

- CHED **808**. Student knowledge of factors for success in chemistry. S. Barrett, S. Wuerz
- CHED **809**. Filtered available phosphate by FIA: A partnership between chemistry and geology. J. Onyeagba, P.J. Iles, R. Kochambilli, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb
- CHED **810**. Utilizing 3-D printing to enhance classroom instruction of dynamic nature of proteins. J. Green, M. Guthrie, L. Manner, J. Bowden, S.S. Ruebush
- CHED **811**. Dip coater. M. Bresnahan, B. Veldman
- CHED **812**. Impact of mindset on the persistence of STEM majors. J. Hackleman, B. Brando, A. Stacy, A.M. Baranger
- CHED **813**. Connecting dots to community through chemistry at St. Xavier University, Chicago. P.M. Brehm, B. Alappat
- CHED **814**. Role models and mentors matter for Tennessee girls in STEM. J.M. Iriarte-Gross, T. Thomas, K. Owens, R. Marlin, A. Williams
- CHED **815**. Synthesis and analysis of fullerenes in the undergraduate physical chemistry laboratory. T.J. Fuhrer, A. Lambert, H. Bell, C. Roper
- CHED **816**. Using a ranking task coupled with semi-structured interviews to characterize upper-division chemistry students' modeling practices in quantum chemistry: A mixed-methods study. C. Crickmore, M.N. Muniz, J. Beck
- CHED **817**. Diffraction: A butterfly experiment. B.A. Bober, M.O. McAnally, I. Jones, H. Shi, M. Su, B. Negro
- CHED **818**. What chemical facts does the public need to know? M. Winkelman, S. Wuerz
- CHED **819**. Chemical safety and chemical disposal. A. Argueta, S. Wuerz
- CHED **820**. Chemical storage in home, shop, and public areas. J. Montoya, S. Wuerz
- CHED **821**. Magic in chemical education. A. Morris, S. Wuerz
- CHED **822**. Factor analysis for academic success in chemistry. B. Claro-Martinez, S. Wuerz
- CHED **823**. Withdrawn.
- CHED **824**. Binary liquid-vapor phase diagrams with desktop gas chromatography. B.A. Rowland, P. Bayliss
- CHED **825**. Philatelic table of the elements as a teaching tool: Topics in health and medicine. B.T. Winn, L.G. French
- CHED **826**. Implementing preferred VARK learning modalities in organic chemistry. K. Page, S.K. Hamilton
- CHED **827**. Timing of homework completion vs. performance in general chemistry. M.N. Cosio, V.M. Williamson
- CHED **828**. Optimize of teaching contents and the develop of teaching methods to the compulsory course of general chemistry in universities. D. Tang, Z. Sun, Z. Yu, H. Lv
- CHED **829**. Microwave-assisted Fischer indole synthesis for the organic chemistry laboratory. M. Rico Mendoza, M.T. Wentzel
- CHED **830**. Implementing a flipped classroom and active learning techniques in general chemistry to augment student success at a mid-sized rural university. E. Bladorn, C. Chatha, V. Cherrette, H. Dailey, J. Lopez, H. Mills, C. Park, H. Park, A. Rose, S. Sherry, R. Skorheim, M. Smith, E.C. Wasinger
- CHED **831**. Assessing the levels of models upper-division chemistry students develop and apply in the context of the hydrogen atom: A qualitative investigation. J. Kirsch, J. Beck, M.N. Muniz
- CHED **832**. Effect of online homework on students' performance in introductory chemistry. H. Syu, B. Adair, S.T. Mabrouk
- CHED **833**. Spinning towards low-cost spin coaters. H. Speerstra, B. Veldman
- CHED **834**. Biochemistry research in the general chemistry lab classroom: A pilot study. J. Callus, S. Juris, K. Spencer, J. Tomasik
- CHED **835**. Using analgesia as a theme in the first semester of organic chemistry laboratory. N. Akanda, R. Blough, J. Orlandi, M.J. Castaldi, J.K. Murray
- CHED **836**. Computer-aided Design (CAD), fabrication, and testing of an inexpensive 3D printed filter fluorometer. M.H. Hakim, D.A. Rourke, L.A. Porter
- CHED **837**. Conceptual understanding and context: Free energy. K. Wilson, J. Nyachwaya
- CHED **838**. Role of porphyrins in teaching organic chemistry. Z.J. Gregg, J.C. Quirke, J.M. Quirke
- CHED **839**. Homemade antacid tablets for the antacid titration lab. J. Thom, A. Kwong, W.J. Miller
- CHED **840**. Complete binary phase diagram laboratory for undergraduate physical chemistry courses. T.P. Dorch, B. Veldman
- CHED **841**. Effectiveness of chemical demonstrations in increasing student interest in science. D.G. Watson, Y. Gibson, M. Taylor
- CHED **842**. Development and implementation of popular diets case studies in a biochemistry course for dietetics majors. K. Franklin, A. Gamez, R.M. Hyslop, C.E. Brown
- CHED **843**. Prototyping a simple and inexpensive colorimeter from 2D designs via laser cutting and engraving. H. Irtija, E.D. Banks, L.A. Porter
- CHED **844**. Sustainability in the laboratory: Assessing green chemistry integration in the general chemistry curriculum. M.C. Rivas, L. Armstrong, G. Kerstiens, M.T. Robak, M.C. Douskey, A.M. Baranger
- Section I**  
Moscone Center  
Hall D
- Undergraduate Research Posters**
- Computational Chemistry**  
*Cosponsored by COMP and SOCED*  
N. Di Fabio, Organizer
- 12:00 - 2:00**
- CHED **845**. Generation of new liver X receptor ligands using state-of-the-art computational methods. M. Ndukwe, K. Riley
- CHED **846**. Computational studies of formaldehyde reactions with HCN, ammonia, and pyrrole relevant to prebiotic chemistry. K. Thrush, H. Loli, J. Kua
- CHED **847**. Characterization of the structure of vinyl cations. C. Lodder, B.N. Norris
- CHED **848**. Impact of DNA strand length on duplex stability in solution and in a microarray environment via molecular simulation. B. Rivard, S. Cooper, L. Pelletier, J.M. Stubbs
- CHED **849**. Searching for a Möbius conformation of cyclometaphenylene. S. Cho, S.M. Bachrach
- CHED **850**. Nitrogen-substituted bisaryl dienes in the Diels-Alder reaction. Z. Zayat, S.M. Bachrach
- CHED **851**.  $\alpha$ -Conotoxins peptide mutants as Parkinson's therapeutics: A molecular dynamics study. S. Walker, O.M. McDougal, M. King
- CHED **852**. Energy landscape of unsubstituted seven-membered ring oxocarbenium ion. E. Castele, K.A. Woerpel, J.D. Evanseck
- CHED **853**. Theoretical energy determination of hydroxy-peroxy radicals derived from  $\alpha$ -terpenol using *Ab initio* and density functional theory calculations. A. Alejandro, C. Wilson, S. Drake, K. Dowda, R.S. Dabell, J.C. Hansen
- CHED **854**. Temporary anion states in the field of permanent dipole and quadrupole moments. D.C. Hiener, M.C. Fair, M.F. Falcoetta
- CHED **855**. Conventional strain energies of the oxaphosphetanes and the oxadiphosphetanes. B. Nash, A. Smyly, D.H. Magers, S.A. Smith
- CHED **856**. Investigation of hydroxy-peroxy radicals derived from *R-limonene*: A theoretical approach. C. Calderon, A. Alejandro, M. Dick, T. Murphy, M. Synelnikov, M. Russon, R.S. Dabell, J.C. Hansen
- CHED **857**. Conventional strain energy in ketene acetals and ketene aminals. S.G. Travis, S.A. Smith, D.H. Magers
- CHED **858**. Precision-biased statistical coupling analysis for use in rational protein design. O. Chapman, A.M. Leconte, A. Cavalcanti
- CHED **859**. Molecular simulations reveal the importance of disulfide bridging in PrgW, a putative redox switch for plasmid replication. S. Dornblaser, B. Buttaro, V.A. Voelz
- CHED **860**. Using electronics and sterics to affect the cyclization of angularly benzannulated enediynes. T. Keel, M.H. Daly, B.F. Gherman, J.D. Spence
- CHED **861**. Computational investigation of isoquinoline alkaloids and scaffold replaced derivatives as LXR modulators. D.A. Spadoni, C. Todd, F. Payton-Stewart
- CHED **862**. Propagation of hyperbolic secant wave packets: Visualizing the quantum momentum and potential field with numerical analytic continuation. W. Garrett, C. Lechak, B.A. Rowland
- CHED **863**. Theoretical study of aerosol seeding via homoassociation of methane sulfonic acid. C.M. Kottke, H.K. Hernandez-Soto
- CHED **864**. Computational characterization of the form of Ag(phen) for amination and azirdination reactions. P.M. Birschnbach, J. Scanlon
- CHED **865**. Structure-based prediction of small molecule modulators of DNMT3A. Y. Markov, A. Schlessinger
- CHED **866**. Theoretical study of ligand effects on homogeneous hydrogenation catalyzed by iron-pyridone complexes. E.F. Curl, L. Boisvert, T.V. Harris
- CHED **867**. Mathematical model for copper homeostasis in *Pseudomonas aeruginosa*. J.C. Roth, B. Kozemczak, J. Parmar, P. Mendes
- CHED **868**. Effect of ligand chemistry in mononuclear metal catalysts on the intramolecular features of the water oxidation mechanism. K. Hunter, J. Alvarado, E.A. Jarvis
- CHED **869**. ONIOM model of malonate decarboxylation: Significance of the hydrogen bonding buckle. L. Andreola, I. Pathiraja, S.M. Firestine, A. Tamez, D.J. Fox, J.D. Evanseck
- CHED **870**. Interaction energies of tricoal complexes: Effects of substituent groups. A. Jimenez, K.R. Jorgensen
- CHED **871**. Effect of vacancy defects on ion transfer in carbon nanotubes. B.A. Collins, T.D. Shepherd
- CHED **872**. Coarse-grain simulations of confined water within carbon nanotube systems. J. Chisholm, T.D. Shepherd
- CHED **873**. Is a planar  $C_{16}N_{12}$  possible? M. Alsarraj, M. Vaziri, J. Song
- CHED **874**. Inductive and hyperconjugative effects on carbocations. J.J. Nysschen, B.A. Modhera, E.D. Glendening
- CHED **875**. Energetic and structural analysis of metallo-heterofullerene derivatives of  $C_{20}$ :  $C_{18}M$  ( $M = 3d$  transition metals). J. McDonald, K.A. Beran
- CHED **876**. TD-DFT potential energy surfaces and nonadiabatic dynamics of indole by surface hopping with Newton-X. K.M. Vorwerk, W. Kennerly
- CHED **877**. Computational quantum chemistry studies of metal oxide clusters. S. Partovi, L.M. Thompson, H.P. Hratchian
- CHED **878**. Thermodynamic properties of the loss of  $CH_3SH$  from protonated methionine. D. Devore, P.B. Armentrout, J. Johnston
- CHED **879**. Withdrawn.
- CHED **880**. Theoretical study of the formation of  $CH_3SO_3H$  from the reaction of  $CH_3SO_2H$  and OH radical. W.L. Rebelesky, H.K. Hernandez-Soto
- CHED **881**. Computational study of CO adsorption on a platinum-modified faujasite zeolite. K.A. Parrish, M.D. Fellows, H.K. Hernandez-Soto
- CHED **882**. Gas-phase transition states of proline tripeptides. P. Arcoria, J.C. Poutsma, V.H. Wysocki, A. Somogyi
- CHED **883**. Influence of hyperconjugative and inductive effects on the acidities of carboxylic acids. R.C. Rudisell, E.D. Glendening
- CHED **884**. Effects of basis set on the energy levels of highly charged ions. J. Ortiz-Soto, J.I. Vega-Sánchez, N.A. Lopez, J.A. Santana
- CHED **885**. Theoretical investigation of  $N_2C-CO_2$ . V. Nguyen, D. Corey, J. Song
- CHED **886**. Exploring metal surface catalytic effects on Li-S batteries with DFT calculations. C.R. Bernard, J.A. Santana

- CHED 887.** Absorption and fluorescence of indole and tryptophan by TD-DFT. **J. Gerard, W. Kennerly**
- CHED 888.** Density functional theory investigation of the interaction between acetone and chloroform. **M.E. Furgione, R.J. Olsen**
- CHED 889.** Characterizing the Jahn-Teller effect in manganese trifluoride: A molecular modeling approach suitable for early undergraduate and AP high school chemistry students. **K.A. Shaikh, S. Warrick, L. Gurung, D. Kwak, J.A. Bumpus**
- CHED 890.** Solvent effects in the dynamics on potentials with post-transition state valley ridge inflection points. **F. Malik, Z.C. Kramer, B.K. Carpenter, G.S. Ezra, S. Farantos, S. Wiggins**
- CHED 891.** Computational study of the mechanistic effect of fluorine groups on the ring-opening polymerization of  $\epsilon$ -caprolactone with Al-centered catalysts. **C. Ortiz, A. Longo, J.M. Fritsch, B. Wilson**
- CHED 892.** Computational modeling of sodium laurate surfactant in the presence of aqueous divalent cations at the oil-water interface. **K.T. Chippindale, K.E. Johnson**
- CHED 893.** Thermodynamics and SN2 mechanism of the loss of ammonia from protonated methionine. **A.A. Chen, P.B. Armentrout, J. Johnston**
- CHED 894.** MR-MP energy levels of ions in the Li, Be and B isoelectronic sequences. **N.A. Lopez, J.I. Vega Sánchez, J. Ortiz-Soto, J.A. Santana**
- CHED 895.** Using molecular dynamics simulations to investigate novel reaction events: A case study with iron carbonyls. **J. Liu, L. Wang**
- CHED 896.** Investigation of micelle formation using molecular modeling and NMR. **C. Lewis, F.H. Billiot, E. Billiot, K.F. Morris, Y. Fang**
- CHED 897.** Computational investigations of aldol reactions of aromatic enolates and aldehydes. **A. Zolfaghari, N.M. Wachter, S. Mazumder**
- CHED 898.** Elucidation of electrochromic materials utilizing TDFT. **A.L. Tomlinson, A.R. Green**
- CHED 899.** Computational studies of oxygen bond lengthening with group-10 metal clusters. **D. Gray, M. Paul**
- CHED 900.** Withdrawn.
- CHED 901.** Parameter development for pseudouridine. **A. Ustoyev, M.C. Nagan**
- CHED 902.** Molecular modeling studies on the realkylation of Aged-Acetylcholinesterase (AChE) by Quinone Methide Precursors (QMPs). **R. Hopper, I. Pelfrey, R. McCauslin, R.J. Yoder**
- CHED 903.** DFT analysis of various porpholactone isomers. **R.F. Lalisse, M. Guberman-Pfeffer, J. Gascon, C. Bruckner**
- CHED 904.** Protein-ligand docking with HADDOCK: The effects of input protein conformational differences on the success of docking. **K.R. Reinke, J. Grinstead, A. Bonvin**
- CHED 905.** Substitution group effect on the inhibition of ubiquitin C-terminal hydrolases for Parkinson's disease study: Synthesis and computational analysis. **M. Liang, D. Xiao**
- CHED 906.** Utilization of molecular dynamics to examine the physical properties of hydrocarbon mixtures from 293-373 K. **J. Winkler, T. Knippenberg**

## Section I

Moscone Center  
Hall D

### Undergraduate Research Posters

#### Environmental Chemistry

Cosponsored by ENVR and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

- CHED 907.** Correlation study between particulate matter and PAH concentrations through the bio-monitoring of pine tree leaves. **R. Moran, S. Cortez, S. Deprele**
- CHED 908.** Differential impact of chitin and chitosan on heavy metal pollution in water samples. **J. Caldwell, J. Mendez**
- CHED 909.** Continued investigation of the mechanism of biosorption of lead. **T. Robertson, D.J. Schauer**
- CHED 910.** Atmospheric applications of deliquescence relative humidity determined by quartz crystal microbalance. **A.C. Burrows, H. Holst, C.M. Strollo**
- CHED 911.** Impact of the position of the chloro-substituent in chloroformate reactivity. **J. Wirick, M.J. D'Souza**
- CHED 912.** Withdrawn.
- CHED 913.** Changes to As, Cu, Fe, Mn and Zn concentrations in soil resulting from the application of poultry manure. **R.D. Foust, K. Hull**
- CHED 914.** Soil analysis for the greater Albion Community Garden Network. **R. Ford, K.M. Metz**
- CHED 915.** Assessment of heavy metals in subsistence-harvested alaskan pinniped vibrissae. **C. Gotluru, T. Juneja, P. Ferdinando, K. Cash, K. Sekou, A. Hiron, D.G. Giarikos**
- CHED 916.** Laboratory simulation of the open limestone channel at abandoned mine: Swank 13. **J.M. Schulte, P. Youmbi, D. Madl, R. Krupa, J.Z. Bandstra, E.P. Zovinka**
- CHED 917.** Study on the synthesis of ADA chelating cellulose and its adsorptive capability. **L. Yi, S. Wenjian, P. Yang, J. Fangyuan, L. Xiaoxiao**
- CHED 918.** Inventory platform manages chemical risks, addresses chemical accountability, and measures cost-effectiveness. **L. Neff, K. Roeske, M.J. D'Souza**
- CHED 919.** Singlet oxygenation of Lipitor and Lescol. **G.D. Tejada, K.E. O'Shea**
- CHED 920.** Factors controlling the regioselectivity and rate of arene bromination by aqueous BrCl and related brominating agents: Influence of steric effects. **K.R. Martin-Culet, J.D. Sivey**
- CHED 921.** Investigating lead sources near a secondary lead smelting site: Using antimony as a pathfinder element. **D. DeWilde, K. Ryncarz, N. Aist, M. Ketterer, S. Youtsey**
- CHED 922.** Examination of the composition of the lipid component of natural organic matter using ultrafiltration with organic solvents and NMR analysis. **A. Kub, J. Rice**
- CHED 923.** Distinguishing between dissolved reactive phosphate and bio-available phosphate for the development of a biophosphate sensor. **A. Cooper, E. White, C. Lemus, H. Goodson**
- CHED 924.** Photocatalytic degradation of tetracycline using floating PMMA-TiO<sub>2</sub> microspheres. **A.C. Hartley, J.D. Glover, J.E. Boyd**
- CHED 925.** Assessment of hydroxyl radicals production during ultrasonic irradiation for potential treatment of diphenhydramine pollution. **J.M. Rosado, D. Cui, K.E. O'Shea**
- CHED 926.** Photochemical degradation of oil in seawater. **D. Chang, S. Hok, T. Bui, A. Lam, M. Eclevia, W.J. De Bruyn, C.D. Clark**
- CHED 927.** Using 3-component hydrocarbon mixtures to model the properties of catalytic hydrothermal conversion fuels. **S.Y. Ye, M. McLaughlin, D.J. Luning Prak**
- CHED 928.** Ozone in Sequoia National Park: Linking ozone production in the San Joaquin Valley to trends in vegetative impacts in Sequoia National Park from 2000-2016. **C. Buisse, S. Pusede, A. Kotsakis**
- CHED 929.** Effects of anthropogenic activities on the water quality of the Huron River and its contributing streams. **J. Vites, O. Hajihassani**
- CHED 930.** Withdrawn.
- CHED 931.** Groundwater pollution reduction through biochar adsorption of herbicide Dacthal. **O.O. Harrison, E. Baker, S.K. Saha, A. Saha**
- CHED 932.** Modeling the kinetics of trace metal ion speciation: The influence of calcium ion on disjunctive ligand exchange. **L. Rea, N.E. Boland**
- CHED 933.** Human effect on potentially toxic metal concentrations in the soils of Scotland. **K. McCarthy, C. Davidson**
- CHED 934.** Viability of fecal coliform bacteria in beach sand and lake sediments. **C.M. McManus, D.S. Karpovich, J.L. McEvoy**
- CHED 935.** Determination of the mechanism for trihalomethanes and nicotinamide in basic medium for a water disinfection device. **M. Dorko, S. Espy**
- CHED 936.** Effect of silver nanoparticles with varying capping agents on the growth of kale (brassica oleracea). **A. Agloro, A.L. Smalley**
- CHED 937.** Fate and toxicity of BPA in two native plants, blue bush lake beans (*Phaseolus vulgaris*) and switchgrass (*Panicum virgatum*), to explore their phytoremediation potential. **J.C. Murphy, A.K. Merrill, P. Das**
- CHED 938.** Phase transitions of biologically-derived components in sea spray aerosols and investigation into the chemical complexity of aged SSA. **M. Alves, A. Estillere, J. Trueblood, V.H. Grassian**
- CHED 939.** Quantification of 11-nor-9-carboxy-tetrahydrocannabinol in wastewater from Washington State to estimate consumption patterns of cannabis use. **A. LaRock, J. Sadetsky, D. Westerman, D.A. Burgard**
- CHED 940.** Quantification of THC-COOH to estimate cannabis consumption trends via wastewater based drug epidemiology. **J. Sadetsky, A. LaRock, R. Carpenter, D.A. Burgard**
- CHED 941.** Urban and rural land use contributions to phosphorus and E. coli pollution: A case study on Bad Axe Creek. **M. Dobulis, E.M. Greeson, K.L. Kwiatkowski, T. Benedict, O. Bishop, A. Yankley, K. Underwood, C.M. McManus, T. Sivy, D.S. Karpovich**
- CHED 942.** Synthesis of amino acids coupled to 2,6-pyridine dicarboxylic acid, and evaluation of their affinity towards metals. **E. Luta, A. Stedman, S.G. Tajc**
- CHED 943.** Graphene-doped polyethylene electrodes used to produce hydroxyl radicals for water purification. **A. Wallace, L. Slaymaker, R.J. Hamers**
- CHED 944.** Characterizing heavy metal sequestration in a bioswale at Pomona College. **E. Zvans, H. Van Ryswyk, M. Los Huertos**
- CHED 945.** Analyzing the atmosphere of crystal cave: Understanding sources and sinks of trace gases. **A.W. Jarnot, S. Hughes, D.R. Blake**
- CHED 946.** Environmental drivers of cyanobacterial blooms and toxin production in Lake Winnebago, Wisconsin. **A. Tomczyk, S.L. Bartlett, R.M. Kutzner, J. Piatt, T.R. Miller**
- CHED 947.** Algal toxin dynamics and environmental indicators in Green Bay, Wisconsin. **R. Kutzner, S.L. Bartlett, A. Tomczyk, J. Piatt, T.R. Miller**
- CHED 948.** Estimation of the source of atmospheric inputs of selected metals and metalloids to the Pacific northwest (USA). **M. Sousa, C. Welty, D. Price, M. Cummings, F.M. Dunnivant**
- CHED 949.** Absorption and translocation of lead (II) Nitrate within *Coriandrum sativum*. **J. Wilson, D.J. Schauer**
- CHED 950.** Chemistry of imidazole forming reactions and reactive uptake of hydrocarbons. **A. Sager, J.M. Ackendorf, M. Galloway**
- CHED 951.** Photolysis of the suburban-use herbicide trifluralin on retail mulch surfaces. **M. Kaur, F. Pavlovici, K.J. Bisceglia**
- CHED 952.** Gadolinium complexes for catch-and-release of phosphates. **C. Zeller, K. Peterson, S. Harris, V.C. Pierre**
- CHED 953.** Synthesis of water-stable material-organic framework at room temperature. **N. Le, K.T. Jackson, D. Eason, F. Mensah**
- CHED 954.** Effect of substrate on the growth of *Manilkara bidentata* at Finca Nolla Camuy, Puerto Rico: Applications in environmental chemistry. **F.A. Portero Camacho, K.R. Reyes Sanchez, R.J. Mayer Arzuaga**

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.