystal growth on amyloid-like amelogenin fibrils. **S. Akkineni**, S. Engelberth, J. Tao, J. Bonde, S. Habelitz, J. De Yoreo
37. ND-11543: A potent anti-mycobacterial Imidazo[2,1-b]thiazole-5-carboxamide agent. **G.C. Moraski**, Y. Cheng, M. Zimmerman, G. Shetye, S. Cho, S.G. Franzblau, J.S. Schorey, M.J. Miller
38. Spatial distribution of alkalinity and spectrophotometric pH in the upper Clark Fork River, Montana. **F.L. Young**, M.D. Degrandpre, C.M. Beatty, C.E. Wielgasz, P.E. Hurley, H.M. Valett

39. Characterization of the bioabsorption of heavy metals by spruiulina. **M.L. Davis**, T. Masiello
40. Coated zeolite for malodor control. **L.I. Robins**, C. Seek, J. Williams
41. Investigation of mononuclear actinide polyoxomatalates as potential single-molecules magnets. **I. Colliard**, L. Zakharov, M.D. Nyman
42. Screening of catalysts to enhance oxidative peracetic acid depolymerization of lignin. **R. Ma**, M.V. Olarte, H. Job, X. Zhang
43. Ligand binding on iron oxide nanoparticles: Understanding surface chemistry to empower rational design. **K.V. Korpany**, A. Moiseev, S.N. Cross, D. Majewski, M. Glavinović, A.S. Blum
44. Influence of a BODIPY-containing redox active ligand on switchable catalyst behavior. **B. Thompson**, Z.M. Heiden
45. Guanidine appended-BODIPY molecules for use as proton and electron reservoirs. **J.J. Markut**, J.L. Deobald, Z.M. Heiden
46. Understanding CO₂ hydrogenation using ester models: Possibilities and pitfalls in reaching methanol. **B.D. Neisen**, E.S. Wiedner, J.C. Linehan
47. Constructing electron acceptors for probing the mechanism of multi-electron transfer reactions. **J. Wimpenny**, Z.M. Heiden
48. Visible light driven aerobic catalysis using tellurium-containing chromophores. **L. Lutkus**
49. Spectroelectrochemical photoluminescence of TiO₂ nanowires. **R.E. Rex**, F.J. Knorr, J. McHale, Y. Li, J.Z. Zhang, Y. Yang
50. Effect of leucine on dry powder inhaler performance of salbutamol sulphate containing Xylitol crystals. **C. Molina**, A. Nokhodchi
51. Single-crystal-to-single-crystal transformation driven the fabrication of a thermodynamically controlled heterometallic metal-organic framework. **Y. Han**, **M. Sinnwell**, **P.K. Thallapally**
52. Safety is part of everything we do. **F.K. Wood-Black**
53. SCHB at the vanguard of innovation in the chemical community. **J.E. Sabol**, J.L. Bryant, J.C. Giordan

Discovery Hall
Horizon C/D/E

Innovation Fair in Exhibition

Cosponsored by BMGT, PROF and SCHB
Financially supported by ecosVC, Inc.
J. L. Bryant, *Organizer*
J. C. Giordan, *Organizer, Presiding*

6:00 - 8:00

54. Development of a solution-processed transparent conducting film for thin film solar panels. **J. Amador**

Undergraduate Posters

Cosponsored by CHED
C. Heideman, *Organizer, Presiding*

6:00 - 8:00

- 55.** Biomimetic conversion of pentabromopseudilin to its benzofuopyrrole analog with an anti-MRSA activity. **E. Costin, D. Kum, O. Rybakov**, S.K. Bruffy, J. Viramontes, **T.L. Suyama**
- 56.** Mining the Gene Expression Omnibus (GEO) for clues regarding the protective effects of silymarin in the liver. **J.R. Hurworth**, B. Stamper
- 57.** Mitigating dioxin formation from lignocellulose combustion: An experimental and computational approach. **K. Gallo, R. Meehan**, S. O'Brien, J. Valentine, M.E. Cremeens
- 58.** Measuring blood insulin levels using surface-enhanced Raman spectroscopy. **K. Lytle**, J. Coombs, S.R. Goates
- 59.** Antibiotics from actinomycete bacteria with activity against *Pythium*. J. Chung, **A. Hoffman**
- 60.** Exploring combinations of proteases and peptidases for the complete enzyme detoxification of gluten. **K.M. Markham, W.A. Kroes**, N.J. Bratt, D.D. Ojennus
- 61.** Determination of macrolide antibiotics in fish tissue by liquid chromatography with UV detection. **C. Cunningham**, C. Freeman, **E. Lavadour, A. Wirth**, A.G. Cavinato
- 62.** Determination of the major volatile and semi-volatile constituents of the essential oil from *Pinus Strobus Pendula* bark by gas chromatography/mass spectrometry. **N. Nilson**, K.E. Grant
- 63.** Analysis of rat urine and feces to investigate the effect of soft drinks on dietary fluoride uptake. **J.G. Marble, G.D. McQueen, E. Leavitt**, P.J. Iles, S. Moore, R. Kochambilli, **C. Fail**
- 64.** Expanding the analysis of fatty acid methyl esters (FAME) in biodiesel by fourier transform infrared spectroscopy (FT-IR). **E. Cabrera**, W.E. Steiner
- 65.** Isolation of aptamers for detection of *Renibacterium Salmoninarum* in water. **B.G. Staebler-Siewell, B.C. Peterson**, M.D. Hoppe, A.G. Cavinato
- 66.** Development of a low-cost instrument for analysis of lead in tap water. **E. Clarke**, T.L. Sorey
- 67.** Essential oil of *Elaeagnus angustifolia* seed constituents analyzed by gas chromatography / mass spectrometry. **T. Taranto**
- 68.** Low dead volume in spectroscopy. **N. Giauque**, J. Dickson, S.R. Goates
- 69.** Characterization of DNA aptamers for sensor development. **H.M. Breen, J.K. Carter**, A.G. Cavinato
- 70.** Electrospun polyacrylonitrile nanofibers reinforced with nitroxide. **M. Toney**, J. Macossay, S.A. Garza

71. Controlled release of hydroxyapatite nanoparticles via pH responsive polysuccinimide. **M. Toney**, S.G. Boyes, P. Smith
72. Design of nickel nanoparticles for x-ray fluorescence microscopy to visualize cellular metal ion concentrations. M.R. Mackiewicz, **H. Sawab**
73. Computational design of double perovskites for photovoltaic applications. **H. Doran**, R. Berger
74. Tuning the surface architecture of silver nanoparticles for use as anti-viral agents. **H. Wu**, D. Demchenko, K.M. Stedman, M.R. Mackiewicz
75. Band gap and edge engineering of perovskite niobate and tantalate photocatalysts. **G. McClarin**, R. Berger
76. Evaluating research skills development in the undergraduate chemistry laboratory curriculum. **S. Berrett**, R. Sargeant
77. Characterizing screening methods for solar thermal fuel properties of norbornadiene. **R. Szabo**, K. Le, T. Kowalczyk
78. Evaluation of a low cost alternative to a traditional table-top refractometer. **J. Stanger**, D. Loertscher, R. Sargeant
79. Automation for chemistry undergraduates. **M. John**, **P. Conway**, G. Fisher, H. Becerril
80. Influence of phosphine basicity on the addition of protons and electrons to [FeFe]-hydrogenase model complexes. **D. Chudomelka**, J. Wimpenny, Z.M. Heiden
81. In situ high temperature material characterization of proton conducting ceramics using Raman spectroscopy. **D.J. Goettlich**, R.A. Walker, E. Pomeroy
82. Characterization of one-electron organoborohydride oxidation reactions with NMR. **C.J. Allen**, E.R. Abbey
83. Indirect detection of magnesium metal flakes in ammonium nitrate using handheld Raman spectroscopy. O.M. Primera, **A.S. Breton-Vega**, C. Fraga
84. Degradation of nalbuphine. S.R. Goates, **D. Schvaneveldt**, S. Goldrup
85. A chemoenzymatic approach to the total synthesis of epoxyquinol A. **M.S. Duncan**, W.B. Kline, A.J. Stanley, J.A. Collins
86. Organic multistep synthesis lab. **A. Cox**, A.N. Lamm
87. Investigation of hydroquinone ring-cleaving dioxygenase homologs. **M. Maker**, **L. Amorosi**, J. Duncan, T.E. Machonkin
88. Developing a series of hydroquinone ring-cleaving dioxygenase model complexes. **M. Blakeley**, A. Behrman, N.R. Porter, A. Speelman, P.L. Holland, T.E. Machonkin
89. Isolation of saturated pyrrolizidine alkaloids from *Arnebia pulchra*, *Omphalodes verna*, and *Lindelofia anchusioides*. **J.D. Jacobs**, L.K. Johnson, R.A. Davis, B.E. Schroeder, R.B. Kelley

- 90.** Metallodithiolate ligands for reversing metal ion induced aggregation of beta amyloid. M.R. Mackiewicz, **E. Adams**
- 91.** Re-engineering promiscuous cytochrome P450 aromatic *O*-demethylase for lignin bioconversion. **Q. Doolin**, M. Machovina, J.L. DuBois
- 92.** Determination of pyrrolizidine alkaloids in *Heliotropium molle* from the plant family Boraginaceae. **C.J. Burghard**
- 93.** Analyzing the impact on modifying the course structure in organic chemistry. **B. Koster**, C. Wilson, J. Kent, S. Hodapp, R. Sargeant
- 94.** Platinum(II)-catalyzed additions to conjugated alkynones. J.W. Hartman, **B. Howard**
- 95.** Isomerization reaction coordinate study of solar thermal fuel systems using density functional theory (DFT). **K. Yokuda**, T. Kowalczyk
- 96.** Study of the volatile and semi-volatile constituents found in bark from *abies magnifica var. shastensis* by gas chromatography/mass spectrometry. **K. Trujillo**, K.E. Grant
- 97.** Gibbs ensemble Monte Carlo simulations of adsorption in zeolitic imidazolate framework materials. **G. Greene**, Y.A. Houndonougbo
- 98.** Molecular dynamics simulations study of ITPA protein substrate complex. **M.G. Metro**, Y.A. Houndonougbo

MONDAY MORNING

BSF/CSF
Darwin

Chemistry & Collaboration to Advance Nuclear Technologies

Cosponsored by NUCL
S. A. Bryan, *Organizer*
A. E. Clark, *Organizer, Presiding*
N. Henson, *Presiding*

8:00 Introductory Remarks.

8:05 99. Interfacial Dynamics in Radioactive Environments and Materials (IDREAM): An Energy Frontier Research Center that fosters collaboration to accelerate progress towards environmental cleanup. **S.B. Clark**

8:45 100. Education on nuclear and radiochemistry: DOE-funded traineeship at Washington State University and Colorado School of Mines. **N.A. Wall**, M.P. Jensen, K.L. Nash, D. Wall, S.B. Clark, J. Shafer

9:10 101. Experimental thermodynamics and solid-state chemistry on actinide-containing materials. **X. Guo**

9:35 102. Nano x-ray microscopy: The ultimate in non-destructive, 3D material analysis down to 50 nm resolution even in low-Z materials. **J. Jennings**

10:00 Intermission.

10:20 103. Fundamental radiation chemistry questions within the nuclear fuel cycle. **D.R. Peterman**

10:45 104. Actinide / lanthanide differentiation supported by novel aminopolycarboxylates: Structure-complexation study. **P.R. Zalupski**, C. Heathman, T.S. Grimes, V. Bryantsev, S. Jansone-Popova

11:10 105. Twenty years of collaborating for safe nuclear waste management and fundamental actinide chemistry. **M.D. Nyman**

11:35 106. Teaching and research collaboration mission of the WSU Nuclear Science Center. **D.E. Wall**

EMSL
1075

Geochemical Transformations in Natural & Engineered Systems

Cosponsored by GEOC
E. S. Ilton, M. K. Nims, S. Saslow, *Organizers*
E. J. Bylaska, *Organizer, Presiding*
E. Ilton, *Presiding*

8:00 Introductory remarks.

8:05 107. Oxalate promoted Cr(VI) adsorption of hematite nanocubes via forming iron-oxalate-Cr(VI) ternary surface complexation. **X. Huang**, X. Hou, F. Song, K. Rosso, J. Zhao, L. Zhang

8:30 108. Uranium incorporation in iron (oxyhydr)oxides. **M.E. McBriarty**, S.N. Kerisit, E.J. Bylaska, J.A. Soltis, S. Shaw, K. Morris, E.S. Ilton

8:55 109. Atomic-scale structural and chemical investigation of UO₂ surface oxidation. **S. Spurgeon**, J. Stubbs, E. Ilton, E. Buck

9:20 110. Processes and reactions controlling aqueous iodine species transformations and interactions with minerals at the Hanford site. **N.P. Qafoku**, A. Lawter, J.E. Szecsody, C. Bagwell, M. Truex

9:45 Intermission.

10:00 111. Sediment manganese oxide content as an indicator of groundwater arsenic pollution potential. **M. Polizzotto**, E. Gillispie, O. Duckworth

10:25 112. Surface interactions of the siderophore desferrioxamine-B with hematite/water interfaces studied using nonlinear spectroscopy techniques. **A.L. Mifflin**

10:50 113. Reduction of hexa-valent chromium with zero valent iron in neutral pH conditions. **J. Williams**, A.A. Maria, H.P. Emerson, Y. Katsenovich, T.G. Levitskaia

11:15 114. Complex soil organic matter interactions with solvated metal ions and mineral surfaces: Insight from classical molecular dynamics and quantum chemistry. **A. Andersen**, N. Govind, A. Laskin

BSF/CSF

Crick

Hanford: History, Chemistry & Modern Solutions

J. Law, A. Lines, *Organizers*

C. Delegard, A. M. Lines, *Presiding*

8:00 Introductory Remarks.

8:10 115. History of radiochemical processing at the Hanford site. **M. Gerber**

8:35 116. First industrial processes for plutonium separation and chemical conversion in the United States and the Soviet Union. **C. Delegard**, V.F. Peretrukhin, S.I. Rovny

9:00 117. Decladding of Hanford N Reactor fuel and pretreatment of resultant waste. **J.L. Swanson**

9:25 118. Characterization of continuous plutonium(IV) oxalate precipitation. **R.C. Hoyt**

9:50 Intermission.

10:05 119. Nuclear Waste Vitrification Project reprocessing campaign compared to Hanford Purex reprocessing. **J. Tingey**

10:30 120. Treating Hanford waste – A summary of past work and future approaches. **R. Peterson**

10:55 121. Salt solubility in highly concentrated Hanford Waste: From Barney to Pitzer to Hofmeister. **J. Reynolds**

11:20 122. Determination of the radiolytic hydrogen generation of ion exchange materials. **H.A. Colburn**, S.A. Bryan, D.M. Camaioni, L.A. Mahoney, S.R. Adami

11:45 Concluding remarks.

BSF/CSF

Mural

Low Temperature Chemical Transformations

R. S. Weber, *Organizer*

S. Akhade, M. Lee, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 123. Enabling low temperature catalysis by tailoring the reaction space. **J. Lercher**

8:40 124. Aqueous phase electrocatalytic hydrogenation of biomass surrogates: A mechanistic study. **U. Sanyal**, L. Meyer, N. Singh, O. Gutierrez-Tinoco, J. Lercher

9:00 125. Modeling specificity in adsorption and charge transfer on solid/liquid interfaces. **D.C. Cantu**, A.B. Padmaperuma, M. Nguyen, S. Akhade, Y. Yoon, Y. Wang, M. Lee, V. Glezakou, R. Rousseau, M. Lilga

9:35 126. Reaction networks and mechanisms in electrocatalytic hydrogenation of carbonyl compounds. **L.C. Meyer**, O. Gutierrez-Tinoco, U. Sanyal, J. Lercher

9:55 Intermission.

10:10 127. Understanding photoelectrochemistry on epitaxial oxide surfaces. **K.A. Stoerzinger**, L. Wang, Y. Du, S. Chambers

10:45 128. Liquid-phase hydrodeoxygenation of lignin-derived phenolics on Pd/Fe: A mechanistic study. **J. Zhang**, J. Sun, B. Sudduth, X. Pereira Hernandez, Y. Wang

11:05 129. Understanding the role of solvent effects in the thermal and electrochemical hydrogenation of organics. S. Akhade, M. Lee, M. Nguyen, V. Glezakou, **R. Rousseau**

11:40 130. Surface dependent acid-base properties and isopropanol decomposition on CeO₂ nanoparticles with well-defined facets. **B. Sudduth**, D. Yun, Y. Wang

BSF/CSF
Pasteur

Molecular Catalysis for Energy Conversions

A. M. Appel, W. J. Shaw, *Organizers*

B. Ginovska, *Organizer, Presiding*

W. Shaw, *Presiding*

8:00 Introductory remarks.

8:05 131. Electron bifurcation. **J.W. Peters**, D.N. Beratan, P.W. King, M.W. Adams

8:45 132. Toward efficient catalysts for energy conversion: From enzymatic function to functional mimics. **S. Raugei**

9:10 133. Dynamic and allosteric modulation of electron transfer in nitrogenase. **L.E. Johnson**, B. Ginovska, S. Raugei

9:35 134. Designing and characterizing protein-iron oxide interfaces and applications for biohybrid engineering. **B. Rad**

10:00 Intermission.

10:15 135. Redox and ligand dependant states of cytochrome P450, cytochrome P450 reductase, and their complexes: Single protein tracking study. **J.A. Brozik**, C. Barnaba, E.L. Taylor, M.J. Martinez

10:40 136. Catalytic conversion of CO₂ to formate by an artificial enzyme. **J. Laureanti**, W.J. Shaw, M.J. O'Hagan

11:05 137. Hydroquinone ring-cleaving dioxygenases: Enzymes and model complexes. **T.E. Machonkin**

11:30 138. Effect of charged groups on Fe porphyrin catalysts for the oxygen reduction reaction. **S.I. Johnson**, D.J. Martin, J.M. Mayer, S. Raugei

EMSL
1079

Synthetic Methodology Development & its Advanced Application in Organic Chemistry

Cosponsored by ORGN

S. K. Nune, *Organizer*

P. K. Koech, D. Malhotra, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 139. Chemical synthesis with unsymmetrical diaryliodonium salt reagents. **D.R. Stuart**

8:35 140. Molecular checkmate: An organic chemistry approach to derive immunogenicity from drug resistance. J. Hantho, A.J. Burt, A. Ryan, A.E. Nielsen, **R.J. Mancini**

9:05 141. Chemoenzymatic approaches to the total synthesis of epoxyquinol A. **J.A. Collins**, M.S. Duncan, W.B. Kline, A.J. Stanley

9:35 Intermission.

9:45 142. Discovery and development of photoredox-mediated metal-free ring-opening metathesis polymerization. **A.J. Boydston**

10:25 143. N-heterocyclic-10-anthryl-isoxazole amides (N-Het-AIMs) have robust antitumor activity against breast and brain cancer. M.J. Weaver, S. Stump, M.J. Campbell, C. Li, D.S. Backos, P. Reigan, H. Beall, **N.R. Natale**

10:55 144. Intramolecular hydroalkylation of *bis*-homoallylic piperazinols. **T.K. Beng**

11:25 Concluding Remarks.

Discovery Hall
Vista

Advances in Computational Chemistry

K. A. Peterson, S. Xantheas, *Organizers*
B. A. Finney, *Presiding*

8:30 Introductory remarks.

8:35 145. Statistical sampling of solvation ensembles and fluctuations in electronic structure relevant to accurate NMR calculations of ²⁷Al. **A.E. Clark**, E. Martinez, G.K. Schenter

9:00 146. Investigating the effect of mutations on the structure and dynamics of inosine triphosphatase pyrophosphatase from molecular dynamics simulations. **Y.A. Houndonougbo**

9:25 147. Comparative analysis of surface configurations of CO adsorbed on hcp and fcc cobalt for the Fischer-Tropsch synthesis. **G.B. Collinge**, N. Kruse, C. Stampfl, J. McEwen

9:50 Intermission.

10:05 148. Adsorption of 2D water on the “29” copper surface oxide: a STM and DFT study. **R. Zhang**, A. Therrien, K. Groden, A. Hensley, A. Schilling, E.H. Sykes, J. McEwen

10:30 149. Modeling molecular aggregation during thin film formation via *in situ* absorbance spectra. **M. Sosa**, K. Wilson, C. Wong

10:55 150. Performance of simple theoretical models for OEO systems: Insight and limitations. **L.E. Johnson**, B. Robinson

Discovery Hall
Horizon E

Best Practices in Undergraduate Chemical Research: Outcomes & Pedagogy

Cosponsored by CHED

Financially supported by Council on Undergraduate Research, Division of Chemistry

K. L. Breno, K. A. Wheeler, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 151. Flexible approaches to undergraduate research requirements. **K.L. Breno**

8:55 152. Stereoselective synthesis of $[\text{Cp}^*\text{Ru}(\eta^6\text{-aryl})]\text{PF}_6$ complexes via a one-pot procedure from ruthenium(III) chloride: a course-based research project by undergraduate students. **D.M. Hitt**, J. Urbanec, M. Malek, P. Fix, K. O'Byrne, C. Spencer, M. Moulton, R. Imhoff, I. Jacobson, J. Kessler, C. Pharr, J.G. Rowley

9:15 153. Building a sustainable undergraduate research program in biochemistry at a small liberal arts university. **D.D. Ojennus**

9:35 154. Selected case studies in undergraduate research & Ignatian pedagogy. **M.E. Cremeens**

9:55 Intermission.

10:15 155. Undergraduate medicinal chemistry research - "Home Ec" for future scientists. **T.T. Denton**

10:35 156. Successes with undergraduates through innovations in solid-state organic chemistry research. **K.A. Wheeler**, L.S. Cantrell, E. Pinter, I.C. Tinsley, B. Wagner

10:55 157. A toxicology-based approach to training and mentoring undergraduate researchers on a health professions campus. **B. Stamper**

11:15 158. Undergraduate research in computational chemistry at Eastern Washington University. **Y.A. Houndonougbo**

Discovery Hall
Horizon D

Transformative Partnership for Academics

K. L. Breno, K. A. Wheeler, *Organizers*

J. F. Corbey, R. G. Surbella, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 159. Research partnerships between Pacific Northwest National Laboratory and academic institutions: Opportunities and benefits. **S. Baskaran**

8:55 160. Scientific opportunities in the WSU PNNL Nuclear Science and Technology Institute. **N. Henson**, A.E. Clark

9:15 161. My professional and academic experience with Pacific Northwest National Laboratory. **M. Athon**

9:35 162. Advantages and disadvantages of large interdisciplinary and multi-institution programs. **A.E. Clark**

9:55 Intermission.

10:15 163. New paradigm in actinide research: Nuclear materials science at the micron-scale. **J. Schwantes**, R. Peterson, D. Reilly, R. Clark, D.E. Perea, R. Buckner, E. Buck, J. Cliff, M. Conroy, T.G. Lach, P. MacFarlan, S.B. Clark

10:35 164. Overview of the radiation detection for nuclear security summer school. **B. Runkle**

10:55 165. Nuclear chemistry at the intersection of science and policy. **C.L. Cahill**

11:15 Panel Q&A.

11:35 Concluding Remarks.

Discovery Hall
Horizon A

The Lens of Support: Support for the Value Chain of Translating Research to Market Solutions

Translating Research to Market Solutions

Cosponsored by BMGT, PROF and SCHB

Financially supported by ecosVC, Inc.

J. L. Bryant, *Organizer*

J. C. Giordan, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 166. Opening overview: The lens of support for the value chain of translating research to market solutions. **J.C. Giordan**, J.L. Bryant

9:15 167. Value TOK brings to STEM research commercialization. **C. Rosenthal**

9:25 168. The value TCI America brings to STEM research commercialization. **P. Waldenmaier**

9:35 169. The value Pacific Northwest National Laboratory (PNNL) and the Technology Deployment and Outreach Office bring to STEM research commercialization. **R. Thomas**

9:45 170. Value Washington State University (WSU) brings to STEM research commercialization. **S. Steiger**

9:55 Intermission.

10:15 Panel Discussion.

10:45 Moderated Q&A.

11:15 Office Hours with the Speakers.

MONDAY AFTERNOON

Discovery Hall
Vista

Advances in Computational Chemistry

K. A. Peterson, S. Xantheas, *Organizers*
Y. A. Houndonougbo, *Presiding*

1:00 Introductory remarks.

1:05 171. Embedding relativistic 2-component Kohn-Sham density functional theory in a non-relativistic quantum environment. **C. Hoyer**, D. Williams-Young, R. Beck, X. Li

1:30 172. Exploring a real-time approach to electronic structure theory. **M. Kiessling**, J.A. Cina

1:55 173. Coupling real-time time-dependent CASSCF with polarizable force field. **H. Liu**, A.J. Jenkins, X. Li

2:20 Intermission.

2:35 174. Ab initio thermochemistry of transuranium molecules: Halides of U, Np, and Pu. **B.A. Finney**, K.A. Peterson

3:00 175. Tuning the structure and oxygen storage properties of BaFeO_{3-δ} through chemical substitution. **D. Tafen**, D. Alfonso, J.W. Lekse, C. Matranga

3:25 176. Core-level spectroscopies with linear-response and real-time time-dependent density functional theory. **N. Govind**, A. Andersen, Y. Zhang, Z. Fox, M. Galib, J. Fulton, M.H. Khalil

BSF/CSF
Darwin

Chemistry & Collaboration to Advance Nuclear Technologies

Cosponsored by NUCL
S. A. Bryan, *Organizer*
A. E. Clark, *Organizer, Presiding*
N. Henson, *Presiding*

1:00 Introductory Remarks.

1:05 177. Hierarchical phenomena associated with Interfacial Dynamics in Radioactive Environments and Materials. **G.K. Schenter**

1:45 178. Study of Al speciation and ion-ion interactions in Hanford Site nuclear wastes by ²⁷Al NMR shielding tensor calculations. **E. Martinez Baez**, C. Pearce, G.K. Schenter, A.E. Clark

2:15 179. Multi-scale models of oxygen on iron-based hydrodeoxygenation catalysts: Elucidating the effect of external electric fields. **J. Bray**, A. Hensley, G.B. Collinge, Y. Wang, C. Stampfl, J. McEwen

2:45 180. The impact of tri-n-butyl phosphate adsorption at the water/n-hexane interface on interfacial properties and the extraction of water into the organic phase. **M. Servis**, A. Casella, A.E. Clark

3:15 Intermission.

3:30 181. Crosslinking and chain scission of irradiated polyethylene. **S.P. Beckman**

4:00 182. Quantum mechanical calculations of substitutional defects in γ -uranium. **D. Pope**, A.E. Clark

4:30 183. Spectroscopic chameleons – speciation and vibrational characterization of aluminate and its dimeric analogues using ab initio molecular dynamics. **M. Pouvreau**, M. Dembowski, S.B. Clark, J. Reynolds, K. Rosso, G.K. Schenter, C. Pearce, A.E. Clark

EMSL
1075

Geochemical Transformations in Natural & Engineered Systems

Cosponsored by GEOC

E. S. Ilton, M. K. Nims, S. Saslow, *Organizers*

E. J. Bylaska, *Organizer, Presiding*

E. Ilton, *Presiding*

1:00 Introductory remarks.

1:05 184. Evaluating natural and engineered materials for technetium and iodine sequestration. **C. Pearce**, E. Cordova, K. Cantrell, J. Morad, W. Garcia, S. Saslow, O. Qafoku, J. Matyas, T. Levitskaia, G. Wang, K. Johnson, M. Rigali, R. Moore, V. Freedman

1:30 185. Modeling nuclear waste glass corrosion across scales. **S.N. Kerisit**, P.C. Rieke, J. Ryan, J. Neeway, E.M. Pierce, J. Du

1:55 186. Molecular dynamics simulation of ballistic effects in simplified nuclear waste glasses. **A. Jan**, J. Delaye, S.N. Kerisit, S. Gin

2:20 187. Study of glassy hillforts for nuclear waste applications. **M. Ahmadzadeh**, J. Marcial, J. McCloy

2:45 Intermission.

3:00 188. Geochemistry in natural ecosystems: Perspectives from EMSL, DOE's national environmental molecular user facility for biological and environmental research. **N.J. Hess**

3:25 189. Effects of hydrated lime on radionuclides stabilization of Hanford tank residual waste. **G. Wang**, K. Cantrell, M. Snyder, M. Bowden, M. Triplett, E. Buck

3:50 190. Ab initio thermodynamics of hydrated magnesium and calcium carbonates in water and supercritical CO₂. **A.M. Chaka**

4:15 191. Parameter-free prediction of the oxide/water interface structure via density functional simulation quantified by x-ray reflectivity. **E.J. Bylaska**, K. Harmon, J. Weare, P. Fenter

BSF/CSF
Mural

Low Temperature Chemical Transformations

R. S. Weber, *Organizer*
S. Akhade, M. Lee, *Organizers, Presiding*

1:00 Introductory remarks.

1:05 192. Tungsten-incorporated vanadia SCR catalysts, a structural interpretation. **N. Jaegers**, Y. He, C. Wang, M. Hu, I.E. Wachs, Y. Wang, J.Z. Hu

1:25 193. Selectivity control in syngas conversion to light olefins. **X. Pan**, X. Bao

1:45 194. Surface Acetone Reaction on $Zn_xZr_yO_z$: A DRIFTS-MS study. **H. Li**, J. Sun, Y. Wang

2:05 195. Metallic core@shell architectures for industrially relevant catalytic transformations. **C.H. Hendon**

2:35 196. Mapping the reverse water-gas shift reaction network over Pd/Al₂O₃ using *operando* SSITKA coupled with time-resolved IR spectroscopy. **N.C. Nelson**, M. Nguyen, V. Glezakou, R. Rousseau, J. Szanyi

2:55 Intermission.

3:10 197. Condensed-phase low temperature heterogeneous hydrogenation of CO₂ to methanol. **D.J. Heldebrant**

3:40 198. Coordination modes and reactivity of phosphite/triphosphine ligand P(OCH₂PPh₂)₃ towards Ni(II). A. Beganskiene, T.J. Dobson, N.A. Phan, K.E. Johnson, E.J. Valente, **E. Urnezius**

4:00 199. Pt catalysts for low temperature CO oxidation: Determining single-site reactivity via well-defined model studies. **A. Hensley**, K. Groden, A. Therrien, R. Zhang, E.H. Sykes, J. McEwen

4:20 200. Development of regenerative direct formic acid fuel cell system: Investigation of electrocatalytic trends of Pd-based bimetallic surfaces for formic acid oxidation. **S. Ha**

4:40 201. Tailoring the Activity of Pt/CeO₂ Catalysts via High Temperature Synthesis. **X. Pereira Hernandez**, A. DeLaRiva, D. Kunwar, H. Xiong, B. Sudduth, M. Engelhard, L. Kovarik, Y. Wang, A.K. Datye

BSF/CSF
Pasteur

Molecular Catalysis for Energy Conversions

B. Ginovska, W. J. Shaw, *Organizers*

A. M. Appel, *Organizer, Presiding*

R. Bullock, *Presiding*

1:00 Introductory remarks.

1:05 202. (Electro)catalysis for renewable fuels. **J.Y. Yang**

1:45 203. Rational design of CO₂ hydrogenation catalysts through control of thermodynamic hydricity. **E.S. Wiedner**, J.C. Linehan, A.M. Appel

2:10 204. Computationally guided design of proton reduction catalysts. **T. McCormick**, C.N. Virca, M. Davis

2:35 205. Utilizing BODIPY fragments in molecular catalysis. **Z.M. Heiden**, B. Thompson, N.R. Treich

3:00 Intermission.

3:15 206. Designing ligand frameworks for heterolytic C-H activation: Applications to catalytic C-H functionalization. **E.B. Hulley**

3:40 207. Mechanistic insights from sulfide and oxide catalysts. **R.J. Nielsen**, Y. Huang, S.I. Johnson, Y. Ping, W.A. Goddard

4:05 208. CO₂ hydrogenation catalysts are all wet. S.A. Burgess, K. Grubel, A.M. Appel, E.S. Wiedner, **J.C. Linehan**

4:30 209. Tailoring low-valent dinuclear niobium complexes with pendant amines as molecular electrocatalysts for hydrogen oxidation. **F. Fantuzzi**, M. Nascimento, S. Rauei

Discovery Hall
Horizon E (updated)

Celebrating 50 Years of Project SEED: Opening Doors to Careers in Chemistry

K. L. Breno, K. A. Wheeler, *Organizers*

A. Hoffman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 210. PROJECT SEED: fostering diversity in the next generation of scientists. **A.G. Cavinato**

1:55 211. Project SEED at Boise State University, part 1: Program overview and student experiences. **D.L. Warner**

2:15 212. Integrating professional development into research experiences. **M.R. Mackiewicz**

2:35 Intermission.

2:55 213. Discovering discovery with Project SEED. **A. Hoffman**

3:15 214. Creating a viable research program at a small two-year college. **J.W. Hartman**

3:35 215. Project SEED at Boise State University, part 2: Student experience. **D.L. Warner**

3:55 216. Summer research into mercury sensors and a future in chemistry. **T. McCormick**, J. Dayton, A. Shigemoto

4:15 Concluding Remarks.

Discovery Hall
Horizon A

Lens of Business: Stories from the Front - Commercializing Market Required STEM Innovations & Solutions

Cosponsored by BMGT, PROF and SCHB

Financially supported by ecosVC, Inc.

J. L. Bryant, *Organizer*

J. C. Giordan, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 217. Opening overview - Lens of business: Stories from the front - commercializing market required STEM innovations and solutions. **J.C. Giordan**, J.L. Bryant

1:45 218. Photon Biosciences, LLC brings its front line story to: “Commercializing market required STEM innovations and solutions”. **J.A. Brozik**

1:55 219. The value NexTC Corp brings to stories from the front - Commercializing market required STEM innovations and solutions. **J. Amador**

2:05 220. The value Cytokinetics, Inc. brings to stories from the front - Commercializing market required STEM innovations and solutions. **B.A. Charpentier**

2:15 221. How PNNL contributes to STEM research commercialization. **C. Klasen**

2:25 Intermission.

2:45 Panel Discussion.

3:15 Moderated Q&A.

3:35 Office Hours with the Speakers.

Synthetic Methodology Development & its Advanced Application in Organic Chemistry

Cosponsored by ORGN

S. K. Nune, *Organizer*

P. K. Koech, D. Malhotra, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 222. Isoxazolo[3,4-d]pyridazinones as positive allosteric modulators (PAM) of the metabotropic glutamate receptors, and selective for subtypes 2 and 4. C. Gates, D.S. Backos, P. Reigan, H. Kang, **N.R. Natale**

2:00 223. Ring-opening metathesis polymerization of a macrocyclic stilbene-based monomer. **B.E. Lynde**, R. Maust, P. Li, D. Lee, R. Jasti, A.J. Boydston

2:25 224. Synthesis, characterization and testing of amine-based solvents for carbon dioxide capture. **P.K. Koech**, D. Malhotra, M. Nguyen, D.J. Heldebrant, A. Zwoster, V. Glezakou, F. Zheng, R. Rousseau

2:50 Intermission.

3:05 225. Design, development and synthesis of energy efficient CO₂-binding organic liquids for flue gas clean up. **D. Malhotra**, P. Koech, D.J. Heldebrant, J. Page, D.C. Cantu, V. Glezakou, R. Rousseau, F. Zheng

3:30 226. Light-controlled switchable chemoselectivity for palladium-catalyzed Suzuki cross-couplings. **E. Reeves**, S. Neufeldt

3:55 227. Synthesis of benzodiazaborole derivatives. **D. Puhl**, A.N. Lamm

4:20 Concluding Remarks.

TUESDAY MORNING

Discovery Hall
Horizon A (updated)

Chemical Education: Honoring the Legacy of Jane & Glenn Crosby

Cosponsored by CHED
K. L. Breno, J. L. Bryant, K. A. Wheeler, *Organizers*
J. M. Sophos, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 228. Glenn and Jane Crosby, and the ACS Division of Chemical Education Region Awards for Excellence in High School Teaching. **M.Z. Hoffman**

9:00 229. Doc and Jane: dynamic chemistry duo and master chemistry program builders. **J.W. Kenney**

9:20 230. Being there with chemical education curmudgeons. **J.A. Bell**

9:40 231. Legacy well-earned: Remembrances of the Crosbys and their impact on chemistry. **J. Austill**

10:00 Intermission.

10:20 233. Glenn and Jane Crosby: Recollections of a graduate student, a junior colleague, and department chair. **K. Hipps**

10:40 234. The Crosbys; dear friends. **E. Meyer**

11:00 235. Doc and Jane. **A.D. Crosby**

11:40 Concluding Remarks.

BSF/CSF
Darwin

Chemistry & Collaboration to Advance Nuclear Technologies

Sensor Development & Analytical Measurements for Harsh Environments

Cosponsored by NUCL
A. E. Clark, *Organizer*
S. A. Bryan, *Organizer, Presiding*
A. M. Lines, *Presiding*

8:00 Introductory Remarks.

8:05 236. Electrochemical sensors for biomedical and environmental applications. **W.R. Heineman**

8:45 237. *In situ* analysis of non-pertechnetate ⁹⁹Tc in Hanford tank waste. **S.D. Branch**, A.D. French, A.M. Lines, C. Soderquist, B.M. Rapko, W.R. Heineman, S.A. Bryan

9:10 238. Real-time, on-line monitoring for the characterization of radionuclides in complex processing streams. **A. Lines**, S.R. Adami, S.I. Sinkov, A. Casella, G.B. Hall, J. Allred, G.J. Lumetta, S.A. Bryan

9:35 239. Monitoring liquid:liquid interfacial reactions and phase transfer kinetics of tributyl phosphate and its degradation products. **S. Howett**, D. Bottenus, A.M. Lines, C. Louie, S.A. Bryan, C. Delegard, S.B. Clark, W. Pitts, A. Casella

10:00 Intermission.

10:20 240. Developing and testing a novel micro-Raman/UV-vis probe for spectroscopic interrogation of microfluidic devices. **G. Nelson**, A.M. Lines, J.M. Bello, S.A. Bryan

10:45 241. On-line Raman spectroscopy of phosphoric acid systems to determine pH, phosphate concentration, and speciation. **H. Lackey**, A.M. Lines, G. Nelson, S.A. Bryan

11:10 242. Fast separation of rare earth metals by isotachopheresis in a microfluidic device. **D. Bottenus**, S.D. Branch, J. Katalenich, S.B. Clark, A.M. Lines

11:35 243. Three decades of process monitoring directed toward the nuclear fuel cycle. **S.A. Bryan**, A.M. Lines, G.L. Nelson, J.M. Bello

EMSL
1077

Chemistry of Biofuels & Bioenergy

D. Howe, K. K. Ramasamy, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 244. Drivers, opportunities, and challenges for the emerging alternative jet fuel industry. **M. Wolcott**

8:35 245. Biochemical production of aviation biofuels or bio-jet precursors from lignocellulosic biomass materials. **B. Ahring**, K. Srinivas

8:55 246. Brown gold: producing liquid transportation fuel blendstock from municipal sewage by hydrothermal liquefaction (HTL). **J. Billing**, K. Abrecht, T. Hart, A. Schmidt, S. Fox, D. Anderson, R.T. Hallen

9:15 247. Role of copper stability for the selective alcohol condensation. **M. Guo**, K.K. Ramasamy

9:35 Intermission.

9:50 248. Overview on a carbon-neutral circular economy. **C. Drennan**

10:20 249. Lignin based jet fuel production. **H. Wang**, H. Ruan, B. Yang

10:40 250. From bio aldehydes to high value aromatic precursors. **K. Lin**, K.K. Ramasamy

11:00 251. Ethanol conversion to higher ketones over multifunctional mixed oxide catalysts. **S. Subramaniam**, M. Gray, M. Guo, K.K. Ramasamy

11:20 Concluding remarks.

Chemistry of Nanomaterials

M. G. Warner, R. S. Weber, *Organizers*
C. Barrett, *Presiding*

8:00 Introductory Remarks.

8:05 252. On the local structure and catalytic performance of a NiFe bimetallic catalyst for aqueous phase phenol hydrogenation. **Z. Chase**, H. Shi, J. Fulton, D.M. Camaioni, O. Gutierrez-Tinoco, M. Balasubramanian, Y. Wang, J. Lercher

8:25 253. Utilizing molecularly tethered nanoparticles as a platform for evaluating multimetallic nanoparticle electrocatalysts. **S. Young**, J.E. Hutchison

8:45 254. Synthesis and application of hierarchically porous Zr-based metal-organic framework. **L. Hao**, Q. Zhang

9:05 255. Pore-engineered derivatives of metal-organic frameworks for adsorption cooling applications. **D. Barpaga**, J. Zheng, P. Bhattacharya, B.P. McGrail, **R. Motkuri**

9:25 256. Fluorocarbon R134a uptake in metal-organic frameworks for adsorption chiller applications. **D. Barpaga**, J. Zheng, J.J. Jenks, B.P. McGrail, R. Motkuri

9:45 Intermission.

10:00 257. Use of diatom frustules as effective nano-catalyst supporting substrates. **V. Dereviankin**, N. Day, J. Olsen, J. Thiebes, A. Polliack

10:20 258. Flexible and conducting nanofibers functionalized with photoactive ZnO for advanced water treatment. **G. Capilli**, P. Calza, C. Minero, M. Cerruti

10:40 259. Single particle photoluminescence imaging and charge transport in titanium dioxide. **R.E. Rex**, J. McHale, F.J. Knorr

11:00 260. Demonstration of Fowler-Nordheim tunneling in simple solution-processed thin film. **C.K. Perkins**, M. Jenkins, T. Chiang, R. Mansergh, J.F. Wager, J.F. Conley Jr., D.A. Keszler

11:20 261. Selection of DNA aptamers against epidermal growth factor receptor (EGFR) and Drosophila C virus (DCV) using open qPCR. **T.R. Damase**, P.B. Allen

11:40 262. Designing protein self-assembly: Attention on insulin and human serum albumin. **G. Thakur**, T. Thundat

Discovery Hall
Vista

Condensed Phase & Interfacial Chemistry

L. X. Dang, S. Xantheas, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 263. Effects of a potassium cloud on electron transfer in a bacterial ferredoxin. K. Tran, **T. Ichiye**

8:35 264. Structure and dynamics of aqueous electrolytes at interfaces from ab initio molecular dynamics simulations. **M.D. Baer**

9:05 265. Two-dimensional metal organic framework (MOF) self-assembly at the solution-solid interface. **K. Johnson**, U. Mazur Hipps, K. Hipps, Q. Zhang, M. Hurlock

9:25 266. Self-assembly and functionalization of porphyrins supported on HOPG. **K. Gurdumov**, K. Hipps, U. Mazur Hipps

9:45 267. Site and substrate dependence of molecular desorption in self-assembled monolayers: A case study with coronene on Au(111) and HOPG. **B. Chilukuri**, U. Mazur Hipps, K. Hipps

10:05 Intermission.

10:15 268. Quantifying solvation across biological interfaces: Optical studies of solute permeation into lipid bilayers. **R.A. Walker**, C.A. Gobrogge

10:45 269. E/Z isomers possessing different luminescent properties in the solid state. **M. Hurlock**, Q. Zhang

11:05 270. Solvent-dependent surface behavior of coumarin solutes. **G. Purnell**, R.A. Walker

11:25 271. Anisotropic water next to muscovite (mica) surface. **A. Tuladhar**, Z. Chase, B. Legg, A.D. Winkelman, J. Tao, S. Zhang, M.D. Baer, Z. Wang, C.J. Mundy, H. Wang, J. De Yoreo

11:45 272. Plait point behavior in the aniline + cyclohexane + 2-picoline ternary liquid system. M. McKibben, T. Kallem, **J.C. Williamson**

12:05 Concluding Remarks.

BSF/CSF
Crick

Radiation Effects at Complex Interfaces

Cosponsored by NUCL
S. A. Bryan, B. N. Seiner, *Organizers*
B. Seiner, *Presiding*

8:00 Introductory Remarks.

8:05 273. Defect formation and interfacial damage resistance in ion-irradiated $\text{La}_2\text{Ti}_{2-x}\text{Zr}_x\text{O}_7$ thin films. **S. Spurgeon**, M. Sassi, T. Kaspar, V. Shutthanandan

8:35 274. Ab initio simulations of the effects of structure and composition on electronic excitation induced amorphization of ion-irradiated $\text{La}_2\text{Ti}_{2-x}\text{Zr}_x\text{O}_7$ pyrochlores. **M. Sassi**, S. Spurgeon, T. Kaspar, V. Shutthanandan

9:05 275. Effect of low energy electrons on alumina surfaces: An AFM study. **H.M. Felmy**, M. Adinehnia, K. Hips

9:35 Intermission.

9:50 276. Determining the roles of radiolytic transient intermediates and interfacial species in aluminum oxyhydroxide reactivity. **E. Walter**, Z. Wang, M. Sassi, K. Rosso

10:20 277. Epsilon phase high entropy alloy formation under extreme processing conditions. **R. Devanathan**, W. Jiang, M.A. Conroy, K. Kruska, T.C. Droubay, J.M. Schwantes

10:50 278. Near edge structure of titanium in alpha decay damaged natural brannerite and pyrochlore. **E. Buck**, J. Ward, A. Duffin, D. Reilly

11:20 Concluding Remarks.

EMSL
1079

Advances in Mass Spectrometry & Spectroscopy

Mass Spectrometry & Gas-Phase Ion Separation

Cosponsored by ANYL
P. T. Reilly, N. A. Wall, *Organizers, Presiding*

8:30 Introductory remarks.

8:35 279. Advancing digital waveform technology for mass spectrometry. **P.T. Reilly**, B. Opacic, A.M. Moon, A.P. Huntley, M.E. Reece, N.M. Hoffman

9:05 280. High-pressure, thermally extensive MAS NMR for demystifying water. **N. Jaegers**, M. Hu, Y. Wang, J.Z. Hu

9:25 281. Chemical warfare agent simulatant speciation and detection via atmospheric flow tube-mass spectrometry. **K.A. Morrison**, B. Clowers

9:45 282. Energetic characterization using thermometer ions of a trapped ion mobility mass-spectrometer (TIMS). **C. Naylor**, M. Ridgeway, M. Park, B. Clowers

10:05 283. Selective gas-phase ion-vapor clustering to enhance ion mobility separation factors: Deducing association energies. **P. Kwantwi-Barima**, B. Clowers, C.J. Hogan Jr, H. Ouyang

10:25 Intermission.

10:40 284. Experimental and computational vibrational sum frequency spectroscopy studies of pyruvic acid at the air-water interface. **B. Gordon**, E. Tran, N.A. Valley, F. Moore, G.L. Richmond

11:00 285. TD-GC-MS analysis of volatile organic and sulfur compounds in the Lewis-Clark Valley and surrounding areas. **N.A. Johnston**, J.P. Andrew, B.A. Bundy, B.K. Grimm, M.A. Hamann, D.T. Ketcherside, J. Li, M.Y. Manangquil, D.L. Pittman, P. Scott, R. Uhlorn

11:20 286. Saccharide induced lipid film reorganization studied with vibrational sum frequency generation. **K. Link**, G. Spurzem, R.A. Walker

11:40 Concluding remarks.

EMSL
1075

Geochemistry: General Papers

Cosponsored by GEOC
M. K. Nims, S. Saslow, *Organizers, Presiding*

8:30 Introductory remarks.

8:35 287. Use of rare earth elements as a geographical tracer in the Columbia River Basin via multicollector inductively coupled plasma mass spectrometry. **S.D. Shen**, C. Smith, T. Linley, E. Krogstad, M.K. Nims, J. Janak

8:55 288. Reactivity and transformations of minerals in adsorbed H₂O films. **Q.R. Miller**, J. Loring, E.S. Ilton, O. Qafoku, C.J. Thompson, H.T. Schaefer, B.P. McGrail, K. Rosso

9:15 289. Direction-specific interaction between nanocrystals. **X. Zhang**, Y. He, M. Sushko, J. Liu, L. Luo, J. De Yoreo, S. Mao, C. Wang, K. Rosso

9:35 290. Understanding nanorod dissolution mechanisms by liquid phase electron microscopy: The case of β -FeOOH. **L. Liu**, X. Zhang, E. Nakouzi, L. Kovarik, J.A. Soltis, K. Rosso, J. De Yoreo

9:55 291. Iodine sorption on Hanford sediments. **M. Snyder**, K. Cantrell, M. Truex, N.P. Qafoku, A. Lawter, B. Williams, J. Stephenson

10:15 292. Temperature dependent $\delta^{18}\text{O}$ fractionation in otoliths of juvenile Chinook salmon. **M.K. Nims**, T. Linley, J. Janak, J.J. Moran

10:35 Intermission.

10:50 293. Methane and carbon dioxide permeation through polymer and composite barrier films. **P.Y. Hsieh**

11:10 294. Cement composites with self-healing polymer for geothermal wellbore applications. **K.A. Rod**, C. Fernandez, P. Koech, N. Huerta

11:30 295. Magnetic core-shell composites for extraction of rare earth elements. **M.A. Sinnwell**, S.K. Elsaidi, B.P. McGrail, P.K. Thallapally

11:50 Concluding remarks.

BSF/CSF

Mural

In Situ & Operando Techniques for Electrochemical Systems

G. E. Johnson, R. S. Weber, *Organizers*

V. Prabhakaran, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 296. Molecular investigation of complex electrochemical processes occurring at electrode-electrolyte interfaces using in situ liquid SIMS. **Z. Zhu**

9:05 297. In situ chemical imaging analysis of heterogeneous and reactive interfaces. **V. Murugesan**, K. Han, V. Shutthanandan, S. Thevuthasan, K.T. Mueller

9:35 298. Enhanced redox resilience in ALT doped NiO-YSZ SOFC anodes. **M. Welander**, R.A. Walker

9:55 Intermission.

10:10 299. Understanding the electrochemistry of precisely-defined ions using *in situ* infrared spectroscopy. **V. Prabhakaran**, P. Su, G.E. Johnson, J. Laskin

10:30 300. Production of hydrogen peroxide by electrochemical oxidation and reduction of tellurhodamine chromophores. **J. Lohman**, T. McCormick

10:50 301. Electrochemical techniques for the controlled dissolution of Zirconium-based light water reactor components and their Hydrides. **M. Fujimoto**, N. Canfield, D. Olson, M. Elmore, E. Buck, M.A. Conroy, S. Chatterjee

11:10 Concluding Remarks.

TUESDAY AFTERNOON

Discovery Hall
Horizon E

"Golden Age" of Chemistry

Cosponsored by BMGT, PROF and SCHB
Financially supported by ecosVC, Inc.
J. L. Bryant, J. C. Giordan, M. Grandbois, *Organizers*
M. Grandbois, *Presiding*

1:00 Introductory Remarks.

1:05 302. PNNL: A Partner in Innovation. **J. Lee**

1:35 303. Forming and nurturing science-based and research-based startup companies. **S. Rung**

2:05 304. Lens of the WINE Business and stories from the front: Commercializing in the wine industry from research to market.

2:35 Intermission.

3:00 309. "Golden age" panel discussion. **M. Grandbois**

4:00 Concluding Remarks.

EMSL
1077

Biotechnology: Synthetic Biology &/or Biofuel & Bioproduct Production

N. Washton, *Organizer*
E. Bredeweg, R. Egbert, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 310. Nutrient harvesting to sustain water quality and reduce GHG emissions. **D.A. Burke**

1:25 311. The Agile BioFoundry. **J. Magnuson**, K. Burnum-Johnson, H. De Paoli, K. Pomraning, Y. Kim, J. Kim, S. Tripathi, J. Zucker, N. Munoz-Munoz, M. Burnet, S. Deng, Z. Dai, B. Hofstad, J. Collett, E. Panisko, Y. Gao

1:45 312. Harnessing bacterial metabolic diversity for small molecule discovery. **A. Puri**, E. Mevers, T.R. Ramadhar, A.K. Schaefer, D. Petras, D. Liu, P.C. Dorrestein, P. Greenberg, J. Clardy, M. Lindstrom

2:05 313. Exploiting of sugars and lignin to lipids by co-fermentation of *Rhodococci* strains. L. Xiaolu, Y. He, L. Zhang, H. Ben, Z. Xu, M. Gaffrey, Y. Yang, W. Qian, S. Yang, J. Yuan, S. Baker, **B. Yang**

2:25 314. Multi-scale protein production in a test-tube for versatile applications. **I. Novikova**, T. Moser, N. Sharma, R. Sontag, S. China, J.E. Evans

2:45 315. Design, synthesis and *in vitro* evaluation of rifamycin analogue against a virulent strain of *Mycobacterium tuberculosis* (*Mtb*), H37Rv. **S. Pasupathy**, G. Ramachandran, A. Dusthacker, S. Tripathy, N. Bhardwaj, D. Chatterji

3:05 Intermission.

3:20 316. Metabolomics on *Fusarium graminearum* strains lacking the histone H3 lysine27 methyltransferase, KMT6, yields novel secondary metabolites. **M. Freitag**, D. Adpressa, L. Connolly, Z.M. Konkel, X. Chang, B. Pierce, K.M. Smith, S. Loesgen

3:40 317. Unlocking the pharmacological potential of peptide-based drugs: An NMR approach to verifying the structure of designed *de novo* hyperstable disulfide-rich peptides. **G.W. Buchko**, S.V. Pulavarti, S. Rettie, T. Szyperski, D. Baker, C. Bahl

4:00 318. Spatially-organized kinase-substrate reactions with designed scaffold proteins. **E. Speltz**, J. Zalatan

4:20 319. Harnessing oleaginous yeast for overproduction of lipid-based chemicals and biofuels by building synthetic biology tools and engineering cellular metabolism. **X. Xiong**, R. Ghogare, S. Chen

4:40 320. Experimental evolution reveals favored adaptive routes to cell aggregation in yeast. E. Hope, **C. Amarosi**, A. Miller, K. Dang, C. Smukowski, M. Dunham

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Crick

Chemistry of Nuclear Processing

Cosponsored by NUCL
S. A. Bryan, G. J. Lumetta, *Organizers*
J. F. Corbey, P. R. Zalupski, *Presiding*

1:00 Introductory Remarks.

1:05 321. Understanding the crystallization of gibbsite using high-field ^{27}Al and ^{23}Na MAS NMR spectroscopy. **X. Zhang**, J. Hu, C. Pearce, S.B. Clark, K. Rosso

1:25 322. Sum frequency generation: Vibrational spectroscopy and its application in interfacial chemistry relevant to tank waste reprocessing. **Z. Wang**, A.D. Winkelman, X. Zhang, W. Cui, A. Tuladhar, Z. Chase, M. Sassi, E. Walter, K. Rosso

1:45 323. Support functions for testing of a uranium-plutonium co-decontamination flowsheet. **G.J. Lumetta**, J. Allred, S.A. Bryan, G.B. Hall, T.G. Levitskaia, A. Lines, S.I. Sinkov

2:05 324. Controlled Pu:U Ratios in a modified PUREX (CoDCon) solvent extraction flowsheet. **G.B. Hall**, J. Allred, A.M. Lines, S.I. Sinkov, J. Law, S.A. Bryan, G.J. Lumetta

2:25 Intermission.

2:40 325. Continuing studies into the impacts of gamma radiolysis on ALSEP and related solvent extraction systems. **D.R. Peterman**

3:00 326. Structural investigation of plutonium oxalate species and comparison of their oxide products. **J.F. Corbey**, L. Sweet, S.I. Sinkov, D.E. Meier, A. Casella

3:20 327. Association of T2EHDGA and HEH[EHP] in the ALSEP solvent. **V. Holfeltz**, Y. Chen, R.P. Young, G.J. Lumetta, T.G. Levitskaia

3:40 328. Trivalent actinide / trivalent lanthanide differentiation using *N*-methylpicolinate-ethylenediamine-*N,N',N'*-triacetic acid complexant. **P.R. Zalupski**, C. Heathman, T.S. Grimes, V. Bryantsev, S. Jansone-Popova

4:00 329. Oxidation and extraction of americium(VI) from used nuclear fuel using 2-cm diameter centrifugal contactors. **J. Law**, B. Mincher, R. Tillotson, N. Schmitt

4:20 330. Characterization of surface layers formed on DU10Mo ingots after processing steps and high humidity exposure. **T. Kaspar**, C. Arendt, D. Neal, A. Schemer-Kohrn, S.L. Riechers, R. Shimskey, C. Lavender, V. Joshi

4:40 331. Uranyl peroxide capsule self-assembly in slow motion. **A. Arteaga**, E.N. Glass, L. Zakharov, M.D. Nyman

BSF/CSF
Pasteur

Materials Synthesis across Scales

J. De Yoreo, *Organizer*

D. Gotthold, R. S. Weber, *Organizers, Presiding*

1:00 Introductory remarks.

1:05 332. Observing nucleation fluctuations with in situ AFM. **B. Legg**, M.D. Baer, Y. Min, C.J. Mundy, J. De Yoreo

1:25 333. Functional graphene oxide membranes for water separation. **Y. Shin**, W. Liu, R. Devanathan, L. Fifield, B.J. Hinds, D. Gotthold

1:45 334. Effects of ion associations and solvent dynamics on the formation of cage-like polyanions in tetraalkylammonium silicate solutions. **Y. Chen**, N. Washton, R.P. Young, A.J. Karkamkar, K.T. Mueller, J. De Yoreo

2:05 335. Structure and collective dynamics of boehmite oriented aggregation. **E. Nakouzi**, J.A. Soltis, B. Legg, G.K. Schenter, X. Zhang, T.R. Graham, K. Rosso, L. Anovitz, J. De Yoreo, J. Chun

2:25 336. Poly (2-ethyl-2-oxazoline) coated maghemite nanostructures for magnetically guided cancer therapy: study of entropically driven controlled release of paclitaxel. N. Kumar, L. Behera, B. Ateeq, **V. Verma**

2:45 Intermission.

3:05 337. From nanoscale to macroscale, artificially synthesize protein matrix at solid-liquid interface. **S. Zhang**, H. Pyles, D. Baker, J. De Yoreo

3:25 338. Zirconium and hafnium peroxo oxalate species in slightly acidic conditions. **K. Kozma**, M. Amiri, L. Zakharov, M.D. Nyman

3:45 339. Chromium(III) δ -Keggin polycation, aqueous synthesis, and characterization. **M. Amiri**, W. Wang, K. Kozma, L. Zakharov, M.D. Nyman

4:05 340. Supramolecular assembly of uranyl tetrahalides with substituted methyl-pyridinium cations: structure-property relationships. **N.M. Byrne**, R.G. Surbella, C.L. Cahill

4:25 341. Supramolecular actinide materials: A platform to explore structure-property relationships. **R.G. Surbella**, L.C. Ducati, J. Autschbach, J.M. Schwantes, C.L. Cahill

EMSL
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Chemical Tools & Instrumentation

Cosponsored by ANYL
N. A. Wall, *Organizer, Presiding*
S. Peterson, *Presiding*

1:30 Introductory Remarks.

1:35 342. Organo-sulfur analysis using a water stationary phase in GC-FPD. **K. McKelvie**, K. Thurbide

1:55 343. Temperature effects on thermal effusivity calibration materials. **R. Blaine**

2:15 344. Tracking carbon through the root-rhizosphere-soil system using laser ablation-IRMS. **E.H. Denis**, P.D. Ilhardt, A.E. Tucker, N.L. Huggett, J.J. Moran

2:35 345. Optimizing temperature gradient across sample rotor for high temperature MAS experiments. **H.S. Mehta**, E. Walter, J. Sears, Y. Chen, N. Washton, K.T. Mueller

2:55 346. Lab-based XAFS and XES for materials chemistry research. **E. Jahrman**, G.T. Seidler, W. Holden, A. Ditter, D. Mortensen, T. Fister, S.A. Kozimor

3:15 347. Adsorption and desorption study of a nerve-agent simulant from office materials for forensic applications. C. Fraga, **O.M. Primera**, A.S. Breton-Vega, M. Zumbach, B. Wilkins

3:35 Concluding remarks.

BSF/CSF
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Chemistry & Collaboration to Advance Nuclear Technologies

Sensor Development & Analytical Measurements for Hash Environments

Cosponsored by NUCL
S. A. Bryan, A. E. Clark, *Organizers*
S. Howett, S. I. Sinkov, *Presiding*

1:30 Introductory Remarks.

1:35 348. Infrared reflectance spectroscopy of uranium minerals: Determination of the optical constants n and k . **B. DeVetter**, T. Myers, B. Cannon, N. Scharko, M. Kelly-Gorham, J.F. Corbey, C.T. Resch, T.J. Johnson

1:55 349. A new approach to modeling the extraction of solute species across aqueous-organic interfaces to determine the intrinsic kinetics of interfacial phase transfer. **C. Louie**, C. Ivory, S. Howett, D. Bottenus, S.A. Bryan, A. Casella, C. Delegard, F. Heller, A.M. Lines, G.J. Lumetta, S.B. Clark

2:15 350. Discrimination of uranium ore concentrate via Raman spectroscopy: Effects of excitation wavelength. **B. DeVetter**, Y. Su, R. Tonkyn, L. Sweet, J.F. Corbey, T. Myers, S.A. Bryan, T.J. Johnson

2:35 351. Cat litter, nitric acid, plutonium, and \$2.4 billion dollars: PNNL's role in the investigation into the 2014 contamination at the waste isolation pilot plant. **J.M. Schwantes**, D. Atkinson, E. Buck, C. Fraga, L. Greenwood, B. McNamara, M.J. Minette, R. Scheele, L. Sweet, J. Wahl

3:05 Intermission.

3:25 352. Uranium adsorption in synthesized nanocrystalline zeolite. **C. Padilla-Cintron**, N. Anheier, C. Barrett, T. Pope

3:45 353. Tracking nuclear cable insulation aging via nondestructive methods. **M. Correa**, L. Fifield, Y. Shin, A. Zwoster

4:05 354. Some non-standard applications of optical absorbance spectroscopy for characterization of transuranium materials. **S.I. Sinkov**

4:25 355. Thermometric titration for aluminum and its impact on evaporator/crystallizer operations. **D.L. Herting**, J.R. Jewett

4:45 356. Method development for x-ray diffraction analysis of thin powder deposit samples of simulated radioactive tank waste. **T.M. Ely**, H. Meznarich, S. Bolling, T. Valero, G. Cooke

Discovery Hall
Horizon D

Chemistry Education & Outreach: General Papers

Cosponsored by CHED
K. L. Breno, K. A. Wheeler, *Organizers, Presiding*

1:30 Introductory remarks.

1:35 357. Data acquisition in the chemistry lab. **K.N. Goodwin**, E. Nam

1:55 358. Analytical chemistry in historical archaeology. **L. Bodley**, R. Von Wandruszka

2:15 359. Measuring osmosis across liposome membranes using laser light scattering: An undergraduate biochemistry experiment. T.P. Silverstein, **J.C. Williamson**

2:35 Intermission.

2:45 360. Hands-on NMR for students!: Or how benchtop NMR can help transform your labs. **J. Borau Garcia**, J.F. Araneda, S.D. Riegel

3:05 361. Development of instructional videos and analysis of student utilization patterns for the organic chemistry laboratories. **E. Nishimura**, **J. de Leon**, C. Anderton, R. Sargeant

3:25 362. Results from the first year of a community college S-STEM scholarship program: The SEECRS Scholar Academy. **T.A. Vannelli**, E. Davishahl, J. Babcock, D. Hanley, E. Harri

3:45 Concluding remarks.

Discovery Hall
Vista

Condensed Phase & Interfacial Chemistry

L. X. Dang, S. Xantheas, *Organizers, Presiding*

1:30 Introductory remarks.

1:35 363. Interfacial electrochemistry: Bridging the gap between theory and experiments. **T. Pham**

2:05 364. Electrochemical reduction of CO₂ using Au and CuAu nanoparticles. **E. Andrews**, Y. Fang, J.C. Flake

2:25 365. Elucidating mechanisms of CO₂ mineralization and utilization using petroleum coke ash at mineral-water interfaces: A synchrotron-based study. **S. Pan**, P. Chiang, Y. Chen, K. Shah, T. Chen, S. Pei

2:45 Intermission.

3:00 366. Environmentally sustainable energetic ionic liquid formulations for chemical propulsion. **G.F. Holland**

3:20 367. Fatty acid-modified sawdust aggregators for remediation of crude oil spill. **Y. Shin**, J. Park, E.M. Winder, K. Han, R.T. Jeters, L. Fifield, G. Bonheyo

3:50 368. NMR insights into the solubilization and upgrading of high polyethylene terephthalate loadings in the low-cost, bifunctional ionic liquid cholinium phosphate. **R.P. Young**, J. Sun, D. Liu, A. Cruz Gonzalez, N. Isern, T. Schuerg, J.R. Cort, B.A. Simmons, S. Singh

Discovery Hall
Horizon A (corrected)

Exciting Opportunities in Undergraduate Education

Instructional Strategies that Promote Student Learning

K. L. Breno, K. A. Wheeler, *Organizers*
C. A. Berg, *Organizer, Presiding*

1:30 Introductory remarks.

1:35 369. Scientific Python for chemistry and biochemistry undergraduates. **M. John**, G. Fisher, **H. Becerril**

1:55 370. Case studies in an honors general chemistry course. **K.L. Breno**

2:15 371. The development, implementation, and formalization of an enhanced general chemistry sequence at Oregon State University. **R.L. Nafshun**

2:35 372. Use of adaptive learning courseware in a GOB course: A report on the impact on student performance and attitude towards chemistry. **D.K. Howell**

2:55 Intermission.

3:10 373. Development of an introductory undergraduate nanomaterials curriculum. **L.E. Johnson**, M.S. Johal

3:30 374. Challenges of providing undergraduate research opportunities to students at a community college. **G. Blacken**

3:50 375. Teaching writing in the organic chemistry lab. **K. Goodwin**

BSF/CSF

Mural

In Situ & Operando Techniques for Electrochemical Systems

V. Prabhakaran, R. S. Weber, *Organizers*

G. E. Johnson, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 376. Photoinduced charge flow through molecules at plasmonic nanojunctions. **P.Z. El-Khoury**

2:05 377. Atomic imaging through tip-enhanced Raman scattering. **K. Crampton**, J. Lee, V.A. Apkarian

2:25 378. Soft x-ray approaches to probing electrochemical systems *in situ* and *operando* . **K.A. Stoerzinger**, L. Wang, R. Comes, Y. Du, S. Chambers

2:45 Intermission.

3:00 379. Masking contaminant-induced SOFC anode degradation with H₂: Combined operando Raman and electrochemical studies. **R.A. Walker**, K. Reeping, J. Bohn

3:20 380. *In Situ* observation of catalyst reconstruction during electrochemical CO₂ reduction. **M. Wang**, Z. Feng

3:40 381. *In situ* studies of electrocatalyst for oxygen evolution reaction in acidic condition using a combination of X-ray scattering and spectroscopy. **W. Samarakoon**, M. Wang, Z. Feng

4:00 Concluding Remarks.

WEDNESDAY MORNING

BSF/CSF
Darwin

Recent Developments in Radiochemistry & Radioanalytical Chemistry

Cosponsored by NUCL
S. A. Bryan, *Organizer*
M. J. O'Hara, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 382. Cesium removal from AP-105 Hanford tank waste using spherical resorcinol formaldehyde resin. **S. Fiskum**, A. Rovira, H.A. Colburn, J. Allred, M. Smoot, R. Peterson, K. Colosi

8:25 383. Ion exchange cesium removal from Hanford 241-AP-105 tank waste with spherical resorcinol formaldehyde (SRF) resin part 2. **A. Rovira**, S. Fiskum, H.A. Colburn, J. Allred, M. Smoot, R. Peterson, K. Colosi

8:45 384. Aqueous pertechnetate sensing by square-planar platinum(II) complexes. **S. Chatterjee**, A. Norton, W.B. Connick, T.G. Levitskaia, T.E. Albrecht-Schmitt, J. Christ, R. Dunn, R. Erikson

9:05 385. Gram-scale technetium chemistry. **C. Soderquist**

9:25 386. Atom probe tomography analysis of plutonium metal and oxide. **T.G. Lach**, D.E. Perea, D. Reilly

9:45 Intermission.

10:00 387. Microchemical purification of Pu: Improvements in anion exchange kinetics in single bead separations using bead-in-a-tube and forced convection. **N.E. Uhnak**, S.S. Morrison, M.J. O'Hara, J.W. Grate, N.J. Murray

10:20 388. Modeling radioxenon isotopes in solutions containing ^{240}Pu . **A.M. Ritzmann**, J.M. Johns, D. Abrecht, A.M. Prinke, V.T. Woods, C.J. Gesh, B. Reid

10:40 389. Ra-224 purification using a column based separation method in an alcohol solvent. **I.S. Miller**, G.B. Hall, C. Soderquist, M.J. O'Hara

11:00 390. Electrodeposition of Ra for use as a medical isotope generator. **G.B. Hall**, I.S. Miller, M.J. O'Hara

11:20 391. Development of ^{235}U - ^{231}Pa chronometer for uranium safeguards. **B.N. Robertson**, M.J. O'Hara, V. Remcho, C.J. Palmer, S.L. Petersen, B. Reid, K.A. Burns