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**FIRST-PRINCIPLES STUDY OF DEFECT FORMATION ENERGIES IN GRAPHENE AND CARBON NANOTUBES**

**Marasini, Bishal and Sanjiv Jha**, East Central University

Presence of structural defects in graphene and carbon nanotubes (CNTs) can dramatically modify their properties. We apply first principles density functional computational method to study the formation energies of Stone-Wales defects and di-vacancies in carbon nanomaterials. Our calculations were performed using the Quantum ESPRESSO electronic structure package. Graphene sheets were modeled using 4x4, 5x5, and 6x6 hexagonal supercells containing 32, 50, and 72 carbon atoms, respectively. Armchair (10,10) CNT was modeled using a periodic supercell containing 160 carbon atoms. Stone-Wales defects in carbon nanomaterials were produced by the in-plane rotation of C-C bonds by 90° about their center, whereas the di-vacancy defects were created by removing two adjacent carbon atoms. Our calculated formation energies for studied supercells of graphene were in the range of 4.0 eV to 5.0 eV for Stone-Wales defects, and 6.0 eV to 7.0 eV for di-vacancies. In the case of the (10,10) CNT, the formation energy for Stone-Wales defects was calculated to be 4.39 eV. The computing for this project was performed at the OU Supercomputing Center for Education & Research (OSKER) at the University of Oklahoma (OU).

**AN AUTOMATED QUALITY MEASURE OF SENTENTIAL PARAPHRASES**

**Duong, Thanh, Robert Owens, and Thanh Thieu**, Oklahoma State University

Measuring quality/fluency of sentential paraphrasing is a challenging task that traditionally requires human annotation. By building learning-to-rank machine learning models, we present a novel method that works automatically and balances two conflicting criteria: semantic similarity and lexical diversity. Using machine translation features including edit distance, BLEU, ROUGE, and cosine similarity, we built models to measure quality of differentiation between a paraphrase and its reference sentence. Extrinsic evaluation on STS Benchmark and ParaBank Evaluation datasets resulted in a model ensemble with moderate to high accuracy. We applied our method on both small benchmarking and large-scale datasets as resources for the community.

**TRANSPORT AND RECOVERY OF ALUMINUM OXIDE NANOPARTICLES THROUGH LIMESTONE AND DOLOMITE PACKED COLUMNS**

**Maples, Randall and Mitchell Wallis**, East Central University

Metal oxide nanomaterials are used in applications such as materials coatings, sensors and even drug delivery. Because of this, there is the increased potential of these engineered nanoparticles being released into the environment as contaminants when devices and materials containing these are disposed of. The environmental toxicity of such materials has not been fully fleshed out due to the variety of engineered nanoparticles. It is important to assess the short and long-term fate of these engineered materials and their distribution in groundwater. This study looked at the synthesis, transport and recovery of water dispersible functionalized aluminum oxide nanoparticles through packed stone columns as models for the local groundwater environment.

## **COVALENT FUNCTIONALIZATION OF DEFECTIVE GRAPHENE AND CARBON NANOTUBES BY BENZYNE: A DENSITY FUNCTIONAL THEORY STUDY**

**Brown, Kellan and Sanjiv K. Jha**, East Central University

We performed density functional theory calculations to study the covalent functionalization of pristine and defective graphene and carbon nanotubes (CNTs) with benzyne. Our calculations were carried out using the Quantum ESPRESSO electronic-structure package. Graphene sheets were modeled using 4x4, 5x5, and 6x6 hexagonal supercells containing 32, 50, and 72 carbon atoms, respectively. Armchair and Zigzag CNTs were modeled with periodic supercells containing 128 to 160 carbon atoms. Stone-Wales (SW) defects in carbon nanomaterials were created by rotating C-C bonds by 90° about their center, whereas the double vacancy (DV) defects were created by removing two adjacent carbon atoms from graphene and CNTs. The binding energies of benzyne functionalized graphene and CNTs were examined in cases of graphene and nanotubes containing no surface defects, containing Stone-Wales defects, and containing double vacancy defects. Our calculated results indicate that the presence of structural defects enhances the binding of benzyne to the surfaces of graphene and carbon nanotubes.

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## **COMPOUND OSW-1 INHIBITION OF SSRNA VIRUSES, INCLUDING CORONAVIRUS**

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**Brett Roberts, and Anthony Burgett**, University of Oklahoma Health Sciences Center.

The compound OSW-1, used at 1 - 30 nM concentrations, was shown to significantly inhibit the growth of many (+) ssRNA viruses. OSW-1 is a natural compound that extracted from the bulbs of the Giant Chinchinchee plant *Ornithogalum saundersiae*. The OSW-1 used in this study was synthesized in the laboratory of Dr. Burgett. The viruses tested were Enterovirus D68, Coxsackievirus A9, Coxsackievirus B2, Coxsackievirus B5, Coxsackievirus B6, Human Rhinovirus-1B and Feline Coronavirus. When cells were infected with virus then treated with OSW-1, viral growth was inhibited by as much as 4 logs. OSW-1 also significantly inhibited virus growth when the cells were prophylactically treated with the compound then infected with virus. We show that as a treatment, OSW-1 worked at much lower concentrations than other anti-enterovirus compounds such itraconazole. We also show that OSW-1 will work prophylactically to inhibit virus infection and itraconazole will not.

**\*GRAM-POSITIVE ANTIBACTERIAL SPECTRUM OF A NOVEL MELANIN-INSPIRED ANTIMICROBIAL.**

**Reed, Daniel, Toby Nelson, and Gabriel Cook**, Oklahoma State University

**Franklin R. Champlin**, Oklahoma State University Center for Health Sciences.

The Melanin-inspired core represents a novel compound having the intrinsic ability to act as scaffolding for functional groups which may possess antibacterial properties. The purpose of this study was to investigate the antibacterial potential of Melanin-inspired antimicrobial EIPE-1 and EIPE-HCl which are hydrophobic and hydrophilic, respectively. A standardized disk agar diffusion bioassay was employed to determine the susceptibility and resistance levels of twelve gram-positive and thirteen gram-negative bacteria to the nonpolar and polar EIPE derivatives. Turbidimetric growth curves were generated from batch culture growth kinetic analysis to provide preliminary mechanistic information. Five strains of *Staphylococcus aureus*, plus *Bacillus subtilis* and *Staphylococcus epidermidis* were found to be susceptible to the hydrophobic derivative EIPE-1, while other gram-positive and all gram-negative organisms exhibited resistant phenotypes at the potencies tested. Batch cultural growth kinetics revealed EIPE-1 to cause immediate bacteriolysis of *B. subtilis* and *S. epidermidis* at a concentration of 0.2 µg/mL. The more polar EIPE-HCl derivative failed to inhibit growth of any of the organisms examined. These data support the conclusion that the hydrophobic EIPE derivative EIPE-1 possesses a gram-positive antibacterial spectrum and likely acts in a cytoplasmic membrane-directed manner. The susceptibility of two methicillin-resistant *S. aureus* strains suggests that its mechanism of action does not involve the penicillin-binding proteins of peptidoglycan biosynthesis targeted by mainstream β-lactam antibiotics. The uniform resistance of thirteen phylogenetically disparate gram-negative pathogens supports the notion that intrinsic outer membrane exclusion properties may play a role in the mechanism underlying their intrinsic phenotypic resistance. Further experiments will involve treating gram-negative organisms with an outer membrane permeabilizer in an attempt to increase the efficacy of EIPE-1 by chemical sensitization. Determining the mechanism of resistance to gram-negative organisms will be valuable for expanding the EIPE-1 spectrum and the development of other Melanin-inspired derivatives.

**POSITIVE THINKING AND ANXIETY**

**Mitchell, LaDana and Alicia Limke-McLean**, University of Central Oklahoma

This current research evaluated the effects of increased positive thoughts on anxiety. Anxiety experiences include negative feelings of excessive worry, stress, and discomfort. According to Badpar et al. (2017), thoughts can have an impact on human behavior along with mental and emotional states. The goal of this research is to test if increasing positive thoughts could help to alleviate some of the negative thoughts that accompany anxiety. College students (n=346) at the University of Central Oklahoma were recruited via the university email blast system to take part in an online experimental research study. Half of the participants underwent a positive thinking exercise video and the other half viewed a control video. The Positive Thinking scale (PTS) was used as a measurement for positive thinking (Diener et al., 2009). The Brief Symptom Inventory scale was used as a measurement for anxiety (Derogatis, 1975). A 2 (within: before and after) x 2 (between: positive and control) mixed factorial analysis of variance (ANOVA) was conducted on the data. The gain for positive thinking was marginally greater for individuals who watched the positive thinking video than for individuals who watched the control video. This marginally supports that increased positive thoughts can have a decreasing effect on anxiety.

## **DEVELOPING A PREDICTIVE MODEL FOR UNDERSTANDING THE CLIMATE CHANGE IN THE STATE OF OKLAHOMA**

**Akinwale, Emmanuel and Courtney William**, Oklahoma State University.

Motivated by major challenges arising from the rapid change in the climate behavior around the world, the goal of this research project is to develop a predictive model for understanding the climate change in the state of Oklahoma using a common programming language called python. To this end, we study the last fifty years of historic climate data in the state of Oklahoma collected by the National Oceanic and Atmospheric Administration. To build a robust predictive model, we first need to clean the data to minimize the errors in them such as some missing dates then; we consider three main forecasting models, including the moving average scheme, the standard exponential smoothing, and Holt-Winters exponential smoothing. After implementing preliminary data cleaning and data preparation steps, we train each of the three models to tune their parameters. In the next step, we validate the best model within each category on the climate data of the recent few years. It was shown that the Holt-Winters model fits the Oklahoma climate data the best. This finding is further utilized to forecast the change of climate in Oklahoma in next few years. In addition to the developed predictive model, implementing a decomposition scheme, we discover that the average monthly temperature in Oklahoma has been consistently decreasing in the past few decades, particularly, in the 90s. This also proved that global warming was not the correct terminology to describe the change in the Oklahoma's climate. This research project is supported by Oklahoma Louis Stokes Alliance for Minority Participation (OK-LSAMP), conducted by the two undergraduate research scholars, Emmanuel Akinwale and Courtney Williams, and under the supervision of Dr. Farzad Yousefian a faculty member at the School of Industrial Engineering and Management in Oklahoma State University.

## **EFFECT OF TIME MANAGEMENT ON THE SLEEP HABITS OF AN UNDERGRADUATE STUDENT**

**Mitchell, LaDana and Vickie M. Jean**, University of Central Oklahoma.

Approximately 28 to 64 percent of women were reported to have sleep disorders and time management training could significantly improve the sleep quality. (Wang & Wang, 2018). Effective time management can increase the quality of sleep one receives. Various time constraints can influence a student's sleep such as vigorous course loads along with managing part-time work. Adequate sleep increases academic performance. This study was designed to encourage time management strategies in a 21-year-old female undergraduate Psychology student at The University of Central Oklahoma. Participant collected baseline data for two weeks on hours of sleep to implement behavior modification regimen. This study used a single-subject research design. Measures used to collect data include a Microsoft word document for daily journaling of the time and variables; the Google sheets software was utilized to create the graphs for visual representation of this data. Following the baseline period, the participant collected data for an additional two-weeks on the time went to sleep following the implemented time-management behavior change. Participant also began to collect data on reinforcements given and amount of time to complete assignments. Time management-skills were implemented through the process of operant conditioning using positive reinforcement. Anticipated results are that the participant will sleep at least 8 hours a night after implementing the behavior change time-management strategies.