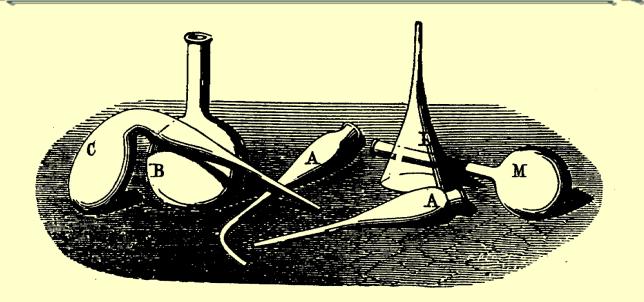




American Chemical Society DIVISION OF THE HISTORY OF CHEMISTRY



PROGRAM & ABSTRACTS

257th ACS National Meeting Orlando, FL March 31 – April 4, 2019

Nicolay V. Tsarevsky, Program Chair

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Final Program

DIVISION OF THE HISTORY OF CHEMISTRY (HIST)

N. V. Tsarevsky, Program Chair

SUNDAY MORNING

Section A

Orange County Convention Center Room W308C

Tutorial & General Papers

N. V. Tsarevsky, Organizer, Presiding

8:20 HIST 1. International places of the periodic table. C.J. Giunta, J.L. Marshall

8:50 HIST 2. Analytical chemistry and the Olympic games: Fighting to catch the cheaters. A.R. Roerdink

9:20 HIST 3. Analysis of plant-derived materials: The early years. N.V. Tsarevsky

9:50 Intermission.

10:00 HIST 4. Rise and fall of melting point: A brief history of once important analytical technique. **V. Dragojlovic**

10:30 HIST 5. William Duane, his radium cow, and the radiation chemistry of water. R.L. Hudson

11:00 HIST 6. Vladimir Vasil'evich Markovnikov: His rule and legacy. D.E. Lewis

11:30 HIST 7. Seeing red: A brief history of red pigments through the ages. E. Bosch

SUNDAY AFTERNOON

Section A

Orange County Convention Center Room W308C

Archaeological Chemistry: Metals & Related Metallic Compounds

M. V. Orna, S. C. Rasmussen, Organizers, Presiding

1:00 Introductory remarks.

1:10 HIST 8. Metals chemistry for the classroom, K-16: A tutorial on low-melting alloys. **A. Rogers**, T. Tieu Ngo, C. Blackwell, W. Arce, C. Baker, M.A. Benvenuto

2:25 HIST 9. Metals of archaeological interest: pedagogical perspectives and possibilities. P.J. Smith, M. Orna

3:10 Intermission.

3:30 HIST 10. Material matter: Exploring ancient pigments in the classroom. **H. Becker**, T. Rutkowski, G. Ersan, V. Imbruce, P. Smart, M.D. Poliks, L. Piper

4:15 HIST 11. Examination of a series of Japanese 100-mon coins by energy dispersive X-ray fluorescence spectrometry. **T. Tieu Ngo**, W. Arce, M.A. Benvenuto

SUNDAY EVENING

Orange County Convention Center Room W308A

5:00 - 7:00 HIST Executive Committee Meeting

MONDAY MORNING

Section A

Orange County Convention Center Room W308C

Archaeological Chemistry: Glasses, Ceramics & Organic Materials

S. C. Rasmussen, Organizer M. V. Orna, Organizer, Presiding

8:05 Introductory Remarks.

8:15 HIST 12. Development of chemical glassware: Evaluating historical narratives via chemical archaeological data. **S.C. Rasmussen**

8:45 HIST 13. XRF investigation on the green lead glass excavated from Wanggung-ri site at Iksan and sarira bottles. **C.H. Do**, G. Kim, B. Yu, J. Song

9:15 HIST 14. WITHDRAWN

9:45 HIST 15. Changes in the body, glaze, and enamel composition of early Meissen porcelain during 1723-ca. 1740. **N. Zumbulyadis**, V. Van Thienen, A. Bezur

10:15 Intermission.

10:30 HIST 16. Analysis of fossilized resin (amber) by carbon-13 nuclear magnetic resonance spectroscopy in solution: A worldwide survey. **J.B. Lambert**, T.A. Contreras, T. Nguyen, J.A. Santiago-Blay

11:00 HIST 17. Metabolomics analysis and its application to biomolecular archaeology of wine. **K. Duffy**, P. van Dommelen, U. Sommer, H. Loney

11:30 HIST 18. Geochemical analysis of ancient and modern soil health in Antigua, West Indies. **A.R. Tricarico**, E.C. Wells

Creating a Common Language for Chemistry: IUPAC's Past, Present & Future Roles

Sponsored by CINF, Cosponsored by HIST

MONDAY AFTERNOON

Section A

Orange County Convention Center Room W308C

Archaeological Chemistry: Color in Archaeology & Pedagogy

M. V. Orna, Organizer S. C. Rasmussen, Organizer, Presiding

1:15 Introductory Remarks.

1:25 HIST 19. Archaeological shades of purple from flora and fauna. Z. Koren

2:10 HIST 20. FTIR spectroscopy and medieval pigments: A long-term love affair. P.L. Lang, H.F. Noneman

2:40 HIST 21. Archaeological blue pigments: Problem children from the get-go. M. V. Orna

3:10 Intermission.

3:25 HIST 22. Color as trace evidence in archaeological materials science and forensic investigations. **I. Kakoulli**

3:55 HIST 23. Discovering hidden layers with X-ray vision: New applications of pXRF to rock art studies. **K.L. Steelman**, V. Roberts, C. Boyd

4:25 HIST 24. Ars pigmentorum: Roman painters and their knowledge of the chemical and physical properties of pigments. **H. Becker**

4:55 HIST 25. At the heart of the madder: Experiments in dye bath chemistry with prehistoric dye plants and alchemical texts. **M.L. LaBerge**

Chemistry in Space: Future Directions

Sponsored by YCC, Cosponsored by AGFD, ANYL, BIOT, BMGT, CHAS, ENVR, FLUO, GEOC, HIST, I&EC, MEDI, POLY and PROF

Creating a Common Language for Chemistry: IUPAC's Past, Present & Future Roles

Sponsored by CINF, Cosponsored by HIST

MONDAY EVENING

Orange County Convention Center West Hall C

Sci-Mix

N. V. Tsarevsky, Organizer

8:00 - 10:00

1-2, 13-14, 17-19, 22, 25. See Previous Listings.

34, 37, 40-41, 43-44, 46-47. See Subsequent Listings.

TUESDAY MORNING

Orange County Convention Center Room W308C

Pioneers of Magnetic Resonance

V. V. Mainz, *Organizer* E. T. Strom, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 HIST 26. Yevgenii Konstantinovich Zavoiskii and the battle for EPR. D.E. Lewis

9:00 HIST 27. Samuel Isaac Weissman: Pioneer of chemical applications of EPR and the way he was. J.R. Norris

Section A

Section A

9:30 HIST 28. George K. Fraenkel: Neglected EPR pioneer. J.H. Freed

10:00 Intermission.

10:15 HIST 29. Harden M. McConnell: The life of a giant in magnetic resonance. L.J. Berliner

10:45 HIST 30. R. Linn Belford: A journey from understanding EPR spectra to multifrequency high field EPR. **A. Smirnov**

11:15 HIST 31. Spin relaxation and the history of EPR. G.R. Eaton, S. Eaton

TUESDAY AFTERNOON

Section A

Orange County Convention Center Room W308C

Pioneers of Magnetic Resonance

E. T. Strom, *Organizer* V. V. Mainz, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 HIST 32. Purcell and Bloch: The discovery and early developments in NMR. V.V. Mainz

1:35 HIST 33. H. S. Gutowsky and the use of NMR in chemistry. H.N. Cheng

2:05 HIST 34. Multi-pronged bite of NMR. P. Laszlo

2:35 HIST 35. Donald E. Woessner: Master of NMR relaxation effects. E.T. Strom

3:05 Intermission.

3:20 HIST 36. John Stewart Waugh and high-resolution NMR in solids. R.G. Griffin

3:50 HIST 37. Sixty years (and counting) of magic-angle spinning for NMR. J.F. Schaefer

4:20 HIST 38. Bid for immortality: A thirty-year race and rivalry between Paul Lauterbur and Raymond Damadian for the invention of MRI. M.A. Meyers, **E.T. Strom**

Section A

Orange County Convention Center Room W308C

Tutorial & General Papers

N. V. Tsarevsky, Organizer, Presiding

8:45 HIST 39. Life of John Lee Comstock: Chemist or plagiarist?. W.P. Palmer

9:15 HIST 40. Gamma Sigma Epsilon: 100 Years of promoting excellence in chemistry. G.R. Boyce

9:45 HIST 41. Vanadium: Chemistry and history. M. Mendoza, I. Villavicencio, C. Hahn

10:15 Intermission.

10:30 HIST 42. Kingsville and uranium: A history of the South Texas uranium belt. C. Hahn, J.T. Medina

11:00 HIST 43. American nuclear chemist: Glenn Seaborg. C. Hahn, D. Rodriguez

11:30 HIST 44. Dorothy Hodgkin: The woman who revolutionized crystallographic investigations. **C. Chi**, **R. Garcia**, C. Hahn

WEDNESDAY AFTERNOON

Section A

Orange County Convention Center Room W308C

Tutorial & General Papers

N. V. Tsarevsky, Organizer, Presiding

12:45 HIST 45. Clendenin, WV: The birth of the petrochemical industry. M.W. Fultz, D. Stone

1:15 HIST 46. Nobel-prize-winning science deniers: Albert Einstein. S. Powell, T.J. Fuhrer

1:45 HIST 47. Nobel-prize-winning science deniers: Paul Dirac. T.J. Fuhrer

ABSTRACTS

HIST 1

International places of the periodic table

Carmen J. Giunta¹, giunta@lemoyne.edu, James L. Marshall². (1) Le Moyne Coll, Syracuse, New York, United States (2) Chemistry, University of North Texas, Denton, Texas, United States

To mark the International Year of the Periodic Table and to illustrate that the table and the elements it houses have been an international enterprise from the start, we have assembled a searchable internet map of locations associated with the periodic table. The map, called Places of the Periodic Table, includes locations where contributors and developers of the periodic table lived or worked, places where elements were discovered, and places associated with the names of elements. The map is built described "Rediscovery largely on places in of the Elements" (http://www.chem.unt.edu/~iimm/REDISCOVERY%207-09-2018/index.htm) and study tour itineraries. Geographical coordinates and addresses are included. Links from the map lead users to further information about the people, places, and events listed.

HIST 2

Analytical chemistry and the Olympic games: Fighting to catch the cheaters

Aaron R. Roerdink, aroerdin@heidelberg.edu. Chemistry and Biochemistry, Heidelberg University, Tiffin, Ohio, United States

Citius, Altius, Fortius (Swifter, Higher, Stronger) is the motto of the modern Olympic Games. The Olympic Charter states the intention of the Games "is to contribute to building a peaceful and better world by educating youth through sport..." Nevertheless, the Olympic Games transformed through the 20th century from their idealized purpose to a platform used by nations to promote their political ideologies. After the fall of the Iron Curtain, it was discovered the successes of athletes from Eastern Bloc countries were fueled by chemical enhancements. In the past twenty years, athletes from all over the globe have continued the practice of enhancing their performances through chemistry as prize money, performance fees, and endorsements have inundated traditionally amateur sports. This project investigates the influence analytical chemistry has had on the Olympic Games. Specifically, the historical development of performance enhancing drugs (PEDs) and the analytical methods used to detect PEDs will be addressed.

HIST 3

Analysis of plant-derived materials: The early years

Nicolay V. Tsarevsky, nvt@smu.edu. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States

Following the discovery of many analytical reactions for the detection and identification of inorganic compounds (e.g., salts present in mineral waters, mineral poisonous substances, etc.) in the 18th and the first half of the 19th century, significant efforts were made to develop qualitative and quantitative analytical methods based on color or precipitation reactions for the detection of complex organic natural compounds such as alkaloids and glycosides. By the early 1880s, several influential monographs dealing with the analysis of plant-derived substances were published, including "Anleitung zur Analyse von Pflanzen" (1858) by Friedrich Rochleder (1819-1874), "Anleitung zur Chemischen Analyse von Pflanzen" (1868) by Georg Christian Wittstein (1810-1887), as well as "Beitraege zur gerichtlichen Chemie" (1872) and especially "Die qualitative und quantitative Analyse von Pflanzen und Pflanzentheilen" (1882) by Johann Georg Noel Dragendorff (1836-1898), in addition to multiple papers dedicated to the subject. These texts introduced important innovations in analytical chemistry that had a major impact on the development of pharmaceutical and forensic science. Some of the most notable discoveries made by the mentioned authors will be described.

HIST 4

Rise and fall of melting point: A brief history of once important analytical technique

Veljko Dragojlovic, vdragojl@fau.edu. Florida Atlantic University, Jupiter, Florida, United States

Throughout XIX and the first half of XX century, melting point was developed into a powerful method for characterization and identification of organic compounds. It was also the time when individual researchers could design and make their own instruments and a great deal of effort was devoted to that end. However, to a modern organic chemist, this once an indispensable method, is an afterthought to a point that it is now customarily reported as "uncorrected."

HIST 5

William Duane, his radium cow, and the radiation chemistry of water

Reggie L. Hudson, reggie.hudson@nasa.gov. Code 691, NASA Goddard Space Flight Center, Greenbelt, Maryland, United States

The name William Duane (1872 - 1935) probably is unknown to most chemists. However, Duane's career is a fascinating study as it covers pioneering studies of atomic structure and radiation effects in the US and Europe. In this ACS presentation, the speaker will describe Duane's early work with Walther Nernst in Germany and with Pierre and Marie Curie in Paris. Duane's extensive study of the radiation chemistry of water in the solid, liquid, and gaseous forms will be highlighted, work that remains important for the speaker's NASA research. In addition, Duane's work in the field of radiology will be

described along with the so-called "radium cow" he introduced to Boston and the "milk" it provided to cancer patients.

HIST 6

Vladimir Vasil'evich Markovnikov: His rule and legacy

David E. Lewis, lewisd@uwec.edu. Chemistry Department, UW-Eau Claire, Eau Claire, Wisconsin, United States

Vladimir Vasil'evich Markovnikov (1838-1904) is best remembered for his empirical rule for addition reactions of unsymmetrical electrophiles to unsymmetrical alkenes (1869), which celebrates its sesquicentennial this year. This rule arose from his doctoral dissertation work, but his contributions are far more than just this one (albeit major) contribution to organic chemistry. Following his time as Professor at Kazan University, Markovnikov went on to build the Organic Chemistry Departments at Novorossiisk University in Odessa (now in the Ukraine), and Moscow. In Moscow, he also moved his research emphasis away from theoretical aspects of organic chemistry, and became one of the pioneers in petroleum chemistry in Russia. In Moscow, also, he mentored some of the brightest members of the next generation of Russian students: organic chemists Nikolai Matveevich Kizhner (1897-1935), Nikolai Yakovlevich Dem'yanov (1861-1937) and Aleksei Yevgen'evich Chichibabin (1871-1945), and an important pioneer of physical chemistry in Russia, Ivan Alexeevich Kablukov (1857-1942). This talk will focus on Markovnikov's Rule and the Moscow era of the career of this great organic chemist.

HIST 7

Seeing red: A brief history of red pigments through the ages

Eric Bosch, ericbosch@missouristate.edu. Chemistry, Missouri State University, Springfield, Missouri, United States

Minerals such as hematite and cinnabar provided natural sources of the red inorganic pigments red ochre and vermillion while plant and insect extracts including madder and cochineal provided dyes that on complexation with aluminum and/or calcium cations provided the red pigments rose madder lake and carmine lake. Early inorganic synthetic methods yielded red lead and vermillion while later inorganic syntheses provided reds including cadmium red that was patented in 1919. Some highlights of the synthesis of organic pigments include alizarin first synthesized in 1869, quinacridone red, perylene maroon and the chance discovery of red diketopyrrolopyrroles in 1974.

HIST 8

Metals chemistry for the classroom, K-16: A tutorial on low-melting alloys

Alexandria Rogers, rogersal@udmercy.edu, Tiffany Tieu Ngo, Clayton Blackwell, William Arce, Charles Baker, Mark A. Benvenuto. Department of Chemistry and Biochemistry, University of Detroit Mercy, Detroit, Michigan, United States

In conjunction with the 2019 National Chemistry week theme "Marvelous Metals," this tutorial will present several ways in which teachers and professors can incorporate metals chemistry in their classrooms. The presentation will include how to safely use several low melting alloys in the classroom, an understanding of alloys and mixtures, how intermolecular forces work, and phase changes. The presentation will also highlight an area where science and art meet – the production of art medals from low melting metals and alloys, and from easy-to-carve forms and materials.

HIST 9

Metals of archaeological interest: pedagogical perspectives and possibilities

Patricia J. Smith², **Mary Virginia Orna**¹, maryvirginiaorna@gmail.com. (1) Chemistry, The College of New Rochelle, New Rochelle, New York, United States (2) ChemSource, Inc., New Rochelle, New York, United States

Two major archaeological eras take their names from metals: the Bronze Age and the Iron Age. Bronze, an alloy of copper and tin (and often smaller amounts of other materials), enjoyed widespread use from the third millennium BCE onwards due to its greater hardness with respect to pure copper or any other hard materials of the time such as ceramics or gold. Weapons, tools, armor, and decorative and building materials made of bronze were therefore more durable and useful than any previously known material. Bronze artifacts also seem to have been used as valuable materials of trade. Its widespread use was only superseded in the 1300s BCE by iron, ushering in the Iron Age, a technological paradigm shift marked by the widespread production of carbon steel, enabling the manufacture of artifacts superior to those made of bronze. This paper will review the history of bronze, iron and other metals in archaeological terms, and then suggest how students can become acquainted with these historic metals via simple activities that will highlight their properties.

HIST 10

Material matter: Exploring ancient pigments in the classroom

*Hilary Becker*¹, hbecker@binghamton.edu, Todd Rutkowski³, Gökhan Ersan², Valerie Imbruce⁴, Pamela Smart⁵, Mark D. Poliks⁶, Louis Piper⁷. (1) Classical and Near Eastern Studies, Binghamton University, Binghamton, New York, United States (2) Department of Art and Design, Binghamton University, Binghamton, New York, United States (3) Department of Physics, Radford University, Radford, Virginia, United States (4) Offie of External Scholarships, Fellowships and Awards, Binghamton University, Binghamton, New York, United States (5) Art History, Binghamton University, Binghamton, New York, United States (6) Binghamton University, Vestal, New York, United States (7)

Department of Physics, Applied Physics and Astronomy, Binghamton University, Binghamton, New York, United States

Materials Matter, a new course at Binghamton University, draws chemistry and physics into conversation with archaeology, art history, and the history of science through an interdisciplinary focus on a particular class of materials-pigments. In its first iteration, co-taught by an archaeologist and a physicist, instruction focused upon all aspects of pigments, considering why pigments have color, their atomic bonding, ancient prices of pigments, and even how innovations in pigments influenced other industries, etc. Class sessions stress humanities research methodologies alongside the quantitative and experimental methods of STEM fields, offering students insights into the process and modes of research early in their college career. Students made frescoes themselves to understand the chemical processes behind the creation of art, and made acrylic paints, while varying different additives, to understand the significance of each ingredient in the process. Students also learned how materials may be studied with experimental techniques such as x-ray fluorescence, x-ray diffraction, multispectral imaging, and electron microscopy, by analyzing pigments and artworks in Binghamton University's Art Museum and in the Analytical and Diagnostics Laboratory. This paper will also highlight the work of the graphic designer who has been involved in planning this course from its inception. His work for Materials Matter is driven by the overarching goal of communicating complex chemical processes by utilizing an integrative visual language. To this end, a graphical framework have been designed to bring into view all aspects of this course in a scalar manner, from the atomic level to the socio-cultural level, so that students can visually map the entire humanistic-scientific domain of one material as we focus upon it different ways. An interactive student app was developed that integrates the various elements of this course using a scalar framework, in order to supplement lecture material and to provide interactive lab assignments.

HIST 11

Examination of a series of Japanese 100-mon coins by energy dispersive X-ray fluorescence spectrometry

Tiffany Tieu Ngo, tieungti @udmercy.edu, William Arce, Mark A. Benvenuto. Department of Chemistry and Biochemistry, University of Detroit Mercy, Detroit, Michigan, United States

A series of Japanese 100 mon coins, from the 1800's, were examined via EDXRF to determine their elemental composition. While bought and sold on the rare coins and antiquities markets today as "brass" or "bronze" coins, they are more complex than just a binary alloy. Elemental findings, including trace element presences, will be presented and discussed.

HIST 12

Development of chemical glassware: Evaluating historical narratives via chemical archaeological data

Seth C. Rasmussen, seth.rasmussen@ndsu.edu. Department of Chemistry and Biochemistry, North Dakota State University, Fargo, North Dakota, United States

Although the use of glass in the fabrication of chemical apparatus is thought to date to at least the first century CE, its use was highly limited due to the low chemical and thermal stability of early soda-lime glass. This changed in the 13th century, when the prospering Venetian glass industry developed a significantly improved glass that allowed its widespread use in chemical apparatus. Glass thus began to replace the more common pottery and copper-based components, resulting in the early development of chemical glassware. The widespread and common use of chemical glassware consistent with the modern view of chemical research is thought have occurred in the early 19th century. By this time period, much of this glassware was fabricated from Bohemian glass, which has led historians to view this as the most suitable glass for chemical glassware. Using various published chemical archaeological data of glass artifacts, the chemical composition of pre- and post-Venetian glass, as well as Bohemian glass, will be compared in order to evaluate their expected chemical and physical properties and thus their respective suitability for chemical glassware. Such an analysis should allow the ability to either more strongly support current historical narratives based on the properties of the respective glasses, or re-evaluate other factors that may have resulted in the shift of Venetian to Bohemian glass for chemical glassware.

HIST 13

XRF investigation on the green lead glass excavated from Wanggung-ri site at Iksan and sarira bottles

Choon H. Do¹, choondo@sunchon.ac.kr, Gyoho Kim², Byung-Yong Yu³, Jonghan Song³. (1) Korean Chemical Industry Specialists Association, Uljin-gun, Gyeong-buk, Korea (the Republic of) (2) Department of Conservation Science for Cultural Properties, Kongju National University, Gongju, Chungnam, Korea (the Republic of) (3) Accelator Lab., Advanced Analysis Center, Korea Institute of Science and Technology, Seoul, Korea (the Republic of)

Many crucibles for glass, bronze and gold production among others were also excavated from the Wanggung-ri site, Iksan for last 20 years. This site has been known as an important workshop site in the 7th century during Baekje or unified Silla period in Korea. Green glassy parts attached to the inside walls of the crucibles were analyzed by XRF. The average composition of the glassy parts were SiO_2 74.7% and PbO 20.7% for weathered samples and 64.4% and 32.5% for no-weathered samples, respectively. Iron, aluminum, copper were also presented as minor components. The XRF results indicated that the lead glass were produced using these crucibles. Other implication of this green glass production may be related to the production of green glass bottles storing sarira, produced during the unified Silla period. The crucibles excavated were also investigated by XRF and microscopy and characterized.

HIST 14

WITHDRAWN

HIST 15

Changes in the body, glaze, and enamel composition of early Meissen porcelain during 1723ca. 1740

Nicholas Zumbulyadis¹, nickz@frontiernet.net, Vince Van Thienen², Aniko Bezur³. (1) Independent Scholar, Rochester, New York, United States (2) Department of Archaeology, Ghent University, Gent, Belgium (3) IPCH, Yale University, West Haven, Connecticut, United States

During the two decades following Böttger's death in 1719, the Meissen Manufactory underwent rapid changes in technology, raw material sources and experimented with various body, glaze and colorant formulations. These rapid changes offer the opportunity for dating objects and reconstructing the evolution of European porcelain using archaeometric techniques. We will report results on the evolution of early Meissen body, glaze, and colorant composition using XRF measurements on three artifacts that are narrowly and reliably dated covering the period between 1723 and ca.1740. Changes in certain minor elements (e.g. Ti, Ba) mirroring the geochemistry of the Erzgebirge region can serve as markers for technological changes during this time. The time line of these compositional changes is interpreted based on an analysis of recipes recorded in the earliest documents of the Meissen Historical Archives. A brief overview of the earliest Meissen archival material will also be given.

HIST 16

Analysis of fossilized resin (amber) by carbon-13 nuclear magnetic resonance spectroscopy in solution: A worldwide survey

Joseph B. Lambert¹, jlambert@trinity.edu, Tayde A. Contreras¹, Truongan Nguyen¹, Jorge A. Santiago-Blay². (1) Dept of Chemistry, Trinity University, San Antonio, Texas, United States (2) Department of Paleobiology, National Museum of Natural History, Washington, District of Columbia, United States

Amber, or fossilized plant resin, has most commonly been used as jewelry and as a source for preserved organisms throughout history. More recently, structural analysis of amber and copal (less mature amber) has gained importance in archaeological and botanical research. Nuclear magnetic resonance (NMR) spectroscopy has been the most successful technique in classifying ambers into different categories based on their structure without altering their chemical makeup. More specifically, solid-state carbon-13 NMR spectroscopy has served as an important technique to categorize amber and copal into five main groups corresponding to their geographic location of origin. Solution-state carbon-13 NMR analysis, which provides more distinct peaks than solid-state NMR spectroscopy, has not previously been used for structural analysis of amber. In this study, 12 amber and copal samples soluble in deuterated chloroform (CDCl₃) were used to determine distinctive structural characteristics for Groups A, B, D, and E. Group C was omitted from this study due to the inability to acquire quality spectra. While solution-state carbon-13 NMR analysis of the 12 amber and copal samples in this study confirmed the existence of specific structural trends that characterize Groups A, B, D, and E, this study

also revealed that there is more spectral variation within each group than apparent from solid-state studies.

HIST 17

Metabolomics analysis and its application to biomolecular archaeology of wine

Kate Duffy¹, cathleenireneduffy@yahoo.com, Peter van Dommelen², Ulf Sommer⁴, Helen Loney³. (1) Scientific Research, Conservation Division, Philadelphia Museum of Art, Philadelphia, Pennsylvania, United States (2) The Joukowsky Institute for Archaeology and the Ancient World, Brown University, Providence, Rhode Island, United States (3) Institute of Science & the Environment, University of Worcester, Worcester, United Kingdom (4) School of Bio-sciences, University of Birmingham, Birmingham, United Kingdom

The grape is arguably the oldest cultivated product in human history and the analysis of its main product, wine, reveals clues to trade and associations in ancient times. Wine was stored in pottery vessels, which if not properly sealed with resin, wicked into clay matrices, polymerizing over time. Researchers have attempted to capitalize on these polymerized compounds by pulverizing and extracting clay sherds before applying analytical instrumentation to the identification of the wine remnants. Two main biomarkers have been employed for the identification of wine residue: tartaric and syringic acids. In order to further mine possible biomarkers for complex archaeological pieces, a metabolomics approach was applied to the analysis of modern day wine and to archaeological samples. Metabolomics, a robust methodology utilized in molecular biology and environmental toxicology, identifies the small molecules that "fingerprint" an originating chemical event. For the first time an untargeted metabolic profiling approach, using high resolution mass spectrometry and multivariate statistical analyses, was applied to wine archaeology to discover and validate novel multi-biomarker signatures of wine. The first objective was to discover a metabolic aging plateau for the chemical compositions of red and white wines, which was achieved by aging liquid samples in a laboratory at 40°C and analyzing the samples using a rapid and non-biased direct infusion mass spectrometry metabolomics approach. Upon determining that the chemical compositions stabilized by six months, a second aging experiment was conducted using model pottery sherds doped with water, white or red wine, with the aim of the analytical and statistical analyses to discover multi-biomarker signatures that indicate the presence of wine in general. Next, these biomarker signatures were translated from a metabolomics discovery platform to a high sensitivity and specificity platform. Finally, the novel multibiomarker signature was validated by analyzing archaeological samples of known context.

HIST 18

Geochemical analysis of ancient and modern soil health in Antigua, West Indies

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The commodification of sugar during the 17th and 18th centuries transformed the livelihoods of individuals across the globe while simultaneously reshaping the ecology of the entire Caribbean region. In Antigua, West Indies these past ecological modifications have directly contributed to increased vulnerability of contemporary populations to climate-driven events. As such, the actions of pre-

Columbian and historic period inhabitants are intertwined with contemporary socio-ecological systems. This research utilizes archaeological chemistry to inform our understanding of the relationship between historic land management practices and contemporary soil health. We analyze two markers of past anthropic activity, soil quality and landscape stability, across three regions (Ayer's Creek Basin, Mercer's Creek Basin, and Indian Creek Basin) in eastern Antigua. Prior archaeological research near Ayer's Creek and Mercer's Creek has revealed a long-term, continuous sequence of occupation dating back 2,000 years suggesting that contemporary environmental health may be the legacy of both past land management practices and the cessation of sugarcane monoculture in 1981. However, it is unknown to what extent historical land use and its interactions with local geology account for these changes. This research integrates archaeological survey, semi-structured interviews, and archival research to inform a behavioral geoarchaeological approach to understanding dynamic, coupled natural-human systems in Antigua, West Indies.

HIST 19

Archaeological shades of purple from flora and fauna

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An incredibly colorful picture emerges from the Ancient Near East that reveals how the dyer and weaver succeeded in creating variegated shades of purple - from bluish to reddish. For the rich, powerful, and priestly, the most eminent purples were produced from *Muricidae* sea snails. The main molluskan species used for such colors was Hexaplex trunculus, with some of these species producing reddishpurple pigments and such colored woolen dyeings, while another variety of the same species produced bluish-purple pigments and dyeings. The use of the other purple-producing Mediterranean mollusks was probably as "color additives" to the *H. trunculus* species in order to produce even redder purple dyeings. For the more common folk who desired purple embellishments on their garments, the most common method of producing such purple colors - the "popular people's purple" - was by combining different dyes. A cornucopia of purple shades were produced from the well-known red-madder and blue-indigo double-dyeing method. However, other surprising chemical and physical combinations have also been observed. Why some combinations were performed to produce the final color is still confounding, and the finding of certain blends is startling. Entomological sources (Ararat cochineal and Kermes insects) were also combined with flora dyestuffs and, strangely enough, even with some molluskan species. These ancient artifacts, with a plethora of purples, span several millennia, and were excavated in various geographical regions that include today's Egypt, Israel, Iran, and Russia. These colorful items, discovered by the presenter via chromatographic (HPLC) and spectrometric (UV/Vis) analyses, will be discussed in the talk.

HIST 20

FTIR spectroscopy and medieval pigments: A long-term love affair

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We review the use of FTIR spectroscopy for the identification of medieval pigments and associated paint materials including additives, media, and grounds. The review will attempt to catalog the most common types of medieval pigments identified by FTIR, along with a description of the nature of the artwork examined (manuscript, fresco, painting, etc.), the sampling methods used (pellet, microscopic fragment, cross-section, etc.), FTIR technique(s) used, and any complementary analytical techniques used. In doing so, we reflect on the overall successes and challenges of the use of FTIR analysis for medieval pigment identification with the aim of providing a comprehensive resource to the art analyst.

HIST 21

Archaeological blue pigments: Problem children from the get-go

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Interest in synthetic blue pigments dates back to the dawn of history. Blue is the oldest known color to be synthesized as a pigment, having been found as a glass frit called Egyptian Blue in Egyptian mural paintings at least 3,000 years old and, as more recent research reveals, in Greek Bronze Age pigments from Knossos dating back to 3,000 BCE. Yet for all this interest, blue is the color that has proved to be the most difficult in developing a durable palette from both natural and synthetic sources. The natural sources, for the most part minerals containing either a sulfur-based chromophore or copper, and the evanescent indigo, were unsatisfactory due to scarcity, expense, and/or instability. Synthetic blues, with the exception of Egyptian Blue, proved to be even more unstable. A surprisingly stable blue from the Maya empire contained an equally surprising chromophore. This paper will document the evolution of blue and its use, and how a gradually increasing understanding of the nature of blue eventually led to other surprising advances in civilization.

HIST 22

Color as trace evidence in archaeological materials science and forensic investigations

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Archaeological monuments and objects, the material remains of our human past, are limited and irreplaceable cultural resources that are under imminent threats from environmentally-linked effects, political conflicts, and looting. As with modern materials, their archaeological counterparts are produced through processes by which raw materials are carefully selected, processed, and transformed into cultural products. In this context, this research examines three of the oldest artificially produced

pigments employed in the decoration of important polychrome monuments and artifacts for over four millennia, Egyptian blue, a sintered polycrystalline compound (frit); madder lake, an organic-inorganic composite and verdigris, a copper acetate, and its organo-metallic complexes. Focusing on Classical antiquity (~400 BC and ~AD 400), from an archaeological perspective, the objective of this research is twofold: first, to explore the structure–property relationships of these pigments and how these relate to the raw materials and operational sequences involved in their manufacture and second, to investigate the meaning, function and use of these coloring compounds in Classical polychromy, alchemy and other chemical arts of the period such as pharmacopeia, wine and perfume making, cosmetics and dyeing. From a materials science perspective, it interrogates the photophysical and chemical properties of these pigments as fingerprint markers for authentication, classification, dating and attribution.



Diffuse light image (a,d) of an Italian 3rd century BC Canosa vase (81.AE.157) from the J. Paul Getty collection and visible-induced NIR and Vis luminescence images showing photon emissions characteristic of Egyptian blue (b) and madder lake (c). The distribution of Egyptian blue and madder lake on the Canosa vase is illustrated in the false-color images c and f respectively.

HIST 23

Discovering hidden layers with X-ray vision: New applications of pXRF to rock art studies

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Exploring new applications of portable X-ray fluorescence spectroscopy to the study of rock art, we report the determination of paint layer stratigraphy based upon measured elemental levels. In Lower Pecos rock art, we were able to discern when red and yellow paints superimpose black paints based on elevated levels of manganese. This ability to see underneath paint layers with "X-ray vision" shows great promise in answering stratigraphic ambiguities, complimenting digital microscopy conducted in

the field. In addition, we collected Munsell color designations for each pXRF analysis location so that we could compare major elemental levels with pigment color and value. We were also able to confirm suspected gunshot damage at a rock art site. These results highlight the advantages of this non-destructive technique.

HIST 24

Ars pigmentorum: Roman painters and their knowledge of the chemical and physical properties of pigments

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The material remains of pigments allow us to have new insight into the choices made in the production of wall paintings, as well as the knowledge that Roman painters had about the pigments that they used. Indeed, Roman painters had incredible knowledge about the chemical and physical properties of pigments. This knowledge base can be explored in three ways. First, there were fraudulent pigments on the market; savvy pigment buyers could learn tips so that they could spot adulterated or fraudulent pigments. These consumer tests relied upon chemical reactions, sensory tests, and even the specific gravity of objects. Using these tests, consumers could be critical of products at the market place and buy better quality materials. Secondly, finds of pigments in pigment shops and workshops in Pompeii and Rome demonstrate that some artists potentially had a range of pigments from which to choose. But artists did not use these pigments indiscriminately, as some pigments were avoided. This is because, as textual evidence indicates, the Romans knew that some pigments were incompatible with the alkalinity of Roman frescoes. Finally, the fact that Roman artists had a refined knowledge of pigments can be demonstrated by looking at how these artists used pigments. At Aventicum (Switzerland), five different white pigments were used in the same room—but all of them in discretely different ways. This, paired with other examples, speaks to a knowledge of the physical properties of pigments (luminosity, mixability, coverage, etc.) that was scrupulously followed.

HIST 25

At the heart of the madder: Experiments in dye bath chemistry with prehistoric dye plants and alchemical texts

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In recent years, an interest in natural botanical dye sources has prompted new research into the cultivation and processing of prehistoric dye plants in Europe and the Near East. Advances in chemical analyses of ancient European textiles have provided more detailed information about dye plants, which were important sources of color in early textile production. Evidence of dye from domesticated madder root (*Rubia tinctorum*) has been reported in the archaeological record of the European Bronze and Iron Ages in textiles preserved in salt mines, bog sites and elite European burials but the picture of madder usage from the Late Bronze Age into the medieval era is still unclear. The use of other indigenous plants related to madder also complicates this picture. A critical review of the history of research on madder and the evidence for its use in archaeological contexts in Europe, along with an experimental

component of the thesis involved growing madder and using madder root as a dye has suggested new paths of research, and "ground-truthed" older data. The preliminary results may shed some light on the distribution of madder through the Iron Age, and may speak to the significance of the color red in European prehistory.

HIST 26

Yevgenii Konstantinovich Zavoiskii and the battle for EPR

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Yevgenii Konstantinovich Zavoiskii (1907-1976) was the first individual to observe the epr signal from a paramagnetic species (in 1944). He reported his discovery to the Lebedev Physics Institute of the USSR Academy of Sciences (FIAN) in Moscow. Instead of finding his discovery hailed as an important advance in the physics of electromagnetic radiation and solids, Zavoiskii was dealt the severe blow of his work being disbelieved by the senior physicists there. It was only at the urging of Pyotr Leonidovich Kapitsa (1894-1984), who suggested that the older physicists may have doubted his results because they did not understand the underlying physics (even Kapitsa himself, a later Nobel laureate, was skeptical), that Zavoiskii built an entirely new instrument in Moscow and demonstrated in person that it did, in fact, work. In this talk, I propose to introduce Zavoiskii, the scientist, and to trace his battle with the older generation of physicists to get his discovery acknowledged as the breakthrough that it was.

HIST 27

Samuel Isaac Weissman: Pioneer of chemical applications of EPR and the way he was

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Samuel Isaac Weissman obtained a PhD (1938) in physical chemistry from the University of Chicago. In 1941 he left Chicago to explore optical properties of rare earths with G. N. Lewis at the University of California, Berkeley. During WWII, Weissman moved to Los Alamos to join the Manhattan Project, the development of the first atomic bomb. Moonlighting, Weissman and colleague David Lipkin were the first to show that phosphorescence from an aromatic molecule was pure dipole radiation from a triplet state. In 1946 Weissman moved to the chemistry department of Washington University, St. Louis and in 1955 became a full professor. There Weissman's interest in EPR became his primary focus. In 1952 Weissman, Pake and Townsend reported the first EPR observation of hyperfine lines. In 1953 Weissman and colleagues Lipkin, Townsend and Paul investigated the chemistry of the anions of aromatic molecules with one unpaired electron and showed that the unpaired electron is distributed over the entire aromatic "free radical". Three years later he and Harden McConnell independently published a quantum mechanical interpretation of the isotopic hyperfine constants of π -radicals, providing detailed information on molecular structure. Beginning in 1957 Weissman exploited spectral line broadening to measure electron and atom transfer exchange reaction rate constants between a free radical and its diamagnetic precursor. In another classical contribution to EPR in 1958, Weissman recognized the significance of the electron dipolar interaction for the observation of triplet EPR spectra. Around 1975, Weissman pioneered the development and application of transient nutation EPR where

the time evolution of the transverse electron spin magnetization is detected in the presence of a weak microwave magnetic field. Beginning in 1995, Weissman and colleagues pioneered the development of pulsed zero-field/low-field EPR combined with fast-field switching to study photoexcited triplet states in molecular crystals. Although Weissman became an emeritus professor in 1980, he remained very active in science and was in the department on most days in discussions with colleagues and students. Collaborations with Professor T. Lin and Dr. David Sloop continued until his death in 2007. To more fully appreciate the man whose career was distinguished by his brilliance in understanding and explaining nature at a fundamental level, examples of his quick and irreverent humor will also be presented.

HIST 28

George K. Fraenkel: Neglected EPR pioneer

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George K. Fraenkel may not be immediately recognizable to chemists but he should be-a towering pioneer in the development and use of ESR techniques to explore the fundamental structure of molecules and their dynamical interactions, he was one of the first chemists in this field. In the 1950s and 1960s he and his students developed unique high-sensitivity, high-resolution spectrometers that allowed them to be the first to detect the ESR spectra of free radicals of guinones, of free radicals in molten sulfur, and of thermochromic compounds. He became a leader in ESR focusing on the electronic structure of aromatic anion radicals in solution, via proton, ¹⁴N, and ¹³C hyperfine splitting, and of their spin relaxation both by linewidth/line-shape analysis (e.g., T₂) and saturation behavior (e.g., T₁). radical anions could readily be generated by electrochemical methods. Numerous George's extensive and varied career went well beyond chemistry beginning in World War II, when he was lead person for developing equipment to measure the explosive power of bombs. In 1965 he became chair of Columbia's Chemistry department, and three years later dean of their Graduate School. While he had hoped to split his time between the deanship and his lab, he immediately found himself confronting the major student unrest against the Vietnam War, and reluctantly ceased all research activities until he finally returned to the Chemistry department for the last five years of his professional life. However, the EPR methods he developed have been applied to many areas of research in physics, biology, and medicine; as one example, modern structural and dynamical studies of proteins implicated in such diseases as ALS, Alzheimer's, and Parkinson's are direct descendants of the work George pioneered. And since 2014, his memory has been honored by the George K. Fraenkel Fund Award for young physical chemists.

HIST 29

Harden M. McConnell: The life of a giant in magnetic resonance

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Harden Marsden McConnell passed away October 8, 2014 after a struggle with cancer. This account attempts to briefly cover his life history and some of his major contributions to magnetic resonance and

EPR from the author who was a PhD student as well as a participant and observer in several of the major developments that he contributed to science and the world. His research contributions to magnetic resonance, especially electron spin resonance, were seminal and have impacted physics, chemical physics, biochemistry and immunology to list only a few fields. He was a great mentor, friend and human being.

HIST 30

R. Linn Belford: A journey from understanding EPR spectra to multifrequency high field EPR

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Lifelong scientific journey of Linn Belford had started with undergraduate research at University of Illinois. It did not involve magnetic resonance but rather ¹³C kinetic isotope effects. From Urbana Linn moved to Berkeley for PhD studies of electronic structure of metal chelates under direction of the future Nobel Laureate Melvin Calvin. It is there at Berkeley Linn came across EPR for the first time. Together with his wife Geneva Belford, a Berkeley graduate, he took another long journey - a road trip back to Urbana to join the faculty at the age of only 23. Linn continued his studies of metal complexes and this naturally brought him back to EPR. While early day EPR instrumentation was rather cumbersome, interpretation of complex spectra was even more challenging. Before 1970s Linn already made seminal contributions towards EPR spectra analysis. One of the studies of copper complexes resulted in a wellknown HOB model because it was authored by Hitchman, Olson and Belford. In 1973 Linn outlined an elegant eigenfield approach for calculating EPR spectra of high spin systems. Linn was one of the first to recognize that changing magnetic field would be particularly advantageous for EPR. From 1985 Linn was co-directing Illinois EPR Research Center where the world's first S-band (2 to 4 GHz) pulsed EPR has been built and many key components of new W-band (95 GHz) EPR have been developed. This was the first national EPR facility offering an unprecedented capability to vary resonant magnetic field over two orders in magnitude. Linn Belford passed away in 2015 after being an active faculty for 50 years. However, his long scientific journey from the theory of coupled spin systems to new EPR instrumentation still continues through the work of his students and the evolution of scientific ideas he was the first to conceive.

HIST 31

Spin relaxation and the history of EPR

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Attempts to understand electron spin relaxation began long before the observation of the EPR phenomenon, and even before the recognition of electron spin. Since the magnetization, M, is proportional to the magnetic field, B, early studies asked 'how does M change when B changes', which is inherently a study of the mechanism of magnetic relaxation. The original focus was on magnetic properties of bulk solid samples, but EPR made it possible to study small numbers of discrete spins. In parallel with the work on magnetism of solids, there were attempts to understand electronic spectra of gas-phase species, such as the H atom. This work led to the idea that magnetic relaxation involved

transitions between quantized electron spin energy levels. Most advances in EPR technology have been based on the current models of spin relaxation, and facilitated further understanding. Now, we have three regimes of EPR, continuous wave, rapid scan, and pulse. Each method drives, and is driven by, our understanding of spin relaxation. Each of the more than 100 EPR experiment types exploit understanding of spin relaxation. Much has been learned and applied, but there are vast vistas beyond our current ability to see.

HIST 32

Purcell and Bloch: The discovery and early developments in NMR

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In 1946, two groups published landmark papers in the *Physical Review*. E. M. Purcell, H. C. Torrey, and R. V. Pound's "Resonance Absorption by Nuclear Magnetic Moments in a Solid," submitted December 24, 1945, and F. Bloch, W. W. Hansen , and M. Packard's "Nuclear Induction," submitted on January 29, 1946. In 1952, Felix Bloch (1905-1983) and Edward Mills Purcell (1912-1997) shared the 1952 Nobel Prize in Physics "for their development of new methods for nuclear magnetic precision measurements and discoveries in connection therewith." This paper will give a short discussion of the lives and scientific accomplishments of Bloch and Purcell and how one discovery founded a field (nuclear magnetic resonance) widely used to study the molecular structure of pure materials, the composition of mixtures, reaction mechanisms, and the human body.

HIST 33

H. S. Gutowsky and the use of NMR in chemistry

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Herbert S. Gutowsky (1919 - 2000) was an eminent scientist, a pioneer in NMR, and a professor (and former head of chemistry department) at the University of Illinois, Urbana-Champaign. He was the first to apply NMR to the field of chemistry. His work helped to make NMR one of the most useful techniques for the analysis of molecular structure and dynamics in liquids, solids, and gases. Examples of the from important contributions his laboratory include: 1) 1948-50. Gutowsky and Pake pioneered the use of NMR to study structure and motion in solids. This work continued in his lab all through the 1970s. 2) 1950-52. He was among the first to determine the origin of chemical shifts, a basic concept for NMR determination. structure 3) 1951-54. He was the first to discover spin-spin coupling in molecular liquids and its implications for molecular the study of structure. 4) 1951-56. He and his team developed the NMR methodologies to study chemical exchange and conformational change in molecules. This work continued in his lab at least until the mid-1970s. 5) 1961-63. He and his coworkers discovered spin rotation relaxation, one of the major relaxation mechanisms in molecular motion. He was active in research until his retirement in 1990. Later In his career, he used NMR to study

complex biological systems and pulsed microwave spectroscopy to study the rotational spectra of weakly bound molecules in the gas phase. The speaker was fortunate to obtain his PhD with Gutowsky, with whom he published four papers. In this talk, the speaker will give a review of Gutowsky's pioneering work and his personal recollections of the exciting research times at Illinois.

HIST 34

Multi-pronged bite of NMR

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Where a sociologist studies the routines, an historian goes for the innovative breaks. While it is true that the vast majority of nmr spectra map out molecular structure, the genuine input of nmr in chemistry was providing other types of information. Dynamic, first and foremost: rate processes in fluxional molecules and coordination complexes; molecular tumbling in fluids; real-time acquisition of internal rotations and atomic inversions, processes of displacements and encapsulations, etc etc. In other words, the field was driven by its inner push forward, much more than from user demand, however strong. This is validated from the instrumental viewpoint: a manufacturer such as Varian Associates making an effort at educating its users; the monthly Newsletter communicating brand-new methodologies; and even some chemists, such as Frank Anet, devising their own instruments. The talk will draw on examples, such as establishing the structure of PF_5 as a trigonal bipyramid, subject to a fluxional process. The very term fluxionality indeed came into the lexicon from the NMR of bullvalene.

HIST 35

Donald E. Woessner: Master of NMR relaxation effects

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Donald E. Woessner received his Ph.D. from Illinois in 1957 with mentor Herb Gutowsky. At Illinois he built the very first pulsed nmr spectrometer ever in a US chemistry department. With the Gutowsky group he published nine papers, setting a record that lasted for 30 years. In 1958 he joined the radiofrequency spectroscopy group at the Dallas Field Research Lab of Mobil R&D Corp. The group had home-built pulsed nmr equipment many years before such instrumentation was commercially available. In the 1958 to early 1970s time period, Woessner carried out important fundamental research on nmr, plus continuing research on the applied uses of nmr in oil production and exploration. In 1962 he published his derivation of what are now known as the Woessner equations, which make it possible to calculate energy barriers for an expanded range of molecular motions. He provided the mathematical framework for isolating methyl rotation from overall motion in certain cases. Woessner retired from Mobil in 1992. He then became an adjunct professor in the Advanced Imaging Research Center at the University of Texas Southwestern Medical School, where he continued to publish important nmr research. He suffered a severe stroke in 2008 nd died from its after effects a few months later. He was one of the rare industrial chemists to win the ACS Southwestern Regional Award, which he received in 1991. His impact on nmr is best summarized by this tribute from Nobel Laureate Paul Lauterbur. "Anyone seriously interested in nmr relaxation phenomena must be familiar with his papers, and he is universally respected in his field. Others have published more papers, been invited to more international congresses, won more awards, and in general been more visible on the scientific scene, but Don has done what many of us often wish we had done; he has just kept producing solid, useful, insightful science."

HIST 36

John Stewart Waugh and high-resolution NMR in solids

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High-resolution solid state NMR experiments first came to fruition in John Waugh's lab in 1968, and involved multiple pulse experiments for homonuclear decoupling, as exemplified by the famous WAHUHA four pulse method. Concurrently, theoretical methods to treat these cyclic, time dependent experiments lead to the development of average Hamiltonian theory (AHT). Today, 50 years after its inception AHT remains the preeminent theoretical approach to understanding time domain NMR. In addition, these initial efforts nucleated investigations of heteronuclear decoupling and of elegant interactions methods to refocus dipolar in solids, the magic echo. In a second set of pioneering papers, Waugh and his students, Alex Pines and Michael Gibby, described double resonance experiments for observation of dilute spins such as ¹³C and ¹⁵N. These dilute spin species were thought to have long T₁'s, so it was proposed to circumvent this problem by cross-polarization (CP) methods introduced originally by Hartmann and Hahn. The addition of continuous wave ¹H decoupling removed the dipolar broadening from the attached ¹H's. An additional benefit of this approach was that it enhanced the polarization of the dilute spins. Subsequently, Schaefer and Stejskal combined CP with magic angle spinning (MAS) to yield the CPMAS method which is the approach that is used universally today to observe many species of dilute spins. The NMR spectrometers that were in use in the late 60's and early 70's were single frequency resonance instruments that produced one or two pulses and were therefore not capable of performing the sophisticated experiments developed by Waugh and his colleagues. Accordingly, he proposed a new spectrometer architecture based on a heterodyne frequency generation system which could be used at multiple frequencies. Today, commercial spectrometers are based on this basic design as are pulse programmers, multiple channel MAS probes, etc.

HIST 37

Sixty years (and counting) of magic-angle spinning for NMR

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In 1959 Raymond Andrew showed line narrowing in NMR spectra of samples spinning at the magic angle (54.7° relative to the applied static magnetic field). Andrew adapted the ultracentrifuge air-bearing design of Jesse Beams to create nearly frictionless sample spinning. The same year, Irving Lowe, a graduate student in the Physics Department at Washington University, separated the air bearings (self-pumped by the Bernoulli effect) from the drive gas, and achieved comparable line narrowing by magic-angle spinning (MAS). Practical spinning speeds were of the order of 5 kHz which was insufficient to

narrow spectra of samples that were proton rich. In 1972 Pines, Gibby, and Waugh showed proton-tocarbon cross polarization (CP) ¹³C NMR spectra of non-spinning organic samples in which the dipolar broadening due to ¹³C coupling to protons was removed by high-power ¹H radio-frequency (rf) irradiation. However, the anticipated result of combining CP and MAS (for resolution and sensitivity enhancement) was ¹³C NMR spectra that would be missing contributions from non-protonated carbons. In 1976 we discovered, however, that the experimental CPMAS spectra had strong contributions from non-protonated carbons. The criterion for success was not that the spinning speed had to be less than the dipolar coupling between ¹H and ¹³C (which was weak for non-protonated carbons), but only less than the usually strong coupling between protons. In 1982, Ed Stejskal designed a stator-rotor combination with pumped air bearings and a separated drive gas. This combination resulted in highly reliable and stable controlled spinning and led to a variety of experiments in which rf pulses were synchronized with spinning. Today, MAS at 200 kHz is practical (for small-diameter cylindrical rotors and larger-diameter spherical rotors) so that proton decoupling is not needed to obtain liquid-like proton and rare-spin NMR spectra of solids.

HIST 38

Bid for immortality: A thirty-year race and rivalry between Paul Lauterbur and Raymond Damadian for the invention of MRI

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On Mar. 19, 1971 Raymond Damadian, a physician-researcher at the State University of New York Downstate Medical Center in Brooklyn, published the seminal paper that first directed attention to the vast medical potentials of nuclear magnetic resonance (NMR). On Sept. 2, 1971 Paul Lauterbur, a physical chemist at SUNY at Stony Brook, influenced by Damadian's paper, had an epiphany that transformed NMR into a clinical diagnostic method: magnetic resonance imaging (MRI). Today MRI is a billion-dollar industry with more than 70 million diagnostic scans performed worldwide each year. It has revolutionized health care. Damadian and Lauterbur engaged in a fiery dispute that raged for thirty years, marked by raw competitiveness, guile, and dramatic turning points. Damadian, marginalized by the scientific community, was brash and bombastic in his claims for recognition. He was also an ardent creationist. In 2003, Paul Lauterbur was awarded the Nobel Prize in Physiology or Medicine, along with Sir Peter Mansfield of the University of Nottingham. The third of three available slots was conspicuously left open. Whose work earns the hallmark of priority for an original discovery of a scientific truth?

HIST 39

Life of John Lee Comstock: Chemist or plagiarist?

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This study concerns the life of an American chemistry textbook author. He was born in Lyme, Connecticut on 25th September 1789 to Baron Charles von Comstock, who had emigrated from Germany to the United States of America. John Lee Comstock lacked formal education past primary

school, so he was apprenticed to his elder brother, Joseph, who was a physician practising in South Kingston, Rhode Island. He was an assistant to a surgeon in the American War of Independence (1812). After he had served his apprenticeship, he practiced as a doctor in Hartford, Connecticut. Comstock saw himself as a chemist as well as a doctor though his lack of formal education would have hindered his chemical writing, but by plagiarising others, he taught himself sufficient chemistry to be considered a competent author of chemistry texts. Much of this study concerns details of Comstock's life interwoven with stories about the authors that he shamelessly plagiarised. John Lee Comstock died of heart disease on November 21st, 1858 at the age of 71.

HIST 40

Gamma Sigma Epsilon: 100 Years of promoting excellence in chemistry

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Founded at Davidson College in 1919, Gamma Sigma Epsilon is a national chemistry honor society that promotes academic excellence, undergraduate research, and service to the community and profession. On the occasion of the society's centennial celebration, this seminar will describe the origins and symbols of the society, contributions to the field, key figures, and important events in its history. Selected contributions of historical significance from the executive national committee and the over 85 active chapters will be presented. Lastly, the current activities of the society and future aims, goals, and commitments will be discussed.



HIST 41

Vanadium: Chemistry and history

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Vanadium is the 21st most abundant element in Earth's crust and a very valuable element for its uses and unique properties. However, the discovery and naming of Vanadium was a lengthy and multifaceted process, as it was discovered twice. The first discovery took place in the year 1801 in Mexico City, and it was achieved by Andres Manuel del Rio. The second discovery was accomplished thirty years later by Nil Gabriel Selfstrom in Stockholm. Still, a pure sample was not synthesized until 1869 by Henry Roscoe in the city of Manchester. Furthermore, several different names were assigned to this element during its discovery until a consensus was formed on Vanadium.

HIST 42

Kingsville and uranium: A history of the South Texas uranium belt

Christine Hahn, **Joseph T. Medina**, jtmedina96@gmail.com. Chemistry, Texas A&M University-Kingsville, La Vernia, Texas, United States

The production and refinement of Uranium ore offers countries the opportunity to rise on the world stage with the ability of vast electricity generation by nuclear reactors as well as unlocking the way to nuclear weapon production. While Uranium ore is imported from countries such as Canada and Kazakhstan, nuclear self-sufficiency is still an area of interest. The United States possesses several deposits of uranium including the Texas Gulf Coast with 60 million pounds of Uranium oxide identified and an additional 200 million pounds believed to exist. Within the Texas Gulf Coast Uranium Belt are several refineries one of which is known as the Kingsville Dome. In this presentation the history of the Kingsville Dome facility and its activity shall be discussed alongside the uranium oxide price market for outlooks of future activity and how the mining has affected drinking water quality reports for several cities including Kingsville and Corpus Christi.

HIST 43

American nuclear chemist: Glenn Seaborg

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This talk is about the American Nuclear Chemist Glenn T. Seaborg, his accomplishments, and his contribution to chemistry through research. An element in the periodic table was named after him and he was involved in the discovery and synthesis of 9 other "transuranium elements." These are known as unstable and radioactive elements in the periodic table ranging from half-lives of 2 million years to half-lives of less than fractions of a second. Seaborg was a very important nuclear chemist and had a large influence on America's history. The topic which will be discussed in greater detail is Seaborg's nuclear chemistry accomplishments, discoveries, and his role in the Manhattan project.

HIST 44

Dorothy Hodgkin: The woman who revolutionized crystallographic investigations

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Born on Cairo, Egypt on May 12th, 1910, Dorothy Hodgkin discovered her interest in chemistry and crystals at the age of 10. She went on to study chemistry at Somerville College, Oxford, where she took interest in crystallography and applied it towards the analysis of small organic molecules. Later, Hodgkin became the first British woman chemist to receive the 1964 Nobel Prize in chemistry for discovering the 3D structure of Vitamin B-12 using X-ray crystallography. After 30 years of work, Hodgkin published her final results in determining the structure of insulin and continued to contribute to the fight against diabetes by cooperating with other labs active in insulin research. Hodgkin was also an advocator of world peace, a role that was demonstrated by her work to establish communication between scientists at the height of the Cold War.

HIST 45

Clendenin, WV: The birth of the petrochemical industry

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In October of 1920, Carbide and Carbon Chemicals Corporation was formed as a subsidiary company of Union Carbide and Carbon Company. This company was established with the goal of commercializing the production of several aliphatic compounds by developing an economical process for manufacturing ethylene. A small gasoline extraction plant was then purchased in Clendenin, West Virginia which marked the start of petrochemical industry. With the completion of the hydrocarbon separation plant and ethane cracking plant at that location in the summer of 1921, the Carbide and Chemicals Corporation created the first petrochemical plant capable of separating light hydrocarbons and manufacturing limited quantities of ethylene and its derivatives. The achievements accomplished in the small town of Clendenin grew into a multi-billion-dollar industry that has become useful in virtually every aspect of modern life. Today, ethylene is used in a range of industries and applications including, but not limited to: the automotive industry, the medical industry, metal fabrication, rubber extraction, and the production of automotive and industrial coolants. Ethylene has become one of the largest produced petrochemicals worldwide, and is primarily used to produce: polyethylene (the world's most common plastic; used for garbage bags, food containers, etc.), ethylene dichloride (a precursor used to produce polyvinyl chloride, also known as PVC), and ethylene oxide for synthesis of ethylene glycol (primarily used to produce polyethylene terephthalate, which is used in polyester fibers). The ethane cracking plant built in Clendenin by Union Carbide and Carbon Company is set apart from other achievements in chemistry as it was the first of its kind to be built. This system became the predecessor for future plants built for the purpose of separating light hydrocarbons from natural gasoline for the production of light olefins.

HIST 46

Nobel-prize-winning science deniers: Albert Einstein

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We are writing what will function as chapters in a history book of the topic "Nobel Prize Winning Science Deniers". This book will be used as a text in a general education science course that seeks to identify

the reasons that even the most knowledgeable people in science can allow personal bias to influence their thoughts and cause them to make scientific mistakes. We hope to learn to avoid those pitfalls in our own thought. Albert Einstein was one of the greatest scientists in the early twentieth century. He developed the theory of relativity, and won the Nobel Prize for his explanation of the photoelectric effect, specifically that light travels in small pockets, called quanta or photons. However, Einstein was unable to fully understand the idea that all energy travels in quanta, particularly because the mathematics in quantum mechanics required an observer to force reality. Einstein believed that all of physics was deterministic and any proper theory should be able to account for all measurable phenomena, and this disagreed with the math of quantum mechanics.

HIST 47

Nobel-prize-winning science deniers: Paul Dirac

Timothy J. Fuhrer, tfuhrer@radford.edu. Chemistry/Physics Department, Radford University, Radford, Virginia, United States

We are writing what will function as chapters in a history book of the topic "Nobel Prize Winning Science Deniers". This book will be used as a text in a general education science course that seeks to identify the reasons that even the most knowledgeable people in science can allow personal bias to influence their thoughts and cause them to make scientific mistakes. We hope to learn to avoid those pitfalls in our own thought. Paul Dirac was one of the greatest minds of the early and middle twentieth century and was the first to merge quantum mechanics with special relativity, creating the field we call quantum electrodynamics. But his early work left some of the mathematics of that field incomplete. When Richard Feynman later advanced that work achieving mathematical theory that matched experiment much better than Dirac's work, Dirac would not accept Feynman's work as legitimate because he found the math to be inelegant and believed that any real theory of the universe must be mathematically elegant.