

American Chemical Society

2018 Rocky Mountain Regional Meeting

N. Xu, *Program Chair*

FRIDAY MORNING

General Chemistry

Sheraton Albuquerque Airport
Gran Quivera

P. D. Burton, *Organizer, Presiding*

9:00 Introduction.

9:05 1. Ethnoscience strategies to indigenize science at tribal colleges: Connecting chemistry to the tribal community. **B. DeVore-Wedding**

9:35 2. Regenerable single atom catalysts for alkane conversions. **G. Canning**, M. Senn, H. Xiong, R. Alcala, N. LiBretto, J. Miller, A.K. Datye

10:05 Intermission.

10:30 3. LigandNet: Machine-learning based toolkit for predicting ligand activity to proteins. **S. Sirimulla**

11:00 4. Crowding effect on electron transfer in inducible nitric oxide synthase. **J. Li**, C. Feng

Inorganic Chemistry

Sheraton Albuquerque Airport
Valle Grande

R. M. Chamberlin, *Organizer, Presiding*

9:00 Introduction.

9:05 5. Synthesis and characterization of lanthanide-silica based core/shell nanoparticles for scintillator applications. **F. Guerrero**

9:35 6. Synthesis of manganese-based precursors and nanoparticles for electronic printing applications. **T. Nguyen**, T.J. Boyle, L.J. Treadwell

10:05 Intermission.

10:30 7. New model systems for periplasmic nitrate reductase (Nap) and formate dehydrogenase (Fdh) catalytic intermediates. **K. KC**, M.L. Kirk

11:00 8. Insights into molecular rectification using donor-acceptor molecules. **R. Dangi**

Organic Chemistry

Sheraton Albuquerque Airport
Chaco

D. Yang, *Organizer, Presiding*

9:00 Introduction.

9:05 9. Structure and properties of new push-pull molecules. **G. Bogdanov**, J.P. Tillotson, J.W. Perry, T.V. Timofeeva

9:35 10. Design, synthesis, and evaluation of cystargolide-based β -lactones as potent proteasome inhibitors and anti-cancer agents. **D. Niroula**, R. Tello-Aburto

10:05 Intermission.

10:30 11. Concepts important for proficiency in organic reaction mechanisms. **S. Nedungadi**, M.D. Mosher, R.M. Hyslop, C.E. Brown

FRIDAY AFTERNOON

Analytical Chemistry

Sheraton Albuquerque Airport
Chaco

J. Chen, *Organizer, Presiding*

1:15 Introduction.

1:20 12. Progress report on the design of a flow-based ATR-FTIR Spectrometer. **A. Campanella**, M.D. Mosher

1:50 13. Fluorescent bead-based method to study the phospholipase A2 -lipid membrane interaction. **S. Hossain**, M.E. Piyasena, K. Pai

2:20 14. Method development: Transition characterization of poly(ester urethane) block copolymer elastomer via thermal and mechanical analyses. **A. Edgar**, J. Torres, D. Yang

2:50 Intermission.

3:15 15. Effects of encapsulated cells on the physical-mechanical properties and microstructure of gelatin methacrylate with high degree of functionalization. **S. Krishnamoorthy**, H. Xu, C. Xu

3:45 16. Micromachined aluminum microfluidic devices: Miniaturized tool for biomedical applications. **G.P. Gautam**, M.E. Piyasena

4:15 17. Microsphere-supported lipid bilayers with fluorescent lipid probes for the detection of phospholipase D activity. **R. Gurung**, T. Ogas, P. Patidar, M.E. Piyasena

4:45 18. Kinetics of peroxytaurine reactions. **G. Meyer**, S.J. Karpowicz

Inorganic Chemistry

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R. M. Chamberlin, *Organizer, Presiding*

1:15 Introduction.

1:20 19. Normalized Timescale Method for the determination of order in catalyst for electrocatalytic reactions. **T.A. Stinson**, M.J. Bailey, A.M. Lilio, T.H. Myren, C.G. Huntzinger, M.R. Hudak, O.R. Luca

1:50 20. Manganese N-heterocyclic carbene pincers for the electrocatalytic reduction of carbon dioxide. **T.H. Myren**, A.M. Lilio, C.G. Huntzinger, J.W. Horstman, T.A. Stinson, T.B. Donadt, C. Moore, B. Lama, H.H. Funke, O.R. Luca

2:20 21. Hierarchical zinc oxide nanostructures for the photochemical reduction of bicarbonate to solar fuels. **H. Pan**, V. Risley, K. Martindale, M.D. Heagy

2:50 Intermission.

3:15 22. Molecular rectification behavior of the pyranopterin ligand of molybdoenzymes. **L. Ingersol**, M.L. Kirk

3:45 23. Charge effect on oxygen atom transfer reactivity related to molybdoenzymes. J. Paudel, **A. Pokhrel**, M.L. Kirk, F. Li

4:15 24. Generation and characterization of functional phosphoserine incorporated neuronal nitric oxide synthase holoenzyme. **H. Zheng**, J. He, J. Li, J. Yang, M.L. Kirk, L. Roman, C. Feng

4:45 25. Implications of pyran cyclization and pterin conformation on oxidized forms of the molybdenum cofactor. **J. Yang**, M.L. Kirk, D. Gisewhite, B. Williams, A. Esmail, B.W. Stein, S. Burgmayer

Physical Chemistry

Sheraton Albuquerque Airport
Gran Quivera

D. R. Porterfield, *Organizer, Presiding*

1:15 Introduction.

1:20 26. Synthesis of nitrile-functionalized ladder-type oligo(*p*-phenylene)s for probing electron delocalization. **J. Yan**, A. Ledbetter, E.W. Reinheimer, T. Mani, J.R. Miller

1:50 27. Discrete stochastic solution to lipid bilayer permeation model. **G. Angles**

2:20 28. Counting triplets on single polymer chains for solar cells. **B. Datko**, A. Thomas, M.J. Heeney, J.K. Grey

2:50 Intermission.

3:15 29. Non-reactive binding sites and their role in the $\text{AlVO}_4^+ + \text{CO}/\text{AlVO}_3^+ + \text{N}_2\text{O}$ catalytic cycle. **B. Sweeny**, S.G. Ard, N. Shuman, A.A. Viggiano

3:45 30. How cerium oxide traps high concentrations of thermally stable platinum single atoms. **D. Kunwar**, S. Zhou, A. DeLaRiva, E. Peterson, H. Xiong, **X. Isidro Pereira Hernández**, S. Purdy, R. ter Veen, H. Brongersma, J. Miller, L. Kovarik, S. Lin, H. Guo, Y. Wang, A.K. Datye

4:15 31. Infrared photodissociation spectroscopy of the H_6^+ cation in the gas phase. **D.C. McDonald**, J.P. Wagner, M.A. Duncan

4:45 32. Photoreduction of CHCl_3 in aqueous SPEEK/ HCO_2^- solution involving free radicals. **M.S. Islam**

FRIDAY EVENING

Analytical Chemistry

Sheraton Albuquerque Airport
Tijeras

J. Chen, *Organizer*

6:00 - 8:00

33. Size effect of gold nanoparticles on graphene quantum dots fluorescence intensity. **Y. Zhang**

34. Facile synthesis of graphene quantum dots and their applications in bioimaging. **Z. Schroer**

35. Efficiency enhancement of anaerobic digester in microbial fuel cell through use of *R. Albus*. S. Chung, **D.J. Moon**, J. Kim

Inorganic Chemistry

Sheraton Albuquerque Airport
Tijeras

R. M. Chamberlin, *Organizer*

6:00 - 8:00

36. Silver nanoparticles synthesis in ionic liquids. **S. Wolde**, H. Zhao, M. Watzky

Organic Chemistry

Sheraton Albuquerque Airport
Tijeras

D. Yang, *Organizer*

6:00 - 8:00

37. Progress report on the use of viscometry in DNA-drug interactions. **J. Forster**

38. Microwave assisted synthesis of 3,6-disubstituted pyrazolo[1,5-a]-pyrimidines and progress toward discovery of anticancer activities. J. Singleton, **R. Dass**, M.A. Peterson

39. Efficient microwave assisted synthesis of N'-aryl/(alkyl)-substituted N-(4-hydroxy-6-phenylpyrimidin-2-yl)guanidines: Scope and limitations. **J. Singleton**, P. Machicao, R. Christensen, N. Lohner, M.A. Peterson

- 40.** Synthesis and characterization of high mobility, side-strapped phthalocyanines for organic photovoltaics. **W.G. Benson**
- 41.** On the reduction chemistry of imidazolium salts. **C.G. Huntzinger**, T. Myren, T.A. Stinson, O.R. Luca, M.R. Hudak
- 42.** Olfactory receptor mediated repellency of linalool, geranyl acetate, and EBF in two drosophila species. **P.K. Duran**
- 43.** Progress report on the preparation of O-benzyl-N-(9'-acridinyl)hydroxylamines. **N.K. Robbins**, M.D. Mosher
- 44.** Aldol approach to efficient, stereoselective synthesis of structurally diverse beta-lactones. **S.K. Ganegamage**, R. Tello-Aburto, N. Doleshwar
- 45.** Lewis-acid-mediated union of epoxy-carvone diastereomers with anisole derivatives: Mechanistic insight and application to the synthesis of non-natural CBD analogues. S. Bailey, R. Sapkota, **A.E. Golliver**, B. Dungan, M. Talipov, O. Holguin, W.A. Maio
- 46.** Mechanism of hop oil isomerization. **E. Munder**, M.D. Mosher
- 47.** Oximation of benzalacetone. **R. Owusu Sarpong**, M.D. Mosher

Physical Chemistry

Sheraton Albuquerque Airport
Tijeras

D. R. Porterfield, *Organizer*

6:00 - 8:00

- 48.** Synthesis and characterization of Iron containing MOFs for environmental remediation. **M.I. Chibuike**
- 49.** X-ray and DFT studies of novel thiobarbituric chromophores with nonlinear optical properties. **S. Rigin**, G. Bogdanov, T.V. Timofeeva, J.P. Tillotson

General Chemistry

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Tijeras

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6:00 - 8:00

- 50.** Evaluation of amyloid- β protein as an antimicrobial peptide in Alzheimer's disease. **C. Hunter**, A. Fanni, D. Brown, E.Y. Chi

51. DLSCORE: Deep Learning model for predicting protein-ligand binding affinities. **M. Hassan**, D. Mogollon, O. Fuentes, S. Sirimulla

52. New Mexico Highlands University Chemistry Club. **E.M. Trujillo**

53. Lobo Chemistry Club: American Chemical Society student chapter at University of New Mexico. **N.A. Abeyta, C. Hunter, F. Delacruz, G. Carrion-Gonzales, L. Perez**

54. Get involved with the ACS Division of Chemical Education. **M.A. Horn**