Professor Barry Dellinger

RESEARCH SYMPOSIUM

LOUISIANA STATE UNIVERSITY

MARCH 8-9, 2017

Dr. Barry Dellinger
Louisiana State University
Director, NIEHS LSU Superfund Center

Barry Dellinger, a native of North Carolina and resident of Baton Rouge, Louisiana, married Lynda Donnelly in Dellinger in 1976 and they had one child, Carrie Barrett Dellinger. Barry was born in Charlotte, NC, the only son of Margaret Elizabeth Barrett Dellinger and Harold Gray Dellinger. He went to high school at Anson High and graduated in 1967. He went on to earn his B.S. at University of North Carolina and his PhD in Physical Chemistry at Florida State University. While at FSU he also served in the USAF. He received many prestigious awards, most recently the ACS Award for Creative Sciences and an NIEHS grant awarded which allowed him to found the LSU Superfund Research Center, his lifelong dream. He taught Chemistry at LSU for seventeen years and held the Patrick F. Taylor Endowed Chair for Environmental Chemistry. He had a profound impact on the students, who to this day esteem him as a father. He loved to travel and was allowed to visit many countries and states because of his scientific knowledge. Those who knew him adored him. His wit was only surpassed by his kindness, love for family, and North Carolina basketball.

EDUCATION & RESEARCH SYMPOSIUM

IN HONOR OF

Professor Barry Dellinger

March 8th — WELCOMING RECEPTION

6:00 P.M. – 8:00 P.M.	**Welcoming Ceremony by Drs. Carol Taylor & Gus Kousoulas, Louisiana State University with reception following**

March 9th — RESEARCH SYMPOSIUM

9:00 A.M. – 9:10 A.M.	**Dr. James Wharton, Professor & Chancellor Emeritus** **Louisiana State University** **Welcoming Ceremony**
9:10 A.M. – 9:20 A.M.	**Dr. Carolyn Hargrave, Vice President for Academic Affairs (ret)** **Louisiana State University** **Opening remarks**
9:20 A.M. – 9:40 A.M.	**Dr. Lynn Jelinski, Sunshine Consultants International** **Preserving Dr. Dellinger's Legacy to the Environment**
9:40 A.M. – 9:55 A.M.	**Break**
9:55 A.M. - 10:20 A.M.	**Dr. William Suk, Chief, Hazardous Substances Research Branch** **Director, Superfund Research Program, Division of Extramural Research and Training, National Institute of Environmental Health Sciences** **Reflecting on Barry Dellinger's Contributions to Interdisciplinary Research & Training**
10:20 A.M. – 10:40 A.M.	**Dr. Donald Lucas, Scientist, Lawrence Berkeley National Laboratory** **Environmental Energy Technologies Division, Professional Researcher and Visiting Scholar** **The Science and Politics of Halogenated Hydrocarbons in Combustion and Fires**

Dalton Woods Auditorium – LSU Energy, Coast & Environment (ECE) Bldg.

EDUCATION & RESEARCH SYMPOSIUM

10:40 A.M. – 11: 00 A.M.	**Dr. Heidelore Fiedler, Professor of Chemistry, Örebro University, School of Science and Technology, MTM Research Centre** **From POPs Sources to Human Risk Management – Some Examples at Global Level**
11:00 A.M. – 1:30 PM	**Lunch and Poster Session Judging** **(Overlap Lunch & Poster Session)** **Lunch begins at 11:00 A.M.** **Poster Session begins 11:30 A.M. in ECE Rotunda**
1:30 P.M. – 1:50 P.M.	**Dr. Cathy Koshland, Professor & Vice Chancellor for Undergraduate Education, University of California, Berkeley** **Using science informed metrics to achieve regulatory outcomes**
1:50 P.M. – 2:10 P.M.	**Dr. Robert Louw, Professor Emeritus, Leiden Institute of Chemistry, Universiteit Leiden** **Pathways to Dioxins: Fact or Fancy?**
2:10 P.M. – 2:30 P.M.	**Dr. Erwin Poliakoff, Emeritus Professor - Spectroscopy, Louisiana State University** **X-ray spectroscopy applied to environmental chemistry problems**
2:30 P.M. – 2:50 P.M.	**Dr. Slawo Lomnicki, Assistant Professor of Environmental Sciences, Louisiana State University** **Impact of EPFR Discovery on Environmental Research**
2:50 P.M. – 3:05 P.M.	**Break**
3:05 P.M. – 3:25 P.M.	**Dr. Stephania Cormier, Associate Vice Chancellor for Research, Global Partnerships, Plough Professor of Excellence in Pediatrics, Infectious Disease Scientific Director, Pediatric Asthma Research, Director, LSU Superfund Research Program, University of Tennessee Health Science Center** **A Biologist's Perspective of EPFRs as an Emerging Health Concern**
3:25 P.M. – 3:40 P.M.	**Poster Awards**
3:40 P.M. – 3:50 P.M.	**Trainee Poster Winner 1 (10 minute talk)**
3:50 P.M. – 4:00 P.M.	**Trainee Poster Winner 2 (10 minute talk)**
4:00 P.M. – 4:10 P.M.	**Trainee Poster Winner 3 (10 minute talk)**
4:10 P.M. – 4:20 P.M.	**Dr. K. Gus Kousoulas, Assistant Vice Chancellor for Research and Economic Development, Louisiana State University** **Closing remarks**

Dalton Woods Auditorium – LSU Energy, Coast & Environment (ECE) Bldg.

LSU | Superfund Research Center

Barry Dellinger Symposium

POSTER SESSION

Thursday, March 9, 2017

1. Study of oxidation of Polyaromatic Hydrocarbon (PAH) by Environmentally Persistent Free Radicals (EPFRs) in physiological conditions. Ajit Ghimire, Albert Dela Cruz, Phillip Potter, Farhana Hasan, Balamurugan Subramanian, Slawo Lomnicki; Department of Environmental Sciences, Louisiana State University, Baton Rouge, LA.

2. Inhaled DCB230 particulate matter produce toxicity and adjuvant effects following house-dust mite induction of asthma in mice. Alexandra Noël[1], Ashlyn C. Harmon[1], Balamurugan Subramanian[2], Zakia Perveen[1], Kurt Varner[3], Kelsey Legendre[4], Daniel B. Paulsen[4], Tammy R. Dugas[1], and Arthur L. Penn[1]; Departments of [1]Comparative Biomedical Sciences; [2]Chemistry, and [4]Pathobiological Sciences, Louisiana State University, Baton Rouge, LA. [3]Department of Pharmacology and Experimental Therapeutics, LSU Health Sciences Center, New Orleans, LA.

3. Plants as a New Natural Particulate Matter (PM) Sampler. Chuqi Guo, Farhana Hasan, Albert Leo N. Dela Cruz, Slawo Lomnicki; Department of Environmental Sciences, Louisiana State University, Baton Rouge, LA.

4. The Effect of Metal Speciation in Fly Ash on Environmentally Persistent Free Radical (EPFR) Formation. Elisabeth Feld-Cook[1], Lisa Bovenkamp-Langois[2], Slawomir Lomnicki[3]; [1]Department of Chemistry, [2]Center for Advanced Microstructures and Devices (CAMD), [3]Department of Environmental Sciences, Louisiana State University, Baton Rouge, LA.

5. Exposure and Toxicity Assessment of EPFRs in Brain. Farhana Hasan[1], Annadora Bruce-Keller[2], Slawo Lomnicki[1]; [1]Department of Environmental Sciences, [2]Pennington Biomedical Research Center, Louisiana State University, Baton Rouge, LA.

6. Ultrafast Spectroscopy and Microscopy. Rami Khoury, Jeewan Ranasinghe, Zhenyi Zhang, Raju Kumal, Tony Karam, Louis Haber; Department of Chemistry, Louisiana State University, Baton Rouge, LA.

7. Novel Monofunctional Platinum Complexes with Tridentate Ligands as Potential Anticancer Drugs. Kokila Ranasinghe, Svetlana Pakhomova, Patricia A. Marzilli and Luigi G. Marzilli*; Department of Chemistry, Louisiana State University, Baton Rouge, LA.

8. The Peculiarities of Pyrolysis of Hydrolytic Lignin in Dispersed Gas Phase and in Solid State. Mohamad Barekati-Gourdazi[1], Dorin Boldor[2], Lavrent Khachatryan[3]; [1]Department of Biological & Agricultural Engineering, [2]LSU AgCenter, [3]Department of Chemistry, Louisiana State University, Baton Rouge, LA.

9. Syntesis and Characterization of Zn (II)-phthalocyanine-peptide for Cancer Imaging Synthesis and Characterization of Zn (II)-phthalocyanine-peptide for Cancer Imaging. Elizabeth A. Okoth,[2] Alyssa Stutes[2], Zehua Zhou[2], J. Michael Mathis[1], and M. Graça H. Vicente[2]; [1]Department of Comparative Biomedical Sciences, [2]Department of Chemistry, Louisiana State University, Baton Rouge, LA.

10. QCM Virtual Sensor Array For Volatile Organic Compound Discrimination. Stephanie Vaughan, Nicholas C. Speller, Noureen Siraj, and Isiah M. Warner; Department of Chemistry, Louisiana State University, Baton Rouge, LA.

11. Iron and Copper Synergy in the Formation of PCDD/Fs. Xia Guan, Phillip Potter, Slawo Lomnicki*; Louisiana State University, Department of Environmental Sciences, Baton Rouge, LA.

12. Molecular Diffusion and Photothermal Kinetics Studied by Second Harmonic Generation. Raju Kumal, Huy Nguyen, James Winter, Robin McCarley, Louis Haber; Department of Chemistry, Louisiana State University, Baton Rouge, LA.

13. Exposure to Environmentally Persistent Free Radicals Leads to Decreased Vascular Responsiveness. Ashlyn C. Harmon[1], Alexandra Noël[1], Balamurugan Subramanian[3], Merilyn Jennings[1], Yi Fan Chen[1], Kurt Varner[2], Arthur L. Penn[1], and Tammy R. Dugas[1]; Department of Comparative Biomedical Sciences, Louisiana State University[1], Department of Pharmacology and Experimental Therapeutics, LSU Health Sciences Center, New Orleans, LA[2] Department of Environmental Sciences, Louisiana State University, Baton Rouge, LA[3]

14. Ruthenium-based GUMBOS as photosensitizers in dye-sensitized solar cells. Tia Vargas-Myers, Paulina Kolic, Pratap Chhotaray, Isiah M. Warner; Department of Chemistry, Louisiana State University, Baton Rouge, LA.

15. Targeting Virus DNA-packaging Motor. Misagh Naderi, Lana Thaljeh, Jane A. Rothschlid, Michal Brylinski; Center for Computation and Technology, Biological Sciences, Louisiana State University, Baton Rouge, LA.

16. A new pipeline for molecular fragmentation and construction for de novo drug design and targeted virtual screen. Misagh Naderi, Chris Alvin, Tairan Liu, Supratik Mukhopadhyay, Michal Brylinski; Center for Computation and Technology, Biological Sciences, Louisiana State University, Baton Rouge, LA

17. Angle-Dependent Strong-Field Molecular Ionization Rates with Tuned Range-Separated Time-Dependent Density Functional Theory. Adonay Sissay[1], Paul Abanador[2], Francois Mauger[2], Mette Gaarde[2], Kenneth J. Schafer[2], and Kenneth Lopata[1,3]; [1]Department of Chemistry and [2]Department of Physics & Astronomy and [3]Center for Computation & Technology, Louisiana State University, Baton Rouge, LA.

18. Synthesis, Characterization and Modeling of Gold-Silver-Gold-Core-Shell-Shell Nanoparticles Exhibiting Enhanced Photothermal Effects. Holden T. Smith[1], Tony E. Karam[1,2], Louis Haber[1], Kenneth Lopata[1]; [1]Department of Chemistry, Louisiana State University, Baton Rouge, LA. [2]Arthur Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA.

19. Preparation of Highly Fluorescent Environmentally Persistent Free Radical Surrogates: Surface Modification of Silica-coated Upconversion Nanoparticles with Nickel Oxide. Ansonia Badgett, Elisabeta Mitran, Robin McCarley; Department of Chemistry, Louisiana State University, Baton Rouge, LA.

Poster Title

Study of oxidation of Polyaromatic Hydrocarbon (PAH) by Environmentally Persistent Free Radicals (EPFRs) in physiological conditions.

Ajit Ghimire, Albert Dela Cruz, Phillip Potter, Farhana Hasan, Balamurugan Subramanian, Slawo Lomnicki
Louisiana State University, Department of Environmental Sciences

Abstract

Formation of Polyaromatic hydrocarbons (PAHs) and Environmentally Persistent free radicals (EPFRs) typically occurs side by side during combustion related activities. EPFRs when reacted with O_2 or with aqueous medium either in lungs or in an environment form Reactive Oxygen Species (ROS). The formed ROS can transform PAHs into oxy-PAHs. Since these oxy-PAH are more soluble than their parent PAH, they are more bioavailable and effect the physiological activities. It is generally believed that the cytochrome P450 metabolism converts PAHs to their hydroxylated, toxic form. EPFRs on PM can activate and desorb PAHs to a larger extent causing additional biological stress to their ROS generation capabilities.

For the studies presented, we analyzed the effect of Fenton's reagent and EPFR-laden particles on the formation of oxy-PAHs from anthracene adsorbed on particles. Fenton's solution did not yield any Anthracenol and yielded only one isomer of Anthraquinone. We found the formation of various isomers of Anthracenol and Anthraquinone in the presence of EPFRs in aqueous media, indicating the increased bioavailability of PAHs. Since Fenton's solution did not produce any Anthracenol, it indicates an important role of EPFRs in PAHs activation. The hydroxyl radical concentration gradient around PM can be a critical factor in this process. Additionally, the PAH activation was distinctly higher if PAHs and EPFRs co-inhabited the same particles.

Poster Title

Inhaled DCB230 particulate matter produce toxicity and adjuvant effects following house-dust mite induction of asthma in mice.

Alexandra Noël[1], Ashlyn C. Harmon[1], Balamurugan Subramanian[2], Zakia Perveen[1], Kurt Varner[3], Kelsey Legendre[4], Daniel B. Paulsen[4], Tammy R. Dugas[1], and Arthur L. Penn[1].

Departments of [1]Comparative Biomedical Sciences; [2]Chemistry, and [4]Pathobiological Sciences, Louisiana State University, Baton Rouge, LA. [3]Department of Pharmacology and Experimental Therapeutics, LSU Health Sciences Center, New Orleans, LA.

Abstract

Inhalation of particulate matter (PM) from combustion can exacerbate pre-existing respiratory diseases, including asthma. The cellular and molecular mechanisms by which PM promotes the onset or exacerbation of asthma remain elusive. We used a house-dust mite (HDM)-induced mouse model of asthma to test the hypothesis that inhaled DCB230, which are environmentally persistent free radicals (EPFRs) PM, will aggravate asthmatic responses. Methods: Two groups of C57BL/6 adult male mice were whole-body exposed to DCB230 aerosols at 1.5 mg/m^3 4 hr/day for 10 days with or without previous HDM-induction of asthma. Similarly, two groups were exposed to filtered air with or without HDM. We evaluated mouse lung function, cytology, gene expression and histopathology. Results: DCB230 alone significantly reduced lung tidal volume and dysregulated the expression of 3 genes, Ccl11, Il12b and Tpsb2, which are mediators involved in inflammation. Following the HDM-induction of asthma, DCB230 produced significant toxicity and adjuvant effects in the lungs. Compared to all other groups, the HDM+DCB230-exposed group exhibited significantly increased lung tissue damping, augmented eosinophilic inflammation, and up-regulated expression of 20 asthma genes, including Ccl12, Clca1, Chil1, Il10, Il17a, Il33, and Muc5ac. Conclusion: Our data indicate that inhaled DCB230 exacerbates asthmatic responses in a HDM mouse model.

Poster Title

Plants as a New Natural Particulate Matter (PM) Sampler

Chuqi Guo, Farhana Hasan, Albert Leo N. Dela Cruz, Slawo Lomnicki

Department of Environmental Sciences, Louisiana State University, Baton Rouge, Louisiana

Abstract

Particulate matter (PM) is one of the criteria pollutants. Most research oversimplified PM as a carrier of toxic compounds which eliminates synergistic effects between PM components resulting in new chemical quality or species. Our research focused on the Environmentally Persistent Free Radicals (EPFRs), species resulting from exactly such interaction which can generate reactive oxygen species (ROS) and oxidative stress in biological systems. In this study, we investigated the effects of collection methods to EPFRs on ambient air PM and developed a new "phytosampling" method, enabling easy particle recovery, "in the environment" collection and minimized effects of the collection matrix compared to the standard sampling method. The basic mechanism of this method is particle entrapment by trichomes on the leaf surface. Trapped particles are subject to the same environmental factors as those suspended in air thus are more representative for ambient air PM. This method gives us a chance to get spatial distribution data of PM because of possibility of remote sampling. The experiment results show that the new "phytosampling" method is an effective method and samples collected in the open environment show larger contribution of oxygen centered EPFRs relative to standard air samplers. And spin trapping experiment confirmed the generation of hydroxyl radical of EPFRs in PBS solution.

Poster Title

The Effect of Metal Speciation in Fly Ash on Environmentally Persistent Free Radical (EPFR) Formation

Elisabeth Feld-Cook[1], Lisa Bovenkamp-Langois[2], Slawomir Lomnicki[3]

1. Department of Chemistry, LSU
2. Center for Advanced Microstructures and Devices (CAMD), LSU
3. Department of Environmental Sciences, LSU

Abstract

EPFRs are surface-bound radicals with long lifetimes [hours to weeks]. They typically originate from combustion processes and are associated with emitted solids (i.e. fly ash). EPFRs are intermediates to PCDD/F formation in combustion exhaust but also induce oxidative stress in biological systems. This study aims at determining the relationship of fly ash composition and EPFR formation.

Real world fly ash (RWFA) and synthetically composed fly ash (SFA) were studied to evaluate the relationship between metal oxides, sulfur compounds and EPFR formation. Thorough characterization of RWFA from China & the U.S. revealed large differences in EPFR content. SFA were made to model RWFA composition and determine a driving element in EPFR formation or inhibition.

Sulfur was determined to be an essential element in controlling EPFR inhibition. Low energy X-ray studies performed at CAMD provided detailed information on sulfur speciation. For SFA containing Ca & S, $CaSO_4$ was dominant but $FeSO_4$ & $ZnSO_4$ were present; however, for S-only containing SFA, $ZnSO_4$ & $FeSO_4$ were the dominant species. We hypothesize that sulfur rich waste releases SO_2 during combustion, which blocks the metal active sites for EPFR formation. The mechanisms explored here can potentially be applied to prevent EPFR formation at superfund sites.

Poster Title

Exposure and Toxicity Assessment of EPFRs in Brain

Farhana Hasan[1], Annadora Bruce-Keller[2], Slawo Lomnicki[1]

1. Department of Environmental Sciences, Louisiana State University, Baton Rouge, LA

2. Pennington Biomedical Research Center, Louisiana State University, Baton Rouge, LA

Abstract

Air pollution has been suggested to increase the risk of the central nervous system diseases. Studies show that the chronic inflammation at the blood-brain barrier (BBB) might be the reason. Environmentally Persistent Free Radicals (EPFRs) with particulate matter (PM) are potential suspects in many diseases. The effects of different concentrations of EPFR exposure on brain and BBB injury were investigated. Preliminary data on mice exposed to inhalation of EPFR-PM for seven days, 1 hr/day have shown significant effects on BBB tight junction proteins. We observed a 50% increase in the activation of MMP-9 in the animals exposed to EPFRs compared to the control. Western blot analysis of glial cell markers in mice brains indicated lower expression of glial fibrillary acidic proteins, likely related to BBB damage.

Recent animal studies show that EPFRs induce COX-2 and decrease syn-phospho protein expression in brain cells at high dose, while TLR4 expression increases both at high and low doses. The changes in expression of these proteins could indicate neurotoxicity. We suggest that this is a result of hydroxyl radicals generated by EPFRs and oxidative stress.

Poster Title

Ultrafast Spectroscopy and Microscopy

Rami Khoury, Jeewan Ranasinghe, Zhengu Zhang, Raju Kumal, Tony Karam, Louis Haber

Department of Chemistry, Louisiana State University

Abstract

A femtosecond pump-probe microscopy setup is being constructed in order to study ultrafast phase transitions in metallic and alloy nanomaterials. Preliminary data have been obtained on the imaging of stainless steel and aluminium samples exposed to femtosecond laser pulses with the size of the melt area measured as a function of the average irradiation powers. Additionally, the synthesis and characterization of iron and bimetalliciron-nickel nanoparticles are reported. The growth of the nanoparticles will be monitored in real-time using a technique called in situ second harmonic generation, which has been demostrated here in the study of the growth dynamics of gold nanoparticles and gold nanoclusters reduced to the surface of colloidal TiO2. Overall, a research program is been developed to investigate the ultrafast heating, melting and resolidification dynamics in metallic and alloy materials and nanomaterials for advancing selective laser melting applications.

Poster Title

Novel Monofunctional Platinum Complexes with Tridentate Ligands as Potential Anticancer Drugs

Kokila Ranasinghe, Svetlana Pakhomova, Patricia A. Marzilli and Luigi G. Marzilli*

Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana

Abstract

Pt(II) complexes bind preferentially at N7 of G residues of DNA, causing DNA structural distortions associated with anticancer activity. Anticancer-active monofunctional Pt(II) complexes have bulky carrier ligands that cause DNA adducts to be distorted. Hence, understanding carrier-ligand steric effects is key in designing new monofunctional platinum drugs. Two Pt(II) complexes with imidazolyl-based tridentate ligands were prepared in order to investigate their **G** adducts (**G** is a Pt(II)-bound, N9 guanine or N9 hypoxanthine derivative not linked to another nucleobase). Complexes were characterized using NMR spectroscopy and X-ray crystallography. Solution NMR spectroscopy is the primary tool for studying metal complexes of nucleotides because such adducts rarely crystallize. However, [Pt(*N*(H)1,1′-Me_2dma)(3′-GMPH)]NO_3 was crystallized, allowing, to our knowledge, the first crystallographic molecular structure determination for a 3′-GMP platinum complex. Ligand bulk can be correlated with the degree of impeded rotation of the **G** nucleobase about the Pt–N7 bond, as assessed by the observation of rotamers. Adducts studied here exhibit two new downfield-shifted **G** H8 signals, consistent with **G** bound to platinum by N7 and a syn/anti rotamer mixture.

Poster Title

The Peculiarities of Pyrolysis of Hydrolytic Lignin in Dispersed Gas Phase and in Solid State

Mohamad Barekati-Gourdazi[1], Dorin Boldor[1], Lavrent Khachatryan[2]*

[1] Department of Biological & Agricultural Engineering, LSU and LSU AgCenter, Baton Rouge, Louisiana 70803, USA

[2] Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803, USA

Abstract

The unique decomposition pathways of hydrolytic lignin (HL) dissolved in acetone/water mixture and dispersed by droplet evaporation technique in flow of nitrogen gas has been investigated in conventional reactor at atmosphere condition and temperature region of 400 – 550°C and residence time of 0.3 sec. The results validate the fact that dispersion of the lignin into gas phase by decreasing of the sample size (as well as "minimizing the char area to avoid catalytic contact" of molecular products/radicals with the surface) may open new perspectives to understand the chemistry of depolymerization of lignin. Surprisingly, the expected phenolic compounds were in trace amounts at less than 15% conversion of lignin. The hypothesis about the largely disputed key question on lignin pyrolysis as to whether the phenolic compounds or oligomers (dimers, trimers, etc.) are the primary products is discussed. Additionally, a focus on free radical mechanism of depolymerization of solid lignin by formation of free intermediate radicals from initial lignin macromolecule as well as from inherent, low molecular weight oligomer molecules is developed.

Poster Title

Synthesis and Characterization of Zn (II)-phthalocyanine-peptide for Cancer Imaging

Synthesis and Characterization of Zn (II)-phthalocyanine-peptide for Cancer Imaging.

Elizabeth A. Okoth,2 Alyssa Stutes, 2 Zehua Zhou,2 J. Michael Mathis1 and M. GraÃ§a H. Vicente2

1Department of Comparative Biomedical Sciences, Louisiana State University, Baton Rouge, LA 70803, USA

2Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA

Abstract

Phthalocyanine (Pc) compounds are dyes structurally similar to porphyrins with extended pi systems. They display a strong absorbance in the NIR region, have good chemical, photo and thermal stability and are excellent singlet oxygen generators.[1] These properties make Pcs favorable for many applications such as photosensitizers (ps) in imaging and photodynamic therapy.[2] Conjugation of biomolecules such as oligonucleotides, antibodies, peptides, vitamins, polyethylene glycol groups to Pcs produces amphiphilic ps with enhanced hydrophilicity, serum life, specificity and uptake.[3] Various synthetic peptide sequences target and bind specific tumor associated markers, therefore these Pc-peptide conjugates are expected to be stable in biological media, specific to tumor cells and show enhanced uptake.[3] Although isothiocyanate is a versatile functional group and has been used in porphyrin conjugation to amine functional groups under mild conditions, it has been investigated once by Duan et al as a Pc functional group.[4] In our continued effort to synthesize biocompatible Pc analogues with various functional groups, we report the design, synthesis, spectroscopic characterization and biological evaluation of regioisomerically pure Pc-isothiocyanate and Pc-peptide.

Poster Title

QCM Virtual Sensor Array For Volatile Organic Compound Discrimination

Stephanie Vaughan, Nicholas C. Speller, Noureen Siraj, and Isiah M. Warner

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803

Abstract

The use of quartz crystal microbalance (QCM) sensor arrays for analyses of volatile organic compounds (VOCs) has attracted considerable interest, as compared to traditional techniques such as GC/MS, due to low cost and simplistic operation. Such arrays typically employ various chemosensitive materials as recognition elements. Among these materials, ionic liquids have proven promising due to the interesting properties afforded by this class of tunable characteristics. Conventionally, such arrays have adopted the multisensor array (MSA) approach, which comprises multiple cross-reactive sensors based on chemical affinity. However, there are disadvantages to this approach, including cost, complexity, and sensor drift. Herein, we present an alternative in the form of a QCM virtual sensor array (VSA). This approach is based on exploiting viscoelasticity, film thickness, and harmonics, of a single sensor to produce multiple cross-reactive responses. Thus, through employment of the VSA approach, factors such as cost, complexity, and sensor drift are reduced as compared to MSAs.

Poster Title

Iron and Copper Synergy in the Formation of PCDD/Fs

Xia Guan, Phillip Potter, Slawo Lomnicki*

Louisiana State University, Department of Environmental Sciences, Baton Rouge, USA

Abstract

Polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) originate as byproducts of industrial and thermal processes. Transition metal oxides present in waste incineration systems catalyze the formation of PCDD/Fs through surface reactions involving organic dioxin precursors. The catalytic effects of individual transition metal oxides have been studied. Iron and copper are present in high concentrations in most combustion systems and are known to individually catalyze the formation of PCDD/Fs. The variable makeup of fly ash introduces the possibility of synergistic or inhibiting effects between multiple components. Knowing the roles of each metal will lead to better models for PCDD/F formation prediction. Fly ash surrogates containing different ratios of iron (III) oxide and copper (II) oxide have been made. These Fe_2O_3 /CuO bimetallic surrogates were used to study the cooperative effects between two transition metals. The mixed metal oxides greatly increased the catalytic activity of the fly ash surrogate and led to extremely high PCDD/F yields under pyrolytic conditions. PCDD/F congener are similar to results obtained from monometallic CuO surrogates but total PCDD/F yields increase with Fe_2O_3 concentration. In the bimetallic surrogates, the CuO surface sites are centers for reaction while the Fe_2O_3 affected the bonds in CuO and increased the ability of copper centers to form surface-bound radicals that are precursors to PCDD/Fs.

Poster Title

Molecular Diffusion and Photothermal Kinetics Studied by Second Harmonic Generation

Raju Kumal, Huy Nguyen, James Winter, Robin McCarley, Louis Haber

Louisiana State University, Department of Chemistry

Abstract

Second harmonic generation (SHG) is used to monitor real-time dynamics of molecules at colloidal nanomaterial interfaces. The adsorption and diffusion of malachite green dye molecules at liposome interfaces is measured with SHG at different buffers. Molecular adsorption and diffusion kinetics of positively-charged dyes at the surface of liposomes in different buffer conditions are studied in real time using second harmonic generation. Malachite green is found to diffuse faster in dioleoylphosphatidylglycerol (DOPG) and dioleoylphosphoserine (DOPS) liposomes in a citrate buffer in the absence of salts whereas no adsorption or diffusion is observed in tri-methyl quinone dioleoylphosphoethanolamine (QPADOPE) and dioleoylphosphocholine (DOPC) liposomes. In a different project, second harmonic generation is also used to investigate the photothermal release of microRNA from the surface of gold-silver-gold core-shell-shell plasmonic nanoparticles. The mircroRNA is functionalized to the surface of nanoparticles by an alkane thiol spacer linker using the Diels-Alder chemistry. The plasmon resonance peak of these nanoparticles can be controlled by changing the core and shell sizes. The rate of photothermal release of oligonulceotides in real time is studied at different irradiation laser wavelengths and powers to measure the photothermal cleaving dynamics.

Poster Title

Exposure to Environmentally Persistent Free Radicals Leads to Decreased Vascular Responsiveness

Ashlyn C. Harmon[1], Alexandra Noël[1], Balamurugan Subramanian[3], Merilyn Jennings[1], Yi Fan Chen[1], Kurt Varner[2], Arthur L. Penn[1], and Tammy R. Dugas[1]

Department of Comparative Biomedical Sciences, Louisiana State University, Baton Rouge, LA[1]

Department of Pharmacology and Experimental Therapeutics, LSU Health Sciences Center, New Orleans, LA[2]

Department of Environmental Sciences, Louisiana State University, Baton Rouge, LA[3]

Abstract

Environmentally persistent free radicals (EPFRs) are formed during the combustion of waste at Superfund sites when pollutants are chemisorbed to redox-active transition metals. *In vitro* studies have demonstrated that cells exposed to EPFRs produce increased IL-6, TNF-α and ROS, indicating inflammation which is an initiator of vascular dysfunction. In addition, *in vivo* data demonstrate that adult C57BL/6 mice exposed to 1.5 mg/m^3 of the EPFR DCB230 for either 4 hours or for 10 consecutive days, exhibit significantly reduced NO and increased ET-1, suggesting endothelial dysfunction. However, analysis of BALF and lung tissue for inflammation was unremarkable, indicating the vasculature as a direct target of injury after EPFR exposure. Therefore, we hypothesized that at an intermediate time point, DCB230 exposure will lead to systemic inflammation, resulting in a decrease in vascular responsiveness. Methods: Adult C57BL/6 mice were subjected to whole-body inhalation of 1.5 mg/m^3 DCB230 for 4 hours a day for 3 consecutive days prior to flow cytometry and vessel reactivity analysis. Results: DCB230-exposed mice demonstrated significantly reduced monocytes in circulation and increased lymphocytes versus the air-only control group. Analysis of aortic segments indicated a significant reduction in maximum relaxation in DCB230 versus control mice. Conclusion: Together these data demonstrate that EPFRs lead to alteration of the peripheral inflammatory cell milieu and reduced vascular responsiveness, which may ultimately culminate in the development or exacerbation of cardiovascular disease.

Poster Title

Ruthenium-based GUMBOS as photosensitizers in dye-sensitized solar cells

Tia Vargas-Myers, Paulina Kolic, Pratap Chhotaray, Isiah M. Warner

Louisiana State University, Department of Environmental Sciences

Abstract

GUMBOS were developed as alternative photosensitizing dyes to improve energy conversion efficiency. GUMBOS can be easily tuned by changing the cation or anion, leading to new materials with properties such as increased molar extinction coefficients and broadened absorption spectra, which are beneficial for application in DSSCs. Ruthenium complexes have been frequently used in DSSCs due to the ability to introduce ligands for optimizing spectral properties and energy levels. These strong donor and anchoring group ligands increase charge transfer within the cell, enhancing efficiency. GUMBOS derived from ruthenium-based dyes with bulky anions were synthesized and evaluated as photosensitizing dyes. Tuning the counter-ion exhibited an increase in light absorption as well as a change in energy conversion efficiency, indicating that these GUMBOS dyes can be tuned for enhanced applications in DSSCs.

Poster Title

Targeting Virus DNA-packaging Motor

Misagh Naderi, Lana Thaljeh, Jane A. Rothschlid, Michal Brylinski

Louisiana State University, Biological Sciences, Center for Computation and Technology

Abstract

Developing anti-viral drugs poses major difficulties due to the fact that viruses replicate by hijacking the host cell's machinery. Therefore, finding suitable protein targets to inhibit viral infection without affecting the host is a challenging task. The majority of antiviral drugs that target herpeseviridae, the focus of this experiment, inhibit virus replication by acting as a competitive substrate for the viral DNA polymerase. The assembly of viral capsids and DNA packaging also holds significant potential for drug development; however, the lack of molecular structures of virus DNA packaging proteins makes it difficult to develop inhibitors of this mechanism. Our goal is to construct atomistic models of the entire DNA packaging machinery for cytomegalovirus virus (CMV) and herpes simplex virus 1 (HSV-1). These models will be subsequently used to identify putative target sites for pharmacotherapy focusing on terminase subunit 1, pUl89 (CMV), and pUl15 (HSV-1). Here, we describe structure modeling and functional annotation of homology-based models of pUl89 and pUl15, including the identification and characterization of putative binding sites for ATP and DNA. These confident models will be ultimately used to carry out structure-based virtual screening for the rational design of new antiviral agents.

Poster Title

A new pipeline for molecular fragmentation and construction for de novo drug design and targeted virtual screen

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Abstract

To reduce the exorbitant costs and increase the success rate of drug development, high throughput drug discovery pipelines are now complemented with many computational methods. For example, virtual screening or docking tools are often used to efficiently search large libraries of small molecules to identify hits. Likewise, to generate or optimize leads for specific targets de novo and structure based drug design methods are proved to be instrumental. Here we introduce two software tools, eMolFrag and eSynth, that can be used for fragment-based drug discovery or to be incorporated in the strategies mentioned above to develop new molecular entities with novel chemical scaffolds. This is particularly important in the context of emerging drug resistant pathogens. Given a library of compounds eMolFrag extracts a non-redundant set of building blocks that can be consequently combined to synthesize new molecules using, eSynth, a fragment-based combinatorial chemistry tool. This process is very similar to LEGO and building new constructs using those pieces. This pipeline can be used to investigate the chemical composition of libraries, to add particular moieties to small molecules, or to prepare virtual screening libraries for targeted drug discovery.

Poster Title

Angle-Dependent Strong-Field Molecular Ionization Rates with Tuned Range-Separated Time-Dependent Density Functional Theory

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Abstract

Strong-field ionization and the resulting electronic dynamics are important for a range of processes such as high harmonic generation, photodamage, charge resonance enhanced ionization, and ionization-triggered charge migration. Modeling ionization dynamics in molecular systems from first-principles can be challenging due to the large spatial extent of the wavefunction which stresses the accuracy of basis sets, and the intense fields which require non-perturbative time-dependent electronic structure methods. In this paper, we develop a time-dependent density functional theory approach which uses a Gaussian-type orbital (GTO) basis set to capture strong-field ionization rates and dynamics in atoms and small molecules. This involves propagating the electronic density matrix in time with a time-dependent laser potential and a spatial non-Hermitian complex absorbing potential which is projected onto an atom-centered basis set to remove ionized charge from the simulation. For the density functional theory (DFT) functional we use a tuned range-separated functional LC-PBE*, which has the correct asymptotic 1/r form of the potential and a reduced delocalization error compared to traditional DFT functionals. Ionization rates are computed for hydrogen, molecular nitrogen, and iodoacetylene under various field frequencies, intensities, and polarizations (angle-dependent ionization), and the results are shown to quantitatively agree with time-dependent Schrcodinger equation and strong-field approximation calculations. This tuned DFT with GTO method opens the door to predictive all-electron time-dependent density functional theory simulations of ionization and ionization-triggered dynamics in molecular systems using tuned range-separated hybrid functionals.

Poster Title

Synthesis, Characterization and Modeling of Gold-Silver-Gold Core-Shell-Shell Nanoparticles Exhibiting Enhanced Photothermal Effects

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Abstract

The synthesis, characterization and theoretical models for new plasmonic nanoparticles which are colloidal gold-silver-gold core-shell-shell nanoparticles are reported. These plasmonic nanoparticles are spherical in shape with highly uniform shells which exhibit plasmonic enhancement and controllable extinction spectra ranging from the ultraviolet to the near infrared wavelengths which could lead to advancements in photothermal cancer therapy. The photothermal efficiency is compared to gold nanoparticles and gold nanorods.

Poster Title

Preparation of Highly Fluorescent Environmentally Persistent Free Radical Surrogates: Surface Modification of Silica-coated Upconversion Nanoparticles with Nickel Oxide.

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Abstract

Environmentally persistent free radicals (EPFRs) are found on the surface of metal oxides associated with particulate matter (PM). Several studies have shown direct correlations between ultra-fine particulate matter (PM0.1) exposure and adverse pulmonary health effects. It was found PM0.1 can reach deep in the alveoli of the lungs and it is hypothesized that EPFRs/PM uptake by cells is the probable cause of such health effects. However, the proposed mechanism for cellular uptake of ultra-fine PM has not been confirmed due to a lack of existing traceable materials resembling EPFRs/PM.

To address this limitation, my research focuses on exploring the synthesis of a highly fluorescent surrogate EPFR probe based on upconversion nanoparticles (UCNPs). The aforementioned are unique photoluminescent materials, because of their ability to be excited with near-infrared radiation, with subsequent emission of visible light. Presented here is work on the development of a fluorescent EPFR probe consisting of an UCNP core, coated with silica, and modified with nickel oxide to resemble EPFRs/PM.

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