Regional Undergraduate Poster Competition

Abstracts

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Determining Physicochemical Properties of Metal-Organic Framework (MOF)–Electrolyte Interfaces

Shasanka Lamichhane, Senior, Chemistry, University of Kentucky

Anton Perera, Chemistry, Cave Western Reserve University
Chad Risko, Chemistry, University of Kentucky

Abstract

Metal-organic frameworks (MOF) are a diverse, highly tunable, and porous materials class of interest across fields as diverse as energy conversion and storage, gas adsorption, and drug delivery. For electrochemical-based energy conversion and storage and catalytic applications, there is a need to understand the nature of the MOF interface with electrolyte solutions. Here, we develop and implement a series of equilibrium and non-equilibrium molecular dynamics (MD) simulations to elucidate the interfacial interactions that take place at the MOF-solution interface. As a paradigmatic MOF, we examine the interface of the zeolitic imidazolate framework 8 (ZIF-8) MOF with acetonitrile-based electrolyte solutions. The electrolyte salts include LiPF6, ammonium-PF6, TEMPO (2,2,6,6-tetramethyl-1-piperidinyloxy)-PF6, and mixtures thereof; the latter two models use TEMPO to represent an electroactive molecule undergoing charge/discharge. To expedite the model throughput, we also report on the development of QSolFlow (QSF), a Python platform to automate MD simulations by creating a high-throughput, highly parallelized MD workflow. QSF allows for the rapid generation of MD-derived data that can facilitate the generation of chemical descriptors for machine learning models.

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Interfacial Properties of ZIF-8 in DMF and Water at Variable Temperatures: A Molecular Dynamics Study

Quinn Hall, Senior, Chemistry, University of Kentucky

Chad Risko, Chemistry, University of Kentucky
Shasanka Lamichhane, Chemistry, University of Kentucky

Abstract

Metal organic frameworks (MOFs) are porous materials that contain secondary building units (SBUs), which are inorganic metals that are coordinated with organic linkers. MOFs are of high interest across several technologies, including gas capture, catalysis, and storage, due to their high surface areas and large porosity characteristics. MOF surface properties when interfaced with solutions are not very well understood as these systems are often complex and not readily characterized experimentally. Computer modeling, and in particular molecular dynamics (MD) simulations, provide an opportunity to examine MOF-solution interfaces at atomic and nano scales. Here, using the zeolitic imidazolate framework-8 (ZIF-8) MOF as a paradigmatic system, we investigate interfacial properties of ZIF-8 with water and dimethylformamide (DMF) at two temperatures (80°C and 92°C). We find that the SBU linkers on the surface of ZIF-8 oscillate at higher angles as temperature increases. This motion affects how the solvents can interact with the surface and pores of the MOF. Keeping these factors in mind, conclusions regarding solvent alignment and characterization on the interface of ZIF-8 can be made and further examined for the differing solvents and temperatures.

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Predicting Metabolically-Close Metabolites from Molecular Formula Comparisons

Christina Tran, Senior, Chemistry, University of Kentucky

Hunter Moseley, Molecular and Cellular Biochemistry, University of Kentucky

Abstract

A wide range of metabolites (small biomolecules) associate cellular metabolism with all biological processes, either directly or indirectly. Understanding these associations requires identifying and placing metabolites within the context of cellular metabolism. The small molecule isotope-resolved formula enumeration (SMIRFE) methodology allows for the derivation of elemental molecular formulas from Fourier transform mass spectral peaks. Metabolites related to SMIRFE derived molecular formulas can be used to map to possible neighbor metabolites for metabolic network interpretation. However, many SMIRFE derived molecular formulas are not present in current metabolic databases. This project aims to develop a method that predicts the closest known metabolite by comparing the molecular formula of unknown metabolites to the molecular formula of known metabolites. The Kyoto Encyclopedia of Genes and Genomes (KEGG) is a knowledgebase with extensive metabolic network information, detailing the biochemical pathways, enzymes, and metabolites involved in cellular processes across various organisms. The KEGG RCLASS database categorizes chemical compounds into reaction-based classes based on their involvement in specific biochemical reactions. A dataset connecting atom mappings of compounds between KEGG reaction classes has been developed and designed for efficient data extraction. Next, cross-reaction metabolite pairs that share a majority of atom mappings will be compared to non-reaction metabolite pairs with high Tanimoto coefficients to derive weights and cutoffs for metabolite pairs at different levels of shared atom mappings and number of reaction steps. The ultimate goal of this project is to develop metrics and methods to detect close metabolites that are not present in existing databases. The detection of close metabolites is necessary to map likely neighbor metabolites for metabolic network interpretation of metabolomics datasets with only molecular formula assignments.

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Mass Spectrometry Imaging for Undergraduates II: Freezing, Cryosectioning and DESI Imaging Studies in Common Meats

Rebecca Ratliff, Junior, Chemistry, Indiana State University

Ryan Van Ooteghem, Chemistry and Physics, Indiana State University
Richard Fitch, Chemistry and Physics, Indiana State University

Abstract

Desorption Electrospray Ionization-Mass Spectrometry Imaging (DESI-MSI) is a technique used to locate and identify molecules on surfaces. The electrospray creates a puddle that moves across a surface absorbing and ionizing molecules. Secondary droplets from spray impacting the puddle enter the inlet of the mass spectrometer and are analyzed. Marker lines were used to optimize instrumental parameters (gas flows, solvent flow rates, and sprayer tips, spray/inlet angles/distances) for the best sensitivity. We then studied sample preparation, performing freezing tests of commercial meat specimens (fish, chicken, pork, and steak) in liquid nitrogen and different hydrocarbon slushes. The specimens were embedded in a stabilizing medium of carboxymethyl cellulose (CMC) and gelatin and sectioned in a cryostat. We mounted the sections on microscope slides and imaged them to acquire DESI-MSI data for analysis. The data were processed into images and analyzed for small molecules and lipids. This training will help us image ecological animal specimens for metabolomic studies.

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Chemical Ionization-Tandem Mass Spectrometry for Correlation of GC-MS and LC-MS Data of Natural Extracts

Kevin Goldstein, Junior, Chemistry and Physics, Indiana State University

Jeremy Rix, Chemistry and Physics, Indiana State University
Richard Fitch, Chemistry and Physics, Indiana State University

Abstract

Natural products have historically been a productive source of bioactive compounds for studies in ecology, physiology and medicine. We are interested in poison frogs, which have been a treasure trove of neuroactive alkaloids. Over 1100 unique compounds have been characterized in these anurans. However, the existing literature is dominated by gas chromatographic (GC) data, usually coupled with electron impact mass spectrometry (EI-MS) whereas isolation and characterization of compounds for further study is typically done by liquid chromatographic (LC) methods and where MS is used, it is done in a electrospray (ESI) or atmospheric pressure chemical ionization (APCI) modes which are not comparable with EI. To address this problem, we are building a public database which will include all of the common spectra obtained from poison frog alkaloids, including EI, CI, ESI and associated MS/MS spectra with GC and LC retention indices for reliable and reproducible identification of these important neuroactive compounds to enable data mining for drug discovery efforts. This requires a common mass spectral fingerprint for matching GC and LC data, which can be used to cross-reference the two separation modes. We are addressing this by obtaining data on authentic natural and synthetic standards using CI-MS/MS for GC and ESI-MS/MS for LC. Preliminary data are promising and we are currently evaluating matched mass analyzer platforms (orbitrap with HCD). We are also investigating variable collision energy for providing fragment dense fingerprint MS2 spectra and structurally informative selective fragmentation spectra. This can be of significant utility in a data-dependent analyses for untargeted analysis of natural extracts. Our results to date will be presented.

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Effects of BNC-1 on Cell Survival and Expression of Tac2-N in a Lung Cancer Cell Line

Lauren Hale, Senior, Chemistry, University of Kentucky

Mark Lovell, Chemistry, University of Kentucky

Abstract

Lung cancer is the second most common cancer in both men and women and is most often diagnosed in older individuals (average age ~70). Because of the late diagnosis and limited therapeutic options lung cancer patients often face a poor prognosis. Current standard of care for lung cancer is largely driven by stage but generally involves surgical resection followed by adjuvant systemic therapy most often using a cisplatin-based regimen. Because lung cancer comes with a poor prognosis, there is a critical need for development of additional treatment options. Recent studies have identified a novel oncogene Tac2-N (TC2N), a tandem C2 domain containing protein that is significantly increased in multiple cancers including lung cancer. Although the specific role of TC2N in lung cancer remains unclear, recent data suggest that its overexpression may promote rapid cancerous cell growth and tumor progression through the restriction of p53 signaling, a tumor suppressor mechanism that plays a vital role in maintaining cellular homeostasis and preventing cancer development. Although recent siRNA studies demonstrate that knockdown of TC2N decreases cell proliferation suggesting it might be a suitable therapeutic target, there are currently no small molecule therapeutics that decrease TC2N expression. Based on earlier gene array studies in mice treated with a novel small molecule methyl 2,4-dimethyl-5-oxo-5,6-dihydrobenzo[c][2,7] naphthyridine-1-carboxylate (BNC-1) the Lovell lab demonstrated a significant decrease in expression of TC2N leading to testing of the molecule in a lung cancer cell line (H460). The purpose of this project was to determine whether BNC-1 is capable of decreasing TC2N, leading to decreased decrease cell proliferation in lung cancers. To test the hypothesis that BNC-1 can reduce colony formation in lung cancer cells, preliminary studies were carried out using H460 non-small cell lung cancer cells. In these cell viability studies, H460 cells were plated at a density of 250,000 cells/well in 12 well culture plates and treated for 24 hours with six varying concentrations of BNC-1 ranging from 0.1 μM to 10 μM. Controls cells were treated with 10 μL DMSO. After treatment, cell viability was measured using MTT assay, a method that measures cellular metabolic activity. Results of the assay showed that BNC-1 led to a significant dose dependent decrease in cell viability. From this, we can conclude that BNC-1 is capable of decreasing cell proliferation in lung cancers. Additional studies from the Lovell lab show BNC-1 treatment decreases TC2N.

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Lamin A and How Amino Acid Co Evolution Shape its Function

Aleena Javaid, Senior, Chemistry, University of Kentucky

Ryan Cheng, Chemistry, University of Kentucky

Abstract

Nuclear lamins play a critical role in maintaining nuclear structure and regulating genome function. In this study, we investigated the amino acid coevolution of Lamin A, encoded by LMNA, to uncover structural and functional constraints within the protein.

Amino acid co-evolution is the study of how amino acid positions in a sequence interact structurally or functionally. It can be used to predict structures and identify evolutionary relationship between species. Proteins are made up of amino acids that fold into specific 3D structures to function correctly. The shape of a protein is critical in the amino acid sequence can affect its shape. In coevolution, if an amino acid at one position in the protein changes, it can affect the protein's structure. To compensate for this, another amino acid at a different position may also change (co-adaptive change) to maintain its structure.

Full-length Lamin A sequences were obtained from public repositories and aligned using a PF00038 Hidden Markov Model to generate a multiple sequence alignment (MSA) that distinguishes conserved residues (represented in uppercase) from less conserved regions (lowercase and gaps). We then ran the DCA (Direct Coupling Analysis) to predict the contact pairs (originally computed in alignment coordinates) to full sequence coordinates and generate scatter plots for the top predicted contacts (e.g., top 20, 50, 100, 200, and 400 pairs).

Next, we walked through the full sequence's uppercase residues in order and, starting at a designated pointer in the alignment sequence, locate the first uppercase letter that matches the current full-sequence residue. This procedure records a mapping that captures the order of the uppercase residues (i.e., first uppercase, second uppercase, etc.), their actual indices in the full sequence, the alignment file index (column) where the match is found, and the residue letter. Finally, we produce a table with three key columns: the full sequence position (count order of the uppercase residue), the matching alignment position, and the residue letter.

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Synthesis of Chiral Amines for Piezoelectric Applications

Claire McGuire, Senior, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky
Michael Wells, Chemistry, University of Kentucky

Abstract

As global climate change and its effects accelerate, the need for innovative and sustainable energy becomes increasingly urgent. One energy source that remains largely untapped is piezoelectricity. Piezoelectricity involves the generation of electricity from certain materials in response to mechanical stressors. In order to produce a piezoelectric effect, we must synthesize a non-centrosymmetric material. Our research focuses on creating new materials that can serve as efficient piezoelectric generators. We are developing a synthetic pathway that converts chiral amines into chiral ammonium salts, which are then combined with iron thiocyanate to form new crystal structures. By developing new piezoelectric materials, we hope to contribute to the development of clean power generation technologies for a more sustainable future.

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Inelastic Neutron Scattering Studies of 72Ge

Logan Martin, Senior, Chemistry, University of Kentucky

Erin Peters, Chemistry, University of Kentucky
Blake Lopez, Chemical and Materials Engineering, University of Kentucky

Abstract

Shape coexistence—a phenomenon in which atomic nuclei exhibit multiple distinct shapes at nearly the same energy—has been observed in numerous isotopes, but its persistence throughout the nuclear landscape is still an open question. The Ge isotopes are of current interest for investigating shape coexistence. These isotopes are also of particular interest for neutrinoless double-beta decay (0νββ) studies. Accurate nuclear structure data are essential in calculating the nuclear matrix elements for 0νββ studies.

In this work, the isotope ^{72}Ge is investigated through inelastic neutron scattering. This study extends previous work on neighboring isotopes ^{74}Ge and ^{76}Ge, conducted at the University of Kentucky Accelerator Laboratory (UKAL). Neutrons were produced via the ^{3}H(p,n)^{3}He reaction and directed onto an enriched ^{72}Ge target at incident energies ranging from 2.0 MeV to 4.0 MeV. Emitted γ-rays were detected using a high-purity germanium (HPGe) detector mounted on a goniometer that allows the carriage to rotate around the scattering sample. These two experimental variables enable the construction of excitation functions and angular distributions.

In studying ^{72}Ge, a newly identified 2241 keV γ-ray, along with a correlated 1346 keV γ-ray, suggests the presence of a previously unreported excited state near 3075 keV. The assignment of this new level is supported by consistent neutron energy thresholds and the shapes of corresponding excitation functions.

To further investigate the properties of the observed states, angular distribution measurements were performed at 4.0 MeV. By analyzing the angular dependence of γ-ray intensities, we aim to determine the multipolarities of the observed transitions, providing crucial constraints for spin and parity assignments. These angular distributions not only support the proposed 3075 keV level but also contribute to a more complete picture of nuclear deformation and collective motion in ^{72}Ge. These results offer new insight into the low-lying level structure of ^{72}Ge. Future work will include theoretical modeling to refine our understanding of the nuclear structure in this region.

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Glysoaminoglycan-Interacting Small Molecules (GISMOs): Therapeutics for Transthyretin Amyloidosis

Ryan Leocata, Junior, Chemistry, University of Kentucky

Paul Gregor, Gismo Therapeutics

Abstract

Transthyretin Amyloidosis (ATTR) is a disease caused by disassociation, misfolding and accumulation of transthyretin protein as amyloid fibrils in the heart and nerves resulting in myocarditis, congenital heart failure, and peripheral neuropathy. Through either genetic predisposition or acquired misfolding, ATTR is estimated to affect 1/5,800 people worldwide. The disease state begins in one area and progressively spreads to neighboring regions through a process known as “seeding-and-spreading.” The misfolded and aggregated TTR acts as a “seed,” promoting functional TTR proteins into become amyloidogenic and propagating from one cell to another. Heparin Sulfate-Glycosaminoglycan (HS-GAG) is a cell surface receptor for aggregated TTR, binding of TTR to HS-GAG leads the TTR complex to endocytosis and spread pathological TTR to neighboring cells.

Current treatments for the disease target the stabilization of the tetramer form of TTR in familial ATTR to restore the function of TTR. However, currently, there are no known disease modifying treatments for ATTR. We developed Glycosaminoglycan Interacting Small Molecules (GISMO) inhibiting the interaction between amyloid proteins and HS-GAG. Utilizing competitive inhibitors of TTR binding to the HS-GAG of the cell surface membrane could prevent endocytosis of pathological TTR and eventually block the spreading of the pathology. We have developed an ELISA-based assay system to inhibit interaction between TTR and Heparin (a surrogate of HSPG). With Elisa-based binding assays, we have screened over 1000 compounds and selected compounds that have shown ability to significantly inhibit the binding step of the disease’s pathology.

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TRAPing CreERT2 active cells within Post Injury Time Window

Marissa Harris, Senior, Chemistry, University of Kentucky

Adam Bachstetter, College of Medicine, University of Kentucky

Abstract

TRAP is Targeted Recombination in Active Populations, and its an approach to gain access to neurons that are initiated by distinct stimuli. In TM dependent recombinase CreERT2 the shown in from the loci of immediate early genes Fos. Fos is an Immediate early gene (IEG) that are transcription factors that regulate cellular function by downstream transcriptional programs and neuronal function. Using FosTRAP mice allows the IEG to be used as a marker for neurons that are active during a short time window prior to sacrifice.

FosTrap mice injected to show where CreERT2 is present. Since CreERT2 can only undergo recombination when TM is present and under a limited time window, 24 hours gives a reasonable time for the TM to metabolize and being compare the activated stimuli from 12 hours. With Rosa26 (R26), this allows for high level of expression of a fluorescent protein tdTomato. This, when combined with the CreERT2 expressing cells to undergo recombination and allow the “TRAPed” causing a permanent expression of the effector gene. 24 hours is a good time window because due to IEG transcription CreERT2 is only shown for a limited amount of time and TM is also limited by metabolism and excretion so trapping the neurons around a short time period would yield best results

A total of 10 females will be used in this experiment. Mice will be injected with tamoxifen (150 mg/kg, i.p.) 24 hours prior surgery (CHI or SHAM) and sacrificed 6 days post-surgery time point. Mice will be perfused, the brain collected and fixed in PFA 4% overnight.

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Evaluating the Stability of Iron Electrodes for Organic Electrochemical Transistors via Surface Modification

Nathan Bermeo-Ramirez, Junior, Chemistry, University of Kentucky

Kenneth Graham, Chemistry, University of Kentucky
Jessica Bone, Chemistry, University of Kentucky
Henry Pruett, Chemistry, University of Kentucky

Abstract

Organic electrochemical transistors (OECTs) are a promising device in the field of bioelectronics for their ability to sense low concentrations of ions and convert that signal into an electrical output. OECTs can be used in smartwatches, in vivo sensors, and in agricultural field sensors. In these applications the OECT can sense electrolyte levels in sweat, neurotransmitters like dopamine from the nervous system, and nitrates, moisture, and ammonia in soil. Due to their integration in biological environments, there is a need for non-toxic, biologically compatible, and degradable electrode material for use in the OECT. Currently gold and silver are popular metal choices when constructing an OECT but not cost effective or degradable.

This work evaluates iron as a promising alternative electrode material despite its limited use in organic electronics. Iron is prone to oxidize in biologically relevant conditions. To prevent unwanted oxidation and increase stability, iron surfaces were modified with phosphonic acids then tested for stability in aqueous and non-aqueous solutions. Octylphosphonic acid (OPA) was shown to increase iron stability more than phenylphosphonic and bisphosphonic acid and bare iron. OPA showed higher stability when soaked in water and salt water across 48-hours. Cyclic voltammetry of poly(3-hexyl thiophene) (P3HT) on iron and OPA modified iron showed stability in non-aqueous solutions for 20 cycles. However, when tested in 0.1M NaCl in water, the electrode and polymer degraded within 1 cycle. Given that iron did not demonstrate sufficient stability in the listed experiments, observing and measuring the whole surface coverage of OPA on the iron or changing the self-assembled monomers (SAMs) can motivate future experiments to help increase the stability of iron.

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