US-Africa Forum

Nanotechnology Convergence for Sustainable Energy, Water and Environment

11-15 August, 2019

Book of Abstracts

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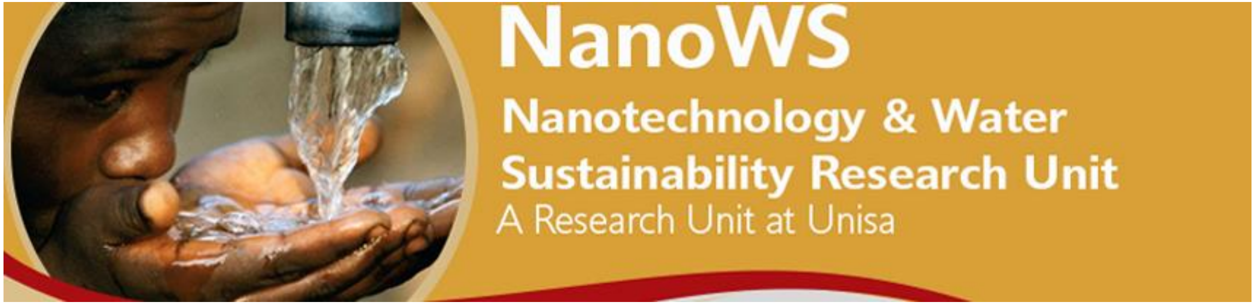

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Session 1

US/Africa Collaborations in Nanotechnology for Energy, Water and the Environment

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This paper presents an overview of some US/Africa collaborations in nanotechnology for sustainable energy, water and the environment with a focus on work done in collaboration with the Pan African Materials Institute (PAMI) at the African University of Science and Technology (AUST). These include efforts to develop materials for solar cells and light emitting devices, wind turbines, porous ceramic water filters, and bioinspired materials for sustainable buildings and transportation systems. In each of these areas, teams of U.S. and African researchers have been engaged in nanotechnology research to develop nanostructured materials that address grand challenge problems in the areas of energy, water and the environment. In the case of materials for energy, novel pressure-assisted cold welding and lamination methods have been developed for the fabrication of organic and perovskite solar cells and light emitting devices, and flexible/stretchable electronic structures. These include perovskite solar cells with power conversion efficiencies as high as 24.1%, and novel LED structures with low turn-on voltages for applications in displays and lighting. Nano-buckled and micro-buckled structures have also been developed for stretchable/flexible solar cells and light emitting devices that can be integrated into electronic textiles, while bamboo nanocomposites have been used to fabricate functioning wind turbines. In the case of ceramic water filters, nano- and micro-porous structures have been developed for the removal of microbial and viral pathogens from water. Nanoparticle structures have also been explored for the disinfection of water, while activated carbon structures and chemical doping have been used to engineer a new generation of ceramic water filters that can remove microbial/viral pathogens and chemical contaminants (fluoride, lead) from contaminated water. Finally, nanostructured biological materials are presented as sources of inspiration for the design of environmentally-friendly buildings and transportation systems. The implications of the results are discussed for future U.S./Africa collaborations in nanotechnology.

Wole Soboyejo was educated in England where he received a BSc degree in mechanical engineering from King’s College London in 1985. He then went on to obtain a PhD in materials science and metallurgy from Cambridge University in 1988, before moving to the United States to work as a Research Scientist at the McDonnell Douglas Research Labs in St. Louis, MO (1988-1992). Since 1992, he has served on the faculty at the Ohio State University (1992-1999), MIT (1997-1998), Princeton (1999-2016), The African University of Science & Technology (AUST) (2011-2014) and the Worcester Polytechnic Institute (WPI) (2016-Present). Soboyejo has also served as President and Provost of AUST (2012-2014), Chair of the African Scientific Committee, and a member of the Scientific Advisory Board of the UN Secretary General (2013-2016). He is currently serving as Senior Vice President and Provost, ad Interim, at WPI.

Safe use of nanomaterials for drinking and industrial water purification

Paul Westerhoff (Arizona State University, Tempe, AZ United States of America)

Over a past two decades the field of environmental nanotechnology and has answered several important questions related to their risks[1], and is now transitioning to the safe use of nanomaterials for treating chemicals in the environment. Based upon market usage, there is good agreement on the types of historic and new engineered nanomaterials in commerce [2]. The field has recognized that the “system” in which nanomaterials (e.g., water, soil, biota, polymers, air, etc.) occur influences their behavior (e.g., dissolution, aggregation, toxicity) [3, 4]. Analytical techniques now exist in numerous research laboratories to measure levels of nanomaterials in water and other systems, although it remains difficult to differentiate engineered from natural nanomaterials [5]. Based upon modeling and direct measurements estimates of human ingestion of engineered nanomaterials and contributions from industrial sectors, it is now possible to estimate concentrations of ENMs in sewage and treated wastewater treatment effluents that enter rivers (Figure 1). Wastewater treatment plants remove >90% of the ENM concentration from water, transferring it to sewage solids [6-8]. For example, even the most widely used ENMs (e.g., TiO_2) occur at parts-per-billion levels in wastewater effluents or rivers[8-10]. Drinking water treatment plants remove >99% of nano-sized materials, leading to parts per trillion of ENMs in tap water [11]. Consequently, based upon very low ENM exposures in drinking water, and even with uncertainty in hazards from human ingestion of ENMs, it can be concluded that ENMs pose low risks in drinking waters[12].

As the risks of ENMs appear low in drinking waters, and the community has developed tools to understand how to detect ENMs in water, there is a growing trend to focus more on the beneficial uses of nanomaterials to treat water than on further studying ENM toxicity in water towards humans. By harnessing the unique properties of ENMs there are new opportunities to use nanotechnology enabled processes to purify drinking or industrial wastewaters, to treat recalcitrant pollutants that conventional water treatment processes poorly remove, consume large amounts of chemicals, or require disposal of large amounts of solid wastes [13]. Life cycle analyses are showing opportunities for nanomaterials in several applications [14-16]. Nanomaterials can be designed to treat water by using various parts of the electromagnetic spectrum, high and selective surface area, electrical conductance, magnetism and tunable hydrophobic/hydrophilic surface properties [13, 17]. The safe use of ENMs for water treatment should be based upon several guiding scientific principles, represented by the following questions: 1) how can we use novel nano-properties for water purification? 2) when are using such novel properties superior to conventional water treatment practices? 3) How can nano-materials be embedded into scaffolding without loosing their functionality? and 4) What safety concerns exist around nano-enabled water technologies? Tunable ENM properties and opportunities to use non-chemical stimuli to activate ENMs in removing pollutants now has the recognized potential to enable fit-for-purpose water treatment through nano-enabled treatment devices that are small, portable, efficient and can be deployed throughout the water grid or in locations “off the water grid” such as homes with private drinking water wells[17].

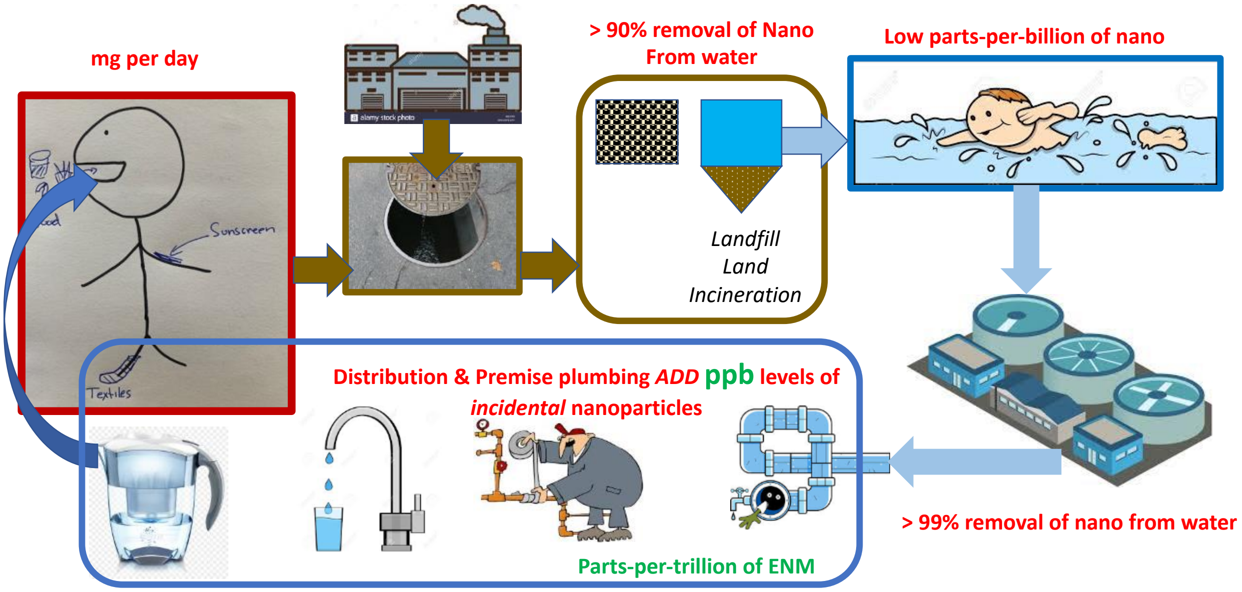

Figure 1 – illustration of human ingestion levels of ENMs, removal rates for ENMs at wastewater and drinking water treatment plants, and order of magnitude estimates for ENMs in various water sources.

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13 August

Session 1

Magnetic nanomaterials and their potential use as analytical sorbents in chemical sciences

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Abstract

Magnetic materials are attractive for incorporating in sorbents for analytical applications because of the easy separation from the sample after extraction especially for aqueous samples. This makes the whole sample preparation step simple and easy. This presentation covers some of the latest trend in the use of magnetic materials for analytical applications in the chemical sciences.

Magnetic Nanoparticles Hyperthermia: The past, the present and the future

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Small is beautiful and powerful. This conclusion is evident if one considers the aim of developing smaller and hence more efficient devices. In recent years, great progress has been made in this respect and nano-sized materials with novel properties have already found or exhibit at least a great potential for applications in the fields of, e.g., optics, magnetism, electricity, catalysis, and biomedicine. Because of their novel magnetic properties, magnetic nanoparticles offer attractive potentials not only for fundamental science value but also for technological innovations. One possible field of application of magnetic nanomaterials is their usage in biology and medicine. One example is the well-established field of magnetic resonance imaging (MRI), where effects of nanoscaled magnets on the proton susceptibility are exploited to increase the contrast in nuclear magnetic resonance imaging. The applicability of such methods relies on the fact that magnetic fields only very weakly interact with organic materials and do not cause known side effects. On the other hand, once magnetic nanoparticles are internalized in a particular organic environment such as, e.g., the human body, external magnetic fields can be applied in order to address these magnetic agents. In general, in addition to imaging methods mentioned above, external static magnetic fields can fix ferromagnetic nanoparticles at a precise position, gradient fields can move them and alternating magnetic fields will yield heating of the nanoparticles. It is the latter effect that opens a completely new route for anti-cancer therapies: Once internalized in tumor tissue, such a heating effect can be utilized for so-called ’Hyperthermia’, i.e. a therapeutic anti-cancer treatment which raises the temperature of tumor tissue in-vivo. This method applies the fact that a cancer cell-killing effect is caused when a temperature above 41-42 ^{o}C is maintained in the target volume. At higher temperatures, the effect is called ’thermoablation’. One outstanding example of the use of superparamagnetic nanoparticles is ’magnetic nanoparticles hyperthermia’ (MNH). In MNH therapy, magnetic nanoparticles are infiltrated deep into tumor tissue and inductively heated by applying alternating magnetic fields.

When aiming at realizing the promises of magnetic nanoparticles hyperthermia as independent therapy of cancer, however, many researches and challenges were required to be done in the last few years from the laboratory scale to preclinical stages. Therefore, the talk focusses on summarizing the work have been done in magnetic nanoparticles hyperthermia in the past and highlighting the present and the future directions to make hyperthermia is the future and most efficient cancer therapy.

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Dr. El-Gendy has been working in the field of magnetic nanoparticles for 17 years. His research expertise includes synthesis, characterization and applications of functionalized magnetic nanoparticles. He received his Ph.D. degree in physics from Heidelberg University, Germany 2011. From 2012-2017, He worked in various research positions on both levels academic and industry, as a postdoctoral researcher and senior scientist at Virginia Commonwealth University (VCU), Virginia (2012-2013, 2015-2017), Nanofoundary LLC., and University of Delaware (UD), Delaware (2013-2015), USA. In fall 2017, he joined department of physics at UTEP as tenure track assistant professor to establish his group in nanomagnetics and biomaterials. His work interests focus on synthesis and optimization of soft and hard magnetic nanomaterials using chemical and physical methods to be used for various types of applications such as hyperthermia treatment for cancer, drug delivery, contrast agent for MRI, rare-earth free permanent magnets, data storage, and magneto-caloric for refrigeration technology. He has published more than 50 high impact scientific papers in peer-review journals and book chapters. He is a reviewer for numerous high ranked scientific journals. In 2018, He published a book of magnetic nanostructured materials by ELSEVIER. He has participated in more than 20 international conferences and been invited for many talks. During 2015-2016, scientific newspapers highlighted his work on novel rare-earth free permanent magnet material. In addition, he holds one US-patent (US2016/0159653A1) and five US-provisional patents (US 62/546, 810), (US 62/278, 228), (US 62/278, 176), (US 62/278, 169), and (US 62/278, 164). In 2017, he has been awarded a highly competitive international young scientist award by national science foundation in China (NSFC). Based on his career achievements, his biography is listed in Marques who's who in America in 2018. Based on his acheivements, he has been awarded building scholar summer sabbatical 2019, funded by US-National Institute of Health (NIH).

Developing convergent technologies that will create better future options for our planet and our species: Abstract for Johannesburg conference

Michael E. Gorman, University of Virginia

The two tour options at the end of this conference illustrate some of the possibilities and problems facing our species:

The human origins site https://www.maropeng.co.za/content/page/fossil-sites-in-the-cradle-of-humankind shows some of the earliest hominids. They were the precursors of our species homo sapiens that now dominates the planet, domesticating many of the other species, introducing new species through genetic modification, developing extraordinary new technological capabilities illustrated by developments in nano, bio, info and cogno. The downside is that our species is causing global warming, which is raising both the temperature and the variance in the climate,

The tour of Nelson Mandela's prison reminds us of the prejudice and hostility our species is capable of. The biggest problem is our inability to work together on issues like climate change, poverty, racism and war. In this presentation I will particularly emphasize climate change but the other issues are just as important and contribute to climate change. The poor often cannot look beyond today or tomorrow—they have to get food and shelter now, and cannot afford to think of environmental consequences. War destroys environments and the people who live in them.

Convergent technologies is one of the potential routes to solving these problems but cannot succeed in doing so unless multiple expertises and stakeholders are involved Convergence requires collaboration across nano, bio, info, cogno, each of which includes specialized expertises and disciplines.

https://www.nsf.gov/od/oia/convergence/characteristics.jsp

Experts within these areas speak different technical languages and are part of different disciplinary cultures and paradigms[1]. They also have preferred methods that can dictate their choice of problems.

The solution is to get these experts into trading zones , where they can begin to exchange ideas and methods around a common goal, gradually developing a creole that allows them to communicate at a level sufficient for coordination and mutual understanding (Gorman, 2010; Collins, Evans & Gorman 2007). Here funding agencies like the NSF with its convergence initiative

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[1] Thomas Kuhn (1962) used the term paradigm to refer to a set of tacit and explicit assumptions that were part of Newtonian physics and were replaced by Einstein's in what Kuhn called a revolution. The heart of Kuhn's argument is that these assumptions become part of normal science—the paradigm clarifies what problems are most important to work on in terms of advancing a particular field, and grad students are inculcated into this way of thinking.

can be helpful—they can provide incentives for these kinds of trading zones, which must include stakeholders as well as scientists and engineers.

One of the additional expertises will be ethics, which needs to be integrated with the ongoing trading zones, exploring ethical implications and opportunities as the research and technology frontier evolves. The ethicists cannot stand apart from the invention of these new technologies; they have to be in a trading zone, too, helping to foresee ethical implications. A particularly important ethical capability is moral imagination (Werhane **), which involves realizing that one's own beliefs and attitudes are mental models and that it is important to share these mental models about desirable and undesirable futures when considering the kinds of opportunities presented by convergent technologies. One of the examples in the talk will be the problem of getting stakeholders and experts to work together on global climate change.

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Session A1

DEVELOPMENT OF FUTURISTIC ON- CHIP CONTAMINANT AND BIO SENSORS WITH Si AMLED OPTICAL SOURCES

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We have in the latter five years developed optical sources on Silicon chip that can be tuned to emit micron and nano dimensioned light emission spots ranging from 450nm - 850 nm. We have also succeeded to develop waveguides that can conduct light up to 150-micron distances on the chip with suitable electronic detectors at the end of the waveguides. We have successfully simulated the propagation of light in these waveguides. We have also successfully designed technology that will allow the light from the waveguide to couple selectively with receptor molecules that is adhered to the surfaces of the waveguide. This implies that contaminant or biospecies atoms may be selectively absorbed to the waveguide and that this absorption will induce an electronic signal that can be detected and processed on the silicon chip. The fact that optical technology is used to detect the absorption of species enables much more sensitive and reliable detection of species, since current on-chip technology normally uses capacitance induced technology or charge on MOSFET gate induced technology. Both these technologies use electrical means of detection and are prone to area wettability effects, digital signal noise interference as well as RF noise interference technology, wheras optical detection technology is immune to these effects. The sensitivity of detection to monolayer atoms are envisaged. The key innovative technology of our designs is the availability of self-developed on-chip micron and nano-dimensioned optical sources. Design and simulation work has more or less been completed. First iteration prototype sensors are currently designed using standard 0.18-micron processing technology. Characterization and further designs will be executed at the UNISA CSET laboratories in Johannesburg in the future using an ultra-high resolution optical and image analysis facility. Collaboration actions have been established with other universities in South Africa, Europe as well as in China.

Nanofibrillar electron-conducting polymer electrode for lithium-air batteries

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Abstract

The quest for batteries with high energy densities has spurred great interest in lithium-air batteries. Lithium-air batteries [Grab your reader's attention with a great quote from the document or use this space to emphasize a key point. To place this text box anywhere on the page, just drag it.]

combine a lithium metal anode with oxygen as the active species in the cathode. Despite their high energy density promise, degradation due to reactive oxygen species such as superoxides and peroxides have proven quite challenging. Conventional lithium-air batteries use carbon as the cathode matrix, but recent work has shown carbon to react with peroxide species. Therefore, there is great need to develop new cathode materials to support oxygen reduction and evolution in a lithium-air battery. To address this challenge, we designed an electron-conducting nanofibrillar polymer electrode, and show that it is capable of supporting oxygen reduction and evolution reactions in a nonaqueous electrolyte. Furthermore, we use X-ray photoelectron spectroscopy to study the stability of the electrode, and propose possible degradation pathways. Our work provides insight into electron-conducting polymers as a viable cathode for lithium-air batteries, as well as their possible limitations.

Chibueze Amanchukwu is currently a TomKat Center Postdoctoral Fellow at Stanford University. His research focuses on the design of electrolytes, and the study of ion transport processes in batteries and electrocatalytic media. In January 2020, he will be starting his independent career as an Assistant Professor in the Pritzker School of Molecular Engineering at the University of Chicago.

Capacity of sunlight driven atmospheric water capture is enhanced by photothermal nanomaterial enabled desiccants

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Removing salts and pollutants from unconventional water supplies (e.g. oceans, brackish groundwater, wastewater, stormwater) and distributing clean water within a municipality can be energy intensive, costly and produces large amounts of waste residual. Atmospheric water capture (AWC) is an alternative method of water production, whereby very low salt content water is removed from air without producing concentrated waste streams to dispose. As a hydrologic reservoir, the atmosphere contains 12,900 km^3 of water, ~14% of the volume of freshwater stored in lakes and rivers combined. Its universal presence suggests that it can be used in a variety of locations from rural homes to disaster relief scenarios and other water-stressed regions. The most advantageous applications for AWC are as an off-grid source of water, i.e. away from both the municipal water and electricity grids. Energy then is provided through the sun, via photovoltaic power or solar thermal heat.

Desiccant materials can capture and concentrate water vapor from regions with a variety of relative humidity (20-100%) and temperature (20-40^{0}C) conditions. However, an ample amount of heat (>175^{o}C for SiO_2) is required to desorb the water vapor from the desiccant prior to condensing it onto a cool surface for collection. We reduced energy demands on bulk heating of desiccants through application of photothermal nanomaterial-enabled desiccants that are light active, producing localized centers of heat directly on the desiccant surface in the presence of sunlight. Nano-enabled desiccants reach desorption temperature 10x faster than commercial silica desiccants, allowing for 3x faster rate of water vapor desorption from the desiccant. The desiccants can be cycled between adsorption/desorption/condensation phases throughout the day to produce >1 L water / gram desiccant / day.

Anjali Mulchandani is a PhD Candidate in Environmental Engineering at Arizona State University. She holds a BS in Civil Engineering from UCLA and MS in Environmental Engineering from Arizona State University. Her research interests explore solving global water, waste and energy challenges by developing novel nano-enabled materials and physical/chemical processes to improve resource sustainability. Two unique resource reservoirs she studies are the atmosphere (to capture drinking water) and sewage sludges (to recover metals, nutrients and energy). Anjali is a National Science Foundation (NSF) Graduate Research Fellow and member of NSF Engineering Research Center on Nanotechnology Enabled Water Treatment.

Size dependent modeling and performance enhancement of nano-scale functionally graded piezoelectric energy harvesters

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Functionally graded materials (FGMs) are a unique type of composite in which the material properties vary in one or more directions from one material to another. FGMs are usually composed of a metal and a ceramic. One special type of FGM is known as a functionally graded piezoelectric materials (FGPM) which can be utilized for energy harvesting applications. The FGPM of interest in this work is composed of Platinum and PZT. FGMs of these types are especially suited for energy harvesting applications because the designer can control their material properties, such as the stiffness and natural frequencies of the energy harvesting system through changes in the FGM composition and material distribution. The variation of the material properties throughout the thickness of the energy harvester causes a shift in the neutral axis of the system. The resulting shift of the neutral axis must be accounted for to obtain effective energy harvester properties and hence the accurate design of the energy harvesting system. In this work, the effect of small-scale phenomenon on the natural frequencies and power density of micro- to nano-scale functionally graded energy harvesters is investigated. The modified couple stress theory is used to account for micro-rotations within the surface elasticity theory is used to account for the residual stresses on the surface of the energy harvester. Both small-scale effects depend on the material parameters that vary throughout the thickness of the FGM. Size-dependent effects have a significant influence on the design and performance of effective micro/nano energy harvesters. Couple stress and surface elasticity both cause significant increases in the effective stiffness of energy harvesting systems. Therefore, neglecting these effects can lead to underestimation of the natural frequencies of the harvester and lead to ineffective designs.

Kevin Larkin is a PhD candidate in the Department of Mechanical & Aerospace Engineering at New Mexico State University. His research interests include nanotechnologies, nonclassical continuum mechanics theories, energy harvesting, and multi-scale modeling. Kevin is currently working as student guest at Los Alamos National Laboratory.

Session A2

Antimicrobial effect and anti-biofouling performance of sulfidized silver nanoparticles on RO Membranes

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Silver, a known biocide, is used for the *in-situ* formation of silver nanoparticles (Ag-NPs) on reverse osmosis (RO) membranes for biofouling mitigation. Biofouling has become an issue because it shortens membrane life expectancy; along with, increasing hydraulic resistance, and decreasing water flux affecting the water treatment process. Ag-NPs are soluble, limiting their effectiveness over a long period of time. This study focuses on functionalizing silver membranes with different concentrations of Na_2S to form a partial Ag_2S layer to slow down the release of silver nanoparticles while maintaining antimicrobial activity. Different concentrations of Na_2S (10^{-1}, 10^{-3}, and 10^{-5} M) were evaluated to identify the degree of sulfidation that can preserve the antimicrobial effect. An *Escherichia coli (E.coli)*-based assay was used to quantify the antimicrobial activity of the functionalized membranes at the different sulfidation levels. As expected, our results showed a negative relationship between sulfidation and antimicrobial activity; silver-functionalized membranes treated with higher concentrations of Na_2S resulted in lower toxicity to *E. coli*. However, when tested in a dynamic cross-flow RO system, the less soluble sulfidized particles were found to be more effective than the more soluble Ag-NPs for biofouling control over the course of 24h. Therefore, retention of the silver coating over time appears to be more important for biofilm control in RO systems than high antimicrobial activity. The concentration 10^{-3} M Na_2S was found to have the best balance between reduced dissolution rate and good antimicrobial and anti-biofouling performance.

Ana C. Barrios is a 3rd year Ph.D. student in the School of Sustainable Engineering and the Built Environment at Arizona State University where she joined Dr. Francois Perreault's research group. She is a member of the NSF Nano-Enabled Water Treatment Engineering Research Center and her research focuses on the mechanisms of interactions of carbon nanomaterials with bacteria and algae. Her interests include safety of nanomaterials and sustainable practices, biological interactions and material transformation after environmental exposure, and water treatment. Before joining ASU, she completed her bachelors and master's degrees in Chemistry at the University of Texas at El Paso.

Facile synthesis of self-assembled BiOI decorated cobalt oxide microspheres and its applications for mineralisation of pharmaceuticals

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Water pollution is the deterioration in quality of waterbodies such as oceans, lakes, ground water, rivers and aquifers, mainly due to human activities that involve the intensive research and commercialisation of different commodities and products for socio-economic development. The development of these industries, their successful operation and their sustainability thereof are of paramount importance towards generation of job opportunities, poverty eradication, and the improvement in health and sanitation. The latter resulted in numerous research and innovation evolution towards eradication of water pollution which is one of the greatest challenges of the 21st century. The issue of water pollution results from numerous human related factors which mostly lead to global warming. Numerous techniques have been developed recently towards eradication or reduction of different pollutants from wastewater except conversional treatment methods. Of the developed methods, photocatalysis using strong visible light active nano materials has gained attention because of the opportunity towards using profuse and abundant visible light. Photocatalysis includes the generation of reactive oxygen species which initiate redox reactions for removal of pollutants from water bodies. Cobalt oxides and Bismuth oxyhalides are known for their strong visible light absorption and photocatalytic properties and the design of photocatalysts involving these semiconductors present the perfect opportunity towards light harvesting. Despite being cheap to synthesise, Co_3O_4 and BiOI have a strong visible light absorption. The synthesised nanocomposites were characterised with XRD, UV-Vis, PL, FTIR, HRTEM and used towards degradation of pharmaceuticals which are one of the major emerging pollutants of the 21st century due to their bioaccumulation and formation of metabolites that may be more hazardous than the parent pharmaceutical. The improved efficiency was determined to be due to the formation of a heterojunction towards mineralisation of selected pharmaceuticals.

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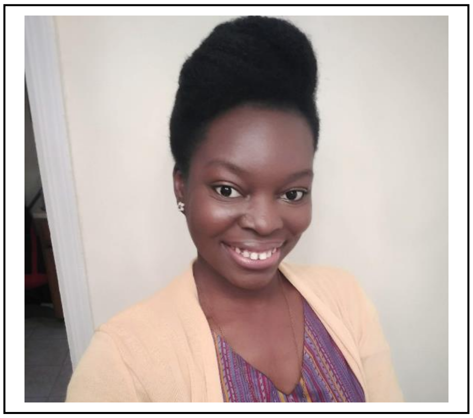
Ceramic Water Filters and Removal Mechanisms of Bacterial, Chemical and Viral Contaminants.

V. Uzonwanne, P. M. Nigay, A. A. Salifu, J. D. Obayemi, C. E. White, A. Nzihou, and W. O. Soboyejo

Abstract

This paper reports on the removal of chemical contaminants from drinking water using activated carbon and hydroxyapatite nanoparticle additives in ceramic water filters (CWFs). Sources of drinking are liable to contamination from industrial wastes and other human activities. The accompanying severe health implications make it necessary to remove these chemicals as part of the water purification process to render the water safe for drinking. Hence, in this work, we explore the doping of micro-and nano-porous CWFs with activated carbon microparticles and hydroxyapatite nanoparticles for the removal of organic (nitrates) and inorganic (lead, excess fluorides) chemicals, respectively, from contaminated water. The mechanisms of removal of these chemicals by the doped-CWFs as well as the effect of the dopants (hydroxyapatite and activated carbon) on the adhesive forces between the chemical contaminants and CWFs are also elucidated. The results highlight dopant-dependent increases in the removal efficiencies of nitrates, lead and fluoride by the CWFs, driven by improved adhesion interactions between the chemical contaminants and the CWFs that are partly due to the increased specific surface areas of the latter. The implications of the results are then discussed for the design of doped-CWFs for the efficient removal of hazardous chemicals during potable water purification.



Vanessa Uzonwanne is a PhD candidate at Worcester Polytechnic Institute in Massachusetts. Her research focuses on studying diseased biological cells as materials by characterizing them with various materials science and mechanical engineering techniques. Currently, she is exploring adhesion as a tool for the treatment of Triple Negative Breast Cancer (TNBC) cells. Her work involves the measurement of adhesion forces and adhesion energies between TNBC and nanoparticles or drugs that are designed to target breast cancer cells/tissues.

Mechanics, dynamics, and vibrations of carbon nanotubes at different stages of a targeted drug delivery process

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Abstract. In this research effort, we study the need for considering mechanics, dynamics, and vibrations points of view in the consideration of carbon nanotube-based targeted drug delivery systems. We consider the CNT acting as a type of capsule or carrier for solid or liquid drug particles that require a targeted release in the body to an unhealthy site, say a tumor. In this case, CNTs are considered as strong candidates due to their high surface-area-to-volume ratio that allows for a high concentration of particle loading. Additionally, after a functionalization process, CNTs have increased solubility and decreased toxicity in the body: an important consideration for biological applications. Now, it should be mentioned that the majority of the studies involving CNT-based targeted drug delivery are performed heavily from a chemistry, biology, and experimental points of view. Researchers studying this topic from a dynamics and vibrations of view are often overlooking the points of view of these other researchers and thus are developing models for non-physical systems with unrealistic assumptions. Therefore, one of the highlights of this research will be the identification of realistic representations of the CNT-based system at different stages of the drug delivery process. This can include, but is not limited to, identifying the effective properties before and after functionalization and loading and developing nonlinear reduced-order models to characterize the static and dynamic stability of the system as it travels through the bloodstream and reaches the injection site. In particular, a focus will be placed on modeling the surrounding viscoelastic medium with respect to the CNT at the point of drug release in the body. Primarily, we will focus on modeling the CNT-based system using beam theory that accounts for attached or encapsulated particles and size dependent phenomena using Eringen’s nonlocal elasticity. We consider this is a considerable contribution to the field, especially for those that have previously studied these types of systems from a mechanics, dynamics, and vibrations point of view that have been making non-physical assumptions. After deriving the governing equations for the system, we will analyze what types of thermal or magnetic loading can be used to release the particles from the CNT once reaching the target site when the CNT is surrounded by the viscoelastic medium, such as the blood or tissues in the body. In analyzing the results for this system, we will be able to share our points of view with experimentalists, chemists, and biologists to advance this growing field more quickly and effectively.

Samantha Ceballes is a Mechanical Engineering Ph.D. student at New Mexico State University (NMSU) in Las Cruces, New Mexico, U.S.A. She received a dual B.S. from NMSU in Mechanical Engineering and Aerospace Engineering in Fall 2017. Upon her graduation, she received the Highest Honors award in the College of Engineering. In the Summer of 2018, Samantha was awarded the National Science Foundation Graduate Student Fellowship Program to fund her graduate studies. Her research interests include nanomechanics, dynamics, vibrations, and reduced-order modeling of nano-scale structures. In particular, Samantha is interested in modeling carbon nantoubes from a structural mechanics, dynamics, and vibrations point of view for bio-mass sensing and targeted drug delivery applications. She can be contacted at sceballe@nmsu.edu

Wednesday 14th August

Session 1

SOVEREIGNTY OF NANOTECHNOLOGY FOR WASTE WATER INQUISITION PROBING SUSTAINABLE DEVELOPMENT

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Abstract

Nanotechnology is to develop and improvise newer materials, devices and systems with fundamentally diffèrent properties by exploiting unique properties of molecular and supramolecular systems at nano level. Almost all the disciplines of science and technology have been inspired by the tools and ideas of nanotechnology, and the innovations continue to be applied in medical technology, lab on chip, sensor technology, energy resources, and environmental protection and preservation. Nanomaterials are nano-sized structures and have extraordinary physical and chemical properties, such as the unique optical, electrical, thermal, magnetic and adsorption characteristics, etc., due to their ultra-small size. Large specific surface areas of nanomaterials can improve the detection sensitivity and miniaturize the devices. Also, these nanomaterials of various compositions, morphologies can provide powerful tools for improving water quality analysis, monitering, detection and remediation. The current talk will summarize progresses and advancement of nanotechnology for wastewater research providing sustainable developments and solutions.

Session A3

Multiscale Simulations of Extracellular Electron Transfer across Multiple-heme Proteins

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Dissimilatory metal-reducing bacteria (DMBR), e.g., *Shewanella oneidensis and Geobacter metallireducens*, are capable of dissimilatory metal-reducing insoluble mineral oxides, such as Fe(III) and Mn(III/IV) oxides, by transferring electrons from the interior of the cell to the exterior through multi-c-type cytochrome nanowire assembly in an anaerobic environment. Extracellular electron transfer (ET) of DMBR has important applications in bioremediation of contaminated water and soil. The interfacial behavior (orientation and structure) of outer-membrane multiple-heme protein is key to extracellular electron transfer (ET) and redox. To tackle computational challenges in across a range of scales, involving protein conformation changes and ET, a multiscale theoretical framework was developed by synergistically combining individual simulation techniques, including mainly molecular dynamics (MD), free energy computation and first-principle kinetic Monte Carlo based on Marcus ET theory and quantum computations. In this work, decaheme MtrF adsorption on an Au (111) surface in water and the ET across the protein were studied as a model system. Our results revealed that the gold surface's dehydration serves as a crucial driving force for protein adsorption due to large surface tension. The most possible adsorption orientation is with the ET terminal (heme5) approaching the gold surface, yielding a pathway for ET between the substrate and the aqueous environment. Upon adsorption, protein's secondary structures and central domains (II and IV) bonded with heme-residues remain relatively stable. MtrF surface mobility is dictated by thiol-gold interaction and strong binding between Au(111) and peptide aromatic groups. The ET transfer rate across protein heme-network along the solvent-to-surface direction is slightly larger than that of the reverse direction, but lower than that of the solvation structure.

Tao Wei is an assistant professor of Chemical Engineering at Howard University, Washington, D.C. He joined Howard in 2017, after four years on the chemical engineering faculty at Lamar University, Texas. Dr. Wei got his PhD degree in Chemical Engineering from University of Southern California in 2008, and trained as a postdoctoral researcher at both Northwestern University and University of Pennsylvania. Dr. Wei's research focuses on fundamental studies of materials interfaces, especially bio-nano hybrids, for the purpose of developing functional materials and biotechnologies to tackle challenges in health, energy and environment. To achieve optimal functional design, he combines in-house developed multiscale simulation frameworks (quantum, atomistic, mesoscopic and continuum scales) with theories (Statistical Mechanics and quantum) with experiments at the interface between chemistry, physics and biology. His research works have been given media highlights by NSF/XSEDE and **Texas Advanced Computing Center (TACC).** His projects on biosensor development are currently funded by NSF and NASA/JPL.

Chitosan-guar gum polymer blend for the removal of mercury in aqueous solution.

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Keywords: mercury, chitosan, guar gum, adsorption, water pollution.

Water pollution by mercury (Hg^{2+}) from industrial activities is of great concern due to its hazardous effects in human beings and the environment. Mercury is non-biodegradable and can easily enter the food chain through accumulation of living organisms. The World Health Organisation (WHO) considers mercury as one of the top ten chemicals of major public health concern with the maximum allowance of 1 ppb in drinking water and maximum uptake of 0.3 mg/week[1]. Various technologies have been developed for the removal of mercury which include filtration, coagulation, precipitation and adsorption. However, most of these methods are not cost effective, have low removal efficiency and need further treatment. Among these technologies, adsorption is considered to be the most economical technique used for the removal of mercury due to its ease of operation, it's applicable at very low concentration, and the availability of wide range of adsorbents[2]. A novel adsorbent used for the removal of mercury from aqueous solution was prepared by solution blending of chitosan and guar gum polymers. Batch adsorption experiments were conducted to study the effect of pH, adsorbent dosage, initial concentration, time and agitation speed for the removal of mercury. The adsorption behaviour was analysed using isotherms and kinetics models. The chitosan-guar gum blend showed to be an effective adsorbent for mercury removal with the adsorption capacity of 92 % at dose (50 mg), pH (12), time (60 min), initial concentration (50 ppm) and agitation speed of 180 rpm.

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A Potential Role for *Shewanella oneidensis* MR-1 and Community 31 in the Dissimilatory Microbial Reduction of Iodate at the Hanford Site

Tafadzwa Chigumira, Ayomikun Olarinoye, Deondre Glover, Dr. Patrick Ymele-Leki, Dr. Yaolin Fennell, Dr. Kimberly Jones
Institution: Howard University, Chemical Engineering Department

Radioiodine-129 (I^{129}) from leaking nuclear waste storage tanks is one of the major contaminants of groundwater at the Hanford Site in Washington State. Speciation of I^{129} in the contaminated groundwater is predominantly as iodate, organo-iodide and iodide. A forthcoming bioremediation solution is to use microbial dissimilatory reduction of iodate to iodide. *Shewanella oneidensis* MR-1 (*S.oneidensis*), a strain of bacteria known to reduce silver and uranium, was investigated in this study for its potential to serve as a bioremediation agent against iodate. For this purpose, *S.oneidensis* was grown in minimal media in the presence of iodate under both aerobic and anaerobic conditions for 24 hours. Iodate speciation was monitored by colorimetric assays with UV Spectrophotometry. Data suggest that *S.oneidensis* could reduce iodate content in the medium by 30.9% in aerobic conditions, whereas no reduction was observed in anaerobic conditions. Additionally, iodate reduction experiments using a community of bacteria collected from groundwater at the Hanford Site, named Community 31, suggest the presence of local iodate reducing bacteria. Results showed that the community may be capable of reducing iodate by 36.3% aerobically. Reduction was not observed in anaerobic conditions. Preliminary experiments testing *S.oneidensis*'s reduction capabilities in concert with Community 31 produced average percent iodate reduction of 36.3% in aerobic conditions and 9.9% in anaerobically.

Findings from these experiments could lead to the development and design of novel facultative anaerobic bioreactors for the bioremediation of groundwater, soils and sediments.

Tafadzwa Lisa Chigumira grew up in Zimbabwe where for much of the population, products beyond clean water and staple foods are luxuries. As a child, she had a difficult time understanding why diseases such as cholera and malaria were particularly devastating for the poor, while people of means where seemingly impervious to the problems. She found hints of solutions in her studies of the sciences and when she moved to the United States of America, she maintained her interest in the field. She was appalled to discover that while cholera and malaria were not in the purview of American problems, conditions such as lead poisoning and cancers from pollutant carcinogens, were devastating particularly for the poor. To better understand and tackle the apparent link between poverty and disease, she completed a Bachelor of Science in Chemical Engineering at the University of South Florida and proceeded to enroll in a Master's in Chemical Engineering at Howard University. Her thesis research at Howard University is centered on the use of microbial agents to tackle groundwater contamination by nuclear waste. In the future she plans on continuing research in groundwater and wastewater treatment. She hopes to gain experience and influence environmental and engineering policy making, as policies can provide protection and preventive measures against the systematic failures that lead to pollution and disease in low income areas.

Fate of natural organic matter at a full-scale drinking water treatment plant in the Gauteng province of South Africa: Insights from optical spectroscopy coupled with chemometric analysis

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Abstract

The transformation of natural organic matter (NOM) due to treatment processes at a water treatment plant (WTP) in South Africa was studied using biodegradable dissolved organic carbon (BDOC) and polarity fraction dynamics with insights from UV-Vis absorbance, fluorescence excitation-emission matrix, and two-dimensional synchronous fluorescence spectroscopy (SFS). The objectives of the study were: (1) to investigate the transformations of NOM brought about by treatment processes applying chemometric analysis and two-dimensional SFS correlations, and (2) to quantify the concentrations and chemical profile dynamics of polarity and BDOC fractions throughout the treatment train. The UV_{254} absorbance along the WTP was reduced by 45% at the final stage. The UV-Vis data fitted onto the Gaussian model showed a decreasing trend in intensity and number of bands down the treatment train. The removal efficiency of NOM components followed the order: humic-like (HL) > tyrosine like (TYL) > fulvic like (FL) > tryptophan like (TPL) > microbial like (MBL). At the source, the relative distribution of the hydrophobic (HPO), hydrophilic (HPI), and transphilic (TPI) fractions was 45, 31 and 24%, respectively. The HPI was recalcitrant to the treatment processes, and the tyrosine-like component of the HPI fraction was conjectured to be a disinfection byproduct limiting reagent. The HL and FL components of the BDOC fraction were the major substrates for bacterial assimilation. According to two-dimensional-SFS correlation (2D-SFS), TYL, TPL, and MBL varied concurrently as water passed through the different treatment stages. For the first time in South Africa, this study has revealed the robustness of a multi-dimensional approach of optical methods coupled with chemometric tools for the assessment of the fate of NOM throughout the treatment processes.

Keywords: biodegradable dissolved organic carbon; natural organic matter; polarity rapid assessment method; Synchronous fluorescence spectroscopy; two-dimensional correlations.

Session A4

Probing the emergence of microscale structure in multicomponent functional membranes

Rachel R. Ford, Joey D. Kim, Mamadou S. Diallo, & Julia A. Kornfield

Sustainable chemistry, resource recovery, and water purification from nonconventional sources necessitates the development of new multicomponent functional materials. Such materials allow one to exploit the favorable properties of different components while mitigating their individual drawbacks, striking a balance between function, stability, and ease of fabrication. Performance of these materials largely stems from complex structure across a broad range of length scales, as sub-nanometer molecular interactions propagate to micrometer-scale phase transitions. Understanding structure formation and the interplay of different components is therefore paramount to realizing the full potential of such functional materials. Herein, we demonstrate a new technique to investigate structure formation using ultra-small angle neutron scattering (USANS). We apply the technique to the emergence of structure during growth of functional polymeric particles in a recently developed class of mixed matrix polymer-polymer (M2P2) membranes.

Rachel R. Ford conducts research as a graduate student in the laboratory of Prof. Julia Kornfield, under the co-advisement of Prof. Mamadou Diallo, at the California Institute of Technology. Ford is a Ph.D. candidate in Chemistry, studying polymer-based membranes for water purification and electrochemical catalysis. In particular, she uses neutron scattering techniques to understand the chemistry and physics of structure formation in a novel class of mixed matrix polymer-polymer (M2P2) membranes, with the aim of tuning the materials to various applications in sustainable chemistry.

Antimicrobial activity of Prunus Africana extract green synthesized copper and silver nanoparticles against Carbapenem resistant Escherichia Coli and Klebsiella Pneumoniae

Kenneth Ssekatawa

ACE II Nanotechnology Center, Makerere University

Atomistic Molecular Simulations of Polyamide Membrane in Desalination at Equilibrium and Nonequilibrium States

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Subnanoporous reverse osmosis (RO) of cross-linked aromatic polyamide (PA) membrane is one of the most promising techniques for water desalination. Fundamental understanding of PA RO membranes at the atomistic level is critical to the enhancement of their separation capabilities, leading to significant societal and commercial benefits. Atomistic molecular dynamics simulations were performed to investigate the relationship between PA membrane microscopic structure and membrane performance, including water permeation, water-ion separation and surface biofouling. A realistic model of cross-linked membrane has been developed by employing in-house developed hierarchical cross-linking procedure. Our results demonstrate that three structural components (parallel stacked benzene rings, T-shaped benzene rings and linearly bonded neighboring rings) as the result of benzene rings' short-range π−π stacked interactions and chemical bonding mainly contribute to the membrane's porosity. Water heterogeneous diffusive dynamics presents as a result of heterogeneous microscopic membrane structure. The membrane's interfacial roughness is crucial to protein attachment and biofouling leads to a decrease of water flux. The pore size distribution with the majority of the pore radiuses around 0.20 nm, gives rise to the membrane's water-ion selectivity. The feasibility of water-ion separation through such subnanopores is indeed controlled by the strength of the ions' dehydration free energy in addition to the size of a hydration cluster. Water molecules in the formation of water chains in less crosslinked area facilitates their transfer through the PA membrane subnanopores. The water flux linearly increases with the increase of the applied pressure drop (5-30 MPa), indicating that the membrane internal overall structure remains unchanged.

Magnetic Nanostructured Materials for permanent magnets and data storage applications

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Magnetic nanostructured materials (MNMs) are involved in all the advanced technology nowadays. While you are reading this abstract maybe few minutes ago you have checked your phone, or you may even be reading this chapter on your tablet or laptop. It is curious that while you try to learn about MNMs, you are surrounded by them. MNMs are used in a wide variety of devices including electronic devices, motors and generators, hard disk drives, magnetic refrigeration and even in general home appliances (e.g. washing machines). Therefore, small is beautiful and powerful. Magnetic nanoparticles can be classified to soft or hard magnetic materials. Soft magnetic materials such as Fe, Co, Ni or their alloys can be used for magnetocaloric effect for magnetic refrigeration as well as medical applications. The other type of the magnetic nanoparticles, which is the focus of this talk, is hard magnetic materials. Co_xC, Mn_xGa, and $CoFe_xC$ nanoparticles are good examples of hard magnets, which have the property of storing magnetic energy even after removing the magnetic field. Such property are commonly used for fabrication of permanent magnets. The main advantage of such particles is due to the higher magnetic anisotropy which can act as good candidate for new generation of magnetic data storage. Magnetic characterization of the novel carbide phase (CoFe2C) revealed thermal stability up to 790 K for particles with a domain size as small as 5 nm and have giant MCE of 4.6×10^6 J/m^3 , which is ten times larger than that of Co nanoparticles. Such colossal anisotropy leads to a thermally stable long-range magnetic order.

Therefore, the talk focusses on the synthesis of CoxC, MnxGa, CoFexC magnetic nanoparticles and their potential for permanent magnets and data storage applications.

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Dr. El-Gendy has been working in the field of magnetic nanoparticles for 17 years. His research expertise includes synthesis, characterization and applications of functionalized magnetic nanoparticles. He received his Ph.D. degree in physics from Heidelberg University, Germany 2011. From 2012-2017, He worked in various research positions on both levels academic and industry, as a postdoctoral researcher and senior scientist at Virginia Commonwealth University (VCU), Virginia (2012-2013, 2015-2017), Nanofoundary LLC., and University of Delaware (UD), Delaware (2013-2015), USA. In fall 2017, he joined department of physics at UTEP as tenure track assistant professor to establish his group in nanomagnetics and biomaterials. His work interests focus on synthesis and optimization of soft and hard magnetic nanomaterials using chemical and physical methods to be used for various types of applications such as hyperthermia treatment for cancer, drug delivery, contrast agent for MRI, rare-earth free permanent magnets, data storage, and magneto-caloric for refrigeration technology. He has published more than 50 high impact scientific papers in peer-review journals and book chapters. He is a reviewer for numerous high ranked scientific journals. In 2018, He published a book of magnetic nanostructured materials by ELSEVIER. He has participated in more than 20 international conferences and been invited for many talks. During 2015-2016, scientific newspapers highlighted his work on novel rare-earth free permanent magnet material. In addition, he holds one US-patent (US2016/0159653A1) and five US-provisional patents (US 62/546, 810), (US 62/278, 228), (US 62/278, 176), (US 62/278, 169), and (US 62/278, 164). In 2017, he has been awarded a highly competitive international young scientist award by national science foundation in China (NSFC). Based on his career achievements, his biography is listed in Marques who's who in America in 2018. Based on his acheivements, he has been awarded building scholar summer sabbatical 2019, funded by US-National Institute of Health (NIH).

Session A5

Atmospheric Water Capture: A decentralized on-demand drinking water technology

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NSF Nanosystems Engineering Research Center for Nanotechnology Enabled Water Treatment

Limited access to clean water due to natural or municipal disasters, drought, or contaminated wells is driving demand for point-of-use and humanitarian drinking water technologies. Whereas centralized potable water costs $1-5 / kilogallon, bottled water costs >$1000 / kilogallon. There is significant economic space for technologies capable of providing the flexibility of bottled water without the infrastructure required for centralized municipal potable water. Atmospheric water capture (AWC) is a competitive technology that provides clean drinking water on demand, does not require fixed physical infrastructure such as pipelines, and does not produce large concentrated waste streams associated with contaminant or salt removal from liquid water supplies.

We have developed geospatial and climatic models for passive solar desiccant driven AWC, in which water vapor is adsorbed onto a desiccant bed at night, desorbed by solar heat during the day, and condensed. AWC volume can vary between 0.5 – 2.5 $L/m^2/day$ as a function of material properties and climatic region of operation, but the quantity of solar thermal energy available to achieve complete desorption of the desiccant can be limiting. Therefore, we developed photothermal nano-enabled desiccants that superheat under sunlight, which increases the rate of desorption, and even allows for more operation of 2 or more AWC cycles per day. Moving from passive to active systems, we are operating commercial dehumidifiers (desiccant and dew point condensation systems) outdoors in a semi-arid climate to benchmark water production, energy efficiency and water quality. The energy cost of AWC is competitive with bottled water. Water quality of desiccant systems exceeds US EPA regulations for tap water, while dew point condensation systems require minor treatment to remove dust.

Anjali Mulchandani is a PhD Candidate in Environmental Engineering at Arizona State University. She holds a BS in Civil Engineering from UCLA and MS in Environmental Engineering from Arizona State University. Her research interests explore solving global water, waste and energy challenges by developing novel nano-enabled materials and physical/chemical processes to improve resource sustainability. Two unique resource reservoirs she studies are the atmosphere (to capture drinking water) and sewage sludges (to recover metals, nutrients and energy). Anjali is a National Science Foundation (NSF) Graduate Research Fellow and member of NSF Engineering Research Center on Nanotechnology Enabled Water Treatment.

Development of a model to be used as an indicator of oily wastewater pollution, fingerprinting and compliance using dimensional analysis.

Lerato Monatisa. Azizallah Izady., Lueta. A. de Kock., Bhekie. Mamba. Thabo T.I. Nkambule., Titus A.M. Msagati
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With the increase in industrial processes and activities, the amount of oil used is also increasing, thus causing more stress in terms of management and treatment of wastewater. Oily wastewater pollution has mainly been reported to cause hazards to both organisms and the environment by endangering aquatic resources, affecting drinking water and groundwater resources, endangering human health; affecting crop production; cause of atmospheric pollution; destructing the natural landscape, and even cause safety issues due to use of coalescence of the oil burner that arise. Due to this, oily wastewater must be treated to comply with state, and local regulations. Industries and Companies that deal with activities that lead to the discharge of oily wastewater need to comply to the regulations which enforce them to ensure that the characteristic of their effluents meet the stipulated criteria. Effluent quality requirements for discharge of oily wastewaters to the municipal streams are determined by local and municipal authorities and, therefore, may vary from place to place. In this project we report on the development of a model that can be used to indicate the quality of oily wastewater discharged into municipal channels by using a measure of evaporation patterns. This is possible because certain parameters normally present in oily wastewater has a direct relationship with the rate and pattern of evaporation. Due to the complexity of the relationship between the parameters that are being measured, it is imperative to employ dimensional analysis based on Buckingham pi theorem for estimating OWE (oily wastewater evaporation) as a function of CWE (clear water evaporation) and climatic parameters. The parameters that are investigated in this project includes climatic parameters: Wind Speed (W), Solar Radiation (R), Air temperature (Ta), while the environmental parameters are: oily wastewater temperature (Tow), Electric Conductivity (EC), Total Dissolved oxygen (TDS), Total Suspended solids (TSS), Biochemical Oxygen Demand (BOD), Chemical Oxygen Demand (COD), Total Petroleum Hydrocarbons (TPH) and Total Organic Carbon (TOC).

Keywords: modeling, evaporation, oily wastewater, environmental parameters, climatic parameters, dimensional analysis

Electrospun Superhydrophobic/Superoleophilic CNTs-modified PVDF Nanofiber Membranes for Oil/Water Separation

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The presence of fats, oils and grease (FOGs) in wastewater systems is a global concern. While water quality remains the critical challenge, the introduction of these FOGs into wastewater poses yet another setback that threatens our ecosystem. The high levels of FOGs in the water bodies is exacerbated by industrial discharge from the leather, textile, food, steel, petrochemical, mining companies as well as urban infrastructure commodities [1]. For example, there are 8 crude oil refinery industries and 16 edible oil refineries in South Africa as reported by Department of Water and Sanitation. These companies dispose approximately 1.4 billion litres of oily wastewater which is subject to treatment by the Wastewater Treatment Plants. However, the complete removal of the FOGs during water purification processes remain a critical challenge [2]. Remarkably, the use of superhydrophobic/superoleophilic based materials is envisaged as an alternative solution for the removal of FOGs where high separation efficiency and selectivity are anticipated [3]. In this work, novel electrospun carbon nanotubes (CNTs)-modified polyvinylidene fluoride (PVDF) were fabricated *via* a facile electrospinning method and tested for removal of the FOGs from water. The PVDF-CNT nanofiber membranes were characterized using FTIR and XRD spectroscopy, SEM, BET, AFM, and TGA among other techniques. The SEM studies confirmed the formation of the uniform nanostructured PVDF-CNT membranes (**Fig. 1**). Additionally, the as-synthesized PVDF-CNT membrane mats were characterised by high mechanical strength and high surface tension. The removal of FOGs was evaluated using filtration systems where excellent removal efficiency was recorded. These PVDF-CNTs nanofiber membranes are anticipated to serve as alternative materials for industrial removal of FOGs from wastewater.

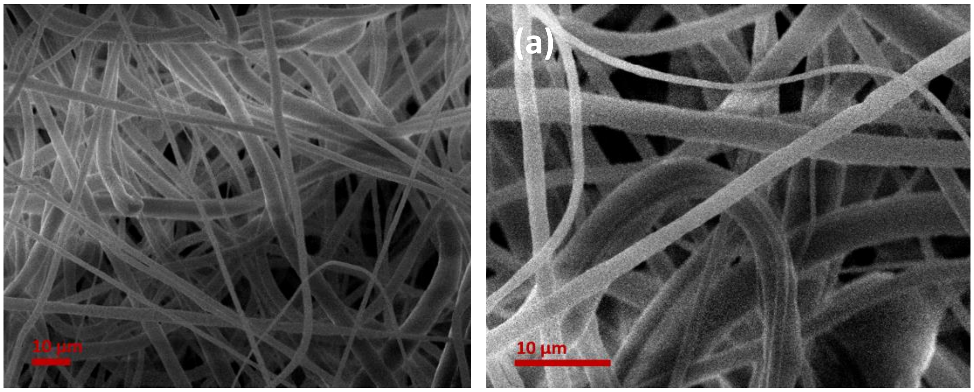

Figure 1: SEM micrograph of CNT-PVDF nanofiber membranes at different magnifications: (a) x1000 and (b) x2500

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Material structure modeling and vibration characteristics of cracked nanocrystalline gyroscopes for sensing applications

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Many of the potential applications for micro/nano-gyroscopes, such as drone guidance or vehicle stability control, call for extremely precise and reliable measurements of rotational velocity. One method for improving the accuracy of MEMS and NEMS cantilever gyroscope models is the inclusion of small-scale effects. The modified couple stress theory and surface elasticity are used to model the behavior of these small-scale systems. Increased model accuracy can also be achieved by accounting for material microstructure. In this work, a multiphase micromechanical model is used to approximate the effective material properties of the nanocrystalline gyroscope. Vibratory micro-/nanoelectromechanical systems such as micro-/nanogyroscopes operate at extremely high frequencies and therefore experience many loading cycles very quickly. These harsh operating conditions often lead to fatigue and cracking in micro structures. Cracks severely affect the static and dynamic behaviors of micro-/nanogyroscopes, resulting in diminished accuracy of measured rotations. In this work, the change in a micro-/nanogyroscopes effectiveness due to the location and severity of a single crack is analyzed. The presence of a crack in a cantilever gyroscope effectively increases the flexibility of the micro-/nano-beam. This produces an increased risk of static pull-in at lower than expected electrode voltages. Additionally, cracks reduce the natural frequency of the gyroscope, leading overall decrease in effectiveness of the gyroscope operating with its original electrostatic forcing conditions.

Nanotechnology for Ceramic Water Filtration

V. Uzonwanne, I. Yakub, A. Plappally, M. Leftwich, K. Malatesta, and W. O. Soboyejo

The persistent demand for clean drinking water in developing countries and regions with contaminated drinking water supply drives the need for continued research efforts towards sustainable water purification methods. This paper reports on the design and optimization of nano- and micro- porous ceramic water filters and colloidal silver coatings for the efficient removal of *Escherichia coli* and disinfection of contaminated water, respectively. In this work, we explore the influence of adhesion and nano-/micro-porosity of the ceramic water filters on the disinfection and removal of *E. coli* from microbially-contaminated water. The adhesion forces are measured using force microscopy techniques. In this way, the trends in the adhesion forces (between the colloidal silver or silver nanoparticles and the porous ceramic water filters or the *E. coli bacteria*) are used to explain the removal of microbial contaminants. Our results also reveal the effective removal of *E. coli (*log reduction values (LRV) of 5.7 - 6.4) for porosities of 36-47 % and pore sizes between ~10 nm and 100 µm. The implications of the results are then discussed for the design of integrated and efficient porous ceramic water filters for effective water purification by adsorption and size exclusion of *E.coli*.

Controlling lithium-ion solvation for improved lithium metal deposition

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Lithium-ion batteries have enabled the portable electronic revolution of the past decade. However, before transportation and electricity generation can be revolutionized by electric vehicles and renewable energy technologies respectively, batteries with much higher energy densities must be developed. The next generation batteries currently being explored (e.g., lithium-sulfur and lithium-air) depend on lithium metal as the anode because lithium has a high gravimetric capacity. Unfortunately, lithium is quite reactive, and it continuously reacts with the electrolyte leading to poor cycle life. To control electrolyte degradation, we explored an unreactive nonpolar alkane as part of the electrolyte mixture to control the electrode-electrolyte interface. We observe that the nonpolar alkane modifies the lithium solvation structure within the electrolyte, changes the lithium deposition morphology, decreases the overpotentials required for deposition and stripping, and more importantly improves cycle life. Our work provides insight into the ion solvation structure and how reactions at the electrode-electrolyte interface can be tuned through careful understanding of ion solvation.

Session 6

SEM-EDX characterization of graphene from maize corn

Moses Kigozi

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Carbon nanotubes acting as nano-scale mass sensors with multiple deposited particles

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This study focuses on the free vibrations of carbon nanotubes (CNTs) with clamped-clamped boundary conditions and multiple deposited nanoparticles. The purpose of this work is to extend the limits of applicability for the theoretical modeling of nanoscale CNT-based mass sensors. Previous studies focused on determining the induced frequency shift or amplitude shifts that arise due to the deposition of a single nanoparticle on or within the CNT. In this effort, the reduced-order model is extended to include an arbitrary number of masses deposited on the CNT. This is a more realistic representation of experiments at the nanoscale. To perform a free vibration analysis, the governing equations are first derived by virtue of Hamilton's principle, considering Euler-Bernoulli beam theory. To account for the effects of mid-plane stretching for end constrained beams, the von Kármán geometric nonlinearity is included and effectively modifies the strain field. Eringen's nonlocal elasticity theory is employed to account for size dependent phenomena. Each deposited particle breaks up the displacement field, leading to continuity equations for the deflection, slope, moment, and shear. After all the governing equations, boundary conditions, and continuity conditions are obtained, a parametric study is performed to determine the impacts of increasing the number of nanoparticles that are deposited onto the CNT on the sensitivity of the carbon-nanotube based sensor. Results show that, even when keeping the total deposited mass constant, the number of particles and their location can significantly shift the natural frequencies and the mode shapes of the nano-sensor.

Structure-property-toxicity relationships of carbon nanomaterials: role of surface chemistry on the mechanisms of interactions with bacteria

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Graphene oxide (GO) is a promising antimicrobial agent with a controllable structure and tunable surface chemistry. However, the properties that define its antimicrobial activity need further understanding to guide GO's design for biocidal applications. To identify the physicochemical determinants of GO's antimicrobial activity, we generated different modified Hummer's GO materials thermally annealed (at 200, 500, or 800 °C) to modify the surface oxygen groups. The plating assay results indicate that at 183, 143, 127 and 86 µg/mL, as received GO (ARGO) and the thermally annealed TGO200, TGO500 and TGO800 reduce E. coli viability by 50% (EC_{50}), respectively. There was a negative correlation between the C/O ratio and the EC 50 value, indicating higher toxicity as ARGO is reduced. To uncover the toxicity mechanism involved at the EC 50 level, a fluorescent dye-based assay was used to measure oxidative stress imposed by GO. An increase in reactive oxygen species (ROS) was generated by ARGO compared to the control, indicating induction of oxidative stress in cells exposed to lower C/O ratio GO. To explain the low oxidative response to TGO exposed cells, plating assays realized after a post-exposure sonication were performed. Results show no significant difference in colony forming units with respect to the control, indicating that physical mechanisms leading to cell entrapment and inhibition of cell growth by GO are present. By comparing different GO samples at their EC_{50} concentrations, this study reveals that reduction of GO sheets alter both the mechanisms of cellular interaction and the degree of toxicity to bacteria cells.

Investigating the effect of polymer architecture and chemistry on structure formation in mixed matrix polymer-polymer membranes

Rachel R. Ford, Orland L. Bateman, Mamadou S. Diallo, & Julia A. Kornfield

Recent advances in the preparation of mixed matrix membranes are providing new opportunities to develop the next generation of multifunctional materials for sustainable chemistry, engineering, and materials (*SusChEM*). One such advance, developed by the Diallo Group, combines the durability of polyvinylidene fluoride (PVDF) with the diverse functionality of hydrophilic polymers. In these mixed matrix polymer-polymer (M2P2) membranes, a hydrophilic polymer precursor is crosslinked *in-situ* in the membrane casting solution to form functional particles anchored in a PVDF matrix. Of particular interest are nitrogen-rich precursors, including hyperbranched polyethyleneimine (PEI) oligomers and low-generation polyamidoamine (PAMAM) dendrimers. Evidence indicates that the architecture of these nitrogen-rich precursors profoundly affects the kinetics of the *in-situ* crosslinking reaction and, ultimately, membrane structure and performance. Herein, we probed the relationship between nitrogen-rich particle precursor and membrane structure using a newly developed ultra-small angle neutron scattering technique, in which we measured structure formation as the crosslinking reaction proceeded.

Poly(ether)sulfone electrospun nanofiber membranes functionalized with graphene oxide quantum dots for antimicrobial applications

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Polymeric electrospun nanofiber membranes (ENMs) have been used in widespread applications in recent years including various water treatment applications. The extensive use of ENMs in water filtration applications is however, limited by bio-fouling; a phenomenon that occurs when pathogenic microbes grow on the surface of the membrane subsequently leading to the formation of an undesirable cake layer. This work describes the development of ENMs with antimicrobial properties prepared by embedding graphene oxide quantum dots (GQDs) into poly(ether) sulfone (PES) nanofiber membranes. FTIR and Raman spectroscopy and other microscopic techniques confirmed the successful incorporation of the GQDs. The work further describes the assessment of antimicrobial effects of the GQD-PES electrospun nanofiber membranes against three bacterial strains namely, *Escherichia coli (E. coli)*, *Staphylococcus aureus (S. aureus)* and *Bacillus cereus (B. cereus)*. The electrospun nanofibers at 10 wt.% of GQDs showed the most active antimicrobial activity against all three bacterial strains tested. The zones of inhibition ranged from 9 to 40 mm. The results demonstrated that incorporating GQDs into the PES nanofiber membranes gives rise to new antimicrobial properties and as a result the novel GQDs-PES nanofiber membrane can be used in water treatment.

Microwave-assisted synthesis of titania-amorphous carbon nanotube and titania-amorphous nitrogen-doped carbon nanotube nanophotocatalyts for the degradation of textile wastewater

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This work reports the synthesis of TiO_2 nanohybrids fabricated using amorphous carbon nanotubes (*a*CNTs) and amorphous nitrogen doped carbon nanotubes (*a*NCNTs) through the microwave assisted hydrothermal method. The physicochemical, optical and thermal properties of the nanohybrids were investigated using various characterization techniques. The nanophotocatalysts were further tested for the removal of Reactive Red 120 (RR 120) and textile dye from real textile wastewater. Fourier transform infrared (FTIR) spectroscopy indicated the presence of surface –OH and –COOH groups and confirmed the presence of carbon residue. The carbon residue was found to consists of *a*CNTs and *a*NCNTs by thermogravimetric analysis (TGA) and differential thermal analysis (DTA). In addition, the synthesis process promoted the removal of graphitic flakes from the outer walls of the *a*NCNTs and *a*CNTs and promoted their incorporated into TiO_2 nanocrystals hence enabling surface plasmon resonance on the TiO_2 and $NTiO_2$ nanocrystals. X-ray photoelectron spectroscopic (XPS) analysis for the TiO_2–*a*NCNT nanohybrids confirmed the C and N doping both due to the amorphous residue from the *a*NCNTs and the carbon residue from the process chemicals. In addition to this, XPS confirmed the presence of surface oxygen-based groups, hence corroborating the observance of wt.% loss corresponding to the loss of surface, adsorbed and chemical water from the nanohybrids. Transmission electron microscopy (TEM) showed that *a*CNTs and *a*NCNTs promote the formation of monodispersed, small (all below 7.4 nm) and well dispersed TiO_2 particles. The incorporation of N into TiO_2 and subsequent hybridization with *a*NCNTs, however, resulted in large particle sizes (16.90 ± 4.11 nm). UV-Vis spectroscopy showed that the $NTiO_2$–*a*NCNT nanohybrids has the lowest energy band gap of 2.97 eV and the lowest PL intensity. The interaction between the TiO_2 and the *a*CNT or *a*NCNTs was confirmed by Raman spectroscopy. Photocatalytic degradation showed that all nanophotocatalysts are able to remove the color in RR 120 and degrade organics in textile waste. The TiO_2–*a*NCNT nanophotocatalysts had superior overall color removal for both RR120 and textile wastewater; achieving a 99% color removal through a combination of photocatalysis and adsorption at a photocatalytic degradation rate constant $3.44 \times 10^{-2} \mathrm{min}^{-1}$.

Poster Session

B1

Investigating the effect of polymer architecture and chemistry on structure formation in mixed matrix polymer-polymer membranes

Rachel R. Ford, Orland L. Bateman, Mamadou S. Diallo, & Julia A. Kornfield

Recent advances in the preparation of mixed matrix membranes are providing new opportunities to develop the next generation of multifunctional materials for sustainable chemistry, engineering, and materials (*SusChEM*). One such advance, developed by the Diallo Group, combines the durability of polyvinylidene fluoride (PVDF) with the diverse functionality of hydrophilic polymers. In these mixed matrix polymer-polymer (M2P2) membranes, a hydrophilic polymer precursor is crosslinked *in-situ* in the membrane casting solution to form functional particles anchored in a PVDF matrix. Of particular interest are nitrogen-rich precursors, including hyperbranched polyethyleneimine (PEI) oligomers and low-generation polyamidoamine (PAMAM) dendrimers. Evidence indicates that the architecture of these nitrogen-rich precursors profoundly affects the kinetics of the *in-situ* crosslinking reaction and, ultimately, membrane structure and performance. Herein, we probed the relationship between nitrogen-rich particle precursor and membrane structure using a newly developed ultra-small angle neutron scattering technique, in which we measured structure formation as the crosslinking reaction proceeded.

B2

The effect of reducing agents on cobalt based catalysts for fischer tropsch synthesis

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Keywords: Fischer Tropsch synthesis, Activation, Syngas, Cobalt, Catalysts, Supports, Activity, Selectivity, Stability

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Fischer Tropsch (FTS) is the newly integrated process for producing high quality fuels from coal, biomass and natural gas over a cobalt or iron catalyst. It is a solution to the world's energy insecurity and stringent environmental regulations. The reduction of the catalyst with H2, CO, and syngas, prior to the reaction plays a vital role in the catalyst activity and selectivity. The use of syngas as both activation and reaction gas could eliminate the use of pure hydrogen (eliminate the hydrogen purification plant) thus potentially dropping the capital and operating cost of the plant, especially for a small plant. In this work, in-Situ XRD was used to monitor the

changing phases of the catalyst during the reduction of 12 wt% Co/Al2O3 by using different reducing agents (H2, and H2/CO) at atmospheric pressure, in a step-wise manner from 0-450 °C. Reduction occurred in two successive steps for all the gases, firstly, the oxide was reduced to CoO and then CoO to metallic fcc cobalt and/or hcp cobalt. Complete reduction to Co° was achieved with H2 reduction and traces of fcc Co° were seen with syngas activation even though the reduction was incomplete. Metallic cobalt started appearing around 310 °C for H2 and 320 °C for syngas. It can be suggested from the results that H2 is a better reducing agent compared to syngas. After the in-situ XRD analysis, two fixed bed reactors were loaded with 1 gram of the catalyst and were used for FTS.The same reduction conditions (P=1 bar gauge, FR=60 (NTP)ml/min, T=350 oC) and reaction conditions (P=20 bar, FR=60 (NTP)ml/min, T=200 °C) were conducted for both reactors, and the only difference is: one was reduced by H2 while the other was activated by syngas. The FTS reaction results show that reducing with H2 results in a higher CO conversion and low methane selectivity compared to syngas activation. One of the possible reasons is that, there could be carbon deposition occurring during the reduction via syngas at 350 oC and the surface carbonaceous deposits are likely to compromise the availability of the active sites. Further work, such as, the effect of reduction temperature, will be done to optimize the use of syngas as an activating agent.

B3

Antimicrobial effect and anti-biofouling performance of sulfidized silver nanoparticles on RO Membranes

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Silver, a known biocide, is used for the *in-situ* formation of silver nanoparticles (Ag-NPs) on reverse osmosis (RO) membranes for biofouling mitigation. Biofouling has become an issue because it shortens membrane life expectancy; along with, increasing hydraulic resistance, and decreasing water flux affecting the water treatment process. Ag-NPs are soluble, limiting their effectiveness over a long period of time. This study focuses on functionalizing silver membranes with different concentrations of Na_2S to form a partial Ag_2S layer to slow down the release of silver nanoparticles while maintaining antimicrobial activity. Different concentrations of Na_2S (10^{-1}, 10^{-3}, and 10^{-5} M) were evaluated to identify the degree of sulfidation that can preserve the antimicrobial effect. An *Escherichia coli (E.coli)*-based assay was used to quantify the antimicrobial activity of the functionalized membranes at the different sulfidation levels. As expected, our results showed a negative relationship between sulfidation and antimicrobial activity; silver-functionalized membranes treated with higher concentrations of Na_2S resulted in lower toxicity to *E. coli*. However, when tested in a dynamic cross-flow RO system, the less soluble sulfidized particles were found to be more effective than the more soluble Ag-NPs for biofouling control over the course of 24h. Therefore, retention of the silver coating over time appears to be more important for biofilm control in RO systems than high antimicrobial activity. The concentration 10^{-3} M Na_2S was found to have the best balance between reduced dissolution rate and good antimicrobial and anti-biofouling performance.

B4

Calcination of Co/TiO_2–PVA nanofibers catalysts for photocatalytic discolouration of Congo red in contaminated water

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The development of calcined Co/TiO_2–PVA nanofibers catalysts was investigated through electrospinning technique. The preparation of Co/TiO_2–PVA composite gel was done by mixing 10% PVA polymer solution and Co/TiO_2 which was pre-synthesized by dry impregnation method. The Co doped TiO_2 nanofibers was heated at 300 °C for 16 hours in a muffin furnace resulting in the calcined catalyst.

The samples were characterized with SEM-EDS, FTIR, XPS, XRD, TGA, and UV–vis DRS. SEM cross-section image of calcined Co/TiO_2–PVA nanofibrous catalyst depicted three layers made of PVA nanofibers, support sheet and Co/TiO_2. UV–vis DRS spectra of samples showed absorbance in the visible range (400 to 800 nm) indicating the suitability of the materials to operate as photocatalysts. The energy band gap was found to 1.86 eV for the photocatalyst based on Tauc plots.

Congo red was used a model organic pollutant. The obtained calcined Co/TiO_2 nanofibrous catalyst was tested in the photodegradation of Congo red dye in aqueous solution. The photodegradation was achieved through simulated solar light irradiation. This comparative study revealed that calcined Co/TiO_2–PVA nanofibers catalyst performed well than the Co/TiO_2 catalyst. Electron holes and hydroxyl radicals played the main role in the decolourisation process of dye (100 %) within 150 min. The results indicate that our developed Co/TiO_2–PVA nanofibers catalyst could be recommended for further heterogeneous catalysis investigations.

B5

Size dependent modeling and performance enhancement of nano-scale functionally graded piezoelectric energy harvesters

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Functionally graded materials (FGMs) are a unique type of composite in which the material properties vary in one or more directions from one material to another. FGMs are usually composed of a metal and a ceramic. One special type of FGM is known as a functionally graded piezoelectric materials (FGPM) which can be utilized for energy harvesting applications. The FGPM of interest in this work is composed of Platinum and PZT. FGMs of these types are especially suited for energy harvesting applications because the designer can control their material properties, such as the stiffness and natural frequencies of the energy harvesting system through changes in the FGM composition and material distribution. The variation of the material properties throughout the thickness of the energy harvester causes a shift in the neutral axis of the system. The resulting shift of the neutral axis must be accounted for to obtain effective energy harvester properties and hence the accurate design of the energy harvesting system. In this work, the effect of small-scale phenomenon on the natural frequencies and power density of micro- to nano-scale functionally graded energy harvesters is investigated. The modified couple stress theory is used to account for micro-rotations within the surface elasticity theory is used to account for the residual stresses on the surface of the energy harvester. Both small-scale effects depend on the material parameters that vary throughout the thickness of the FGM. Size-dependent effects have a significant influence on the design and performance of effective micro/nano energy harvesters. Couple stress and surface elasticity both cause significant increases in the effective stiffness of energy harvesting systems. Therefore, neglecting these effects can lead to underestimation of the natural frequencies of the harvester and lead to ineffective designs.

B6

On-Silicon Chip based Receptor Technology for the Identification of Absorbed CO, CO2 and Bio-species

Timothy Okhai

On-Silicon Chip based Receptor Technology for the Identification of Absorbed CO, CO2 and Bio-species Authors: Timothy A. Okhai 1,2, Lucas W. Snyman 2 and Usisipho Feleni 2 1Clinical Engineering Cluster Group, Department of Electrical Engineering, Tshwane University of Technology, Pretoria, South Africa. 2Unit for Nanotechnology and Water Sustainability Research and Department of Electrical Engineering, College of Science, Engineering and Technology, University of South Africa, Florida, South Africa. Abstract: In this paper, we present possibilities for developing on-chip bio-species biochemical sensors using Si LEDs that operate in the reverse avalanche mode (nomenclated Si AM LED), and in the forward bias mode (Si FB LED). Of particular interest are LEDs that can be fabricated in the Micro- and Nano-scale on standard Silicon Integrated Circuitry, and that emit up to 100 nW of optical power within a broad spectrum in the 450 – 1100 nm range. We have extensively studied the dispersion characteristics for a Si AM LED source that is positioned one micron below surface of a silicon IC [1]-[4]. We will present three sets of designs in order which, in combination with appropriate receptor technology, will enable on-chip detection of (1) carbon monoxide gas concentrations, (2) carbon dioxide gas species, and (3) breast cancer cells using a combination of Si LEDs and quantum dot (QD) materials. In the first design, a Si LED is combined with a micron dimensioned waveguide and a distant Silicon detector, all positioned on the same chip. A crevasse is etched from the surface of the chip and penetrates the evanescent field of the waveguide. As gas molecules are absorbed, the propagated light is dispersed, causing a reduction in detection signal at the detector as a function of propagation wavelength. By studying the wavelength and absorption spectra of different gas species, the positive absorption of CO molecules can be detected. In a second design, a wide propagation channel is designed between the Si LED. A zeolite nano-crystal matrix containing Fe atoms with a large surface area of micropores is drop casted in the crevasse area. A selection of sensors is placed below the crevasse area that can each selectively monitor reflected light in the UV, visible, infrared, and far infrared wavelength region. Again, by comparing the fingerprint combination spectrum of various gases, we hope to positively identify the presence of carbon dioxide and oxygen. In a third design, a TGA Pb-Te synthesized quantum dot (QD) layer is placed in the crevasse. The quantum dot layer is used as a receptor for selectively absorbing Cytochrome P450 enzymes, aptamers or DNA within the layer. Again, the transmittance and reflecting characteristics of the absorbed bio-species in the receptor layer are monitored by a selection of detectors in the UV, visible, infrared and far infrared spectrum. By comparing the unique fingerprints of the bio-species detected by the detectors, we hope to positively identify the

species absorbed within the quantum dot layer. Fabricating these sensors in Micro- and Nano-dimensioned format on chip, offer a large number of specific variant testing, as well as re-vitalising the sensor after each measurement cycle. These features are often not possible with printed circuit on paper sensors. Sensor-on-chip integrated technology also offers the reliable and complex processing of extracted parameters directly on the same chip, and route the outcome of these, even by RF technology, to external display devices. Keywords: Silicon Avalanche Mode LED, Silicon Forward Biased LED, Oxygen, Carbon- monoxide and Carbon-dioxide sensors, Bio-Chemical Sensors on-chip

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B7

Nanotechnology for Ceramic Water Filtration

V. Uzonwanne, I. Yakub, A. Plappally, M. Leftwich, K. Malatesta, and W. O. Soboyejo

Abstract

The persistent demand for clean drinking water in developing countries and regions with contaminated drinking water supply drives the need for continued research efforts towards sustainable water purification methods. This paper reports on the design and optimization of nano- and micro- porous ceramic water filters and colloidal silver coatings for the efficient removal of *Escherichia coli* and disinfection of contaminated water, respectively. In this work, we explore the influence of adhesion and nano-/micro-porosity of the ceramic water filters on the disinfection and removal of *E. coli* from microbially-contaminated water. The adhesion forces are measured using force microscopy techniques. In this way, the trends in the adhesion forces (between the colloidal silver or silver nanoparticles and the porous ceramic water filters or the *E. coli bacteria*) are used to explain the removal of microbial contaminants. Our results also reveal the effective removal of *E. coli (*log reduction values (LRV) of 5.7 - 6.4) for porosities of 36-47 % and pore sizes between ~10 nm and 100 µm. The implications of the results are then discussed for the design of integrated and efficient porous ceramic water filters for effective water purification by adsorption and size exclusion of *E.coli*.

B8

Chalcogenide based semiconductor photocatalysis for photodegradation of organic pollutants in water

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Keywords: Acid blue 40; Chalcogenide semiconductors: photocatalysis; degradation.

Abstract:

Chalcogenide semiconductors have attracted research interest due to their potential applications in electronics, energy storage devices, solar cells and water splitting. In this study CdS/g-C_3N_4 nanocomposite were synthesized using hydrothermal method synthesis. The CdS/g-C_3N_4 nanocomposites were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform-infrared spectroscopy (FTIR), UV-visible spectroscopy, photoluminescence (PL). SEM analysis confirmed the sheet-like morphology of the g-C_3N_4 while the CdS appeared as flower-like microparticles and microspheres. The orange colored nanocomposite showed a low band gap energy and thus could absorb light in the visible region. Photocatalytic activity of the prepared samples for acid blue 40 degradation was evaluated under visible-light irradiation. Results showed that 99% of acid blue 40 was degraded after 180min under illumination of visible light irradiation from a solar simulator. The chalcogenide semiconductor nanocomposites are thus promising materials for solar light photodegradation of organic pollutants in water.

B9

Atmospheric Water Capture: A decentralized on-demand drinking water technology

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NSF Nanosystems Engineering Research Center for Nanotechnology Enabled Water Treatment

Limited access to clean water due to natural or municipal disasters, drought, or contaminated wells is driving demand for point-of-use and humanitarian drinking water technologies. Whereas centralized potable water costs $1-5 / kilogallon, bottled water costs >$1000 / kilogallon. There is significant economic space for technologies capable of providing the flexibility of bottled water without the infrastructure required for centralized municipal potable water. Atmospheric water capture (AWC) is a competitive technology that provides clean drinking water on demand, does not require fixed physical infrastructure such as pipelines, and does not produce large concentrated waste streams associated with contaminant or salt removal from liquid water supplies.

We have developed geospatial and climatic models for passive solar desiccant driven AWC, in which water vapor is adsorbed onto a desiccant bed at night, desorbed by solar heat during the day, and condensed. AWC volume can vary between 0.5 – 2.5 L/m^2/day as a function of material properties and climatic region of operation, but the quantity of solar thermal energy available to achieve complete desorption of the desiccant can be limiting. Therefore, we developed photothermal nano-enabled desiccants that superheat under sunlight, which increases the rate of desorption, and even allows for more operation of 2 or more AWC cycles per day. Moving from passive to active systems, we are operating commercial dehumidifiers (desiccant and dew point condensation systems) outdoors in a semi-arid climate to benchmark water production, energy efficiency and water quality. The energy cost of AWC is competitive with bottled water. Water quality of desiccant systems exceeds US EPA regulations for tap water, while dew point condensation systems require minor treatment to remove dust.

B10

Cysteine-functionalized chitosan magnetite biocomposite for the efficient removal of toxic metal ions in synthetic wastewater

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Abstract

Water pollution due to toxic metal ions is of a great concern owing to their persisting and accumulative behavior in the environment. Chitosan-based nanocomposites are one of the environmentally friendly sorbents that offer high adsorption capacity for the removal of these toxic metals in wastewater. These materials are often crosslinked with reagents such as epichlorohydrin, which tend to interfere with the functional groups of the chitosan structure, resulting in a decrease in adsorption capacity. Therefore, modification of the as-prepared material is required for the introduction of new functional groups. In this study, Cysteine-functionalized chitosan magnetite biocomposite were developed for the highly efficient removal of toxic metals from synthetic wastewater. The biocomposite were prepared by chemical co-precipitation using Fe^{2+} and Fe^{+3} as iron precursors, ammonium hydroxide as a base and Cysteine as capping agent. The structural, surface, and magnetic properties of the prepared chitosan magnetite nanobiocomposite were studied by scanning electron microscope (SEM), Fourier transform infrared spectrum (FTIR) and X-ray powder diffraction (XRD). Adsorption experiments were performed and the effects of different affecting parameters on the adsorption characteristics of were investigated using inductively coupled plasma atomic emission spectroscopy (ICP-OES). The results indicated the suitability of the biocomposite as a potential adsorbent material for the efficient removal of Pb(II) and Cd(II) from wastewater.

Keywords: biocomposites, Chitosan, Adsorption, wastewater, toxic metals

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B11

Mechanics, dynamics, and vibrations of carbon nanotubes at different stages of a targeted drug delivery process

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Abstract. In this research effort, we study the need for considering mechanics, dynamics, and vibrations points of view in the consideration of carbon nanotube-based targeted drug delivery systems. We consider the CNT acting as a type of capsule or carrier for solid or liquid drug particles that require a targeted release in the body to an unhealthy site, say a tumor. In this case, CNTs are considered as strong candidates due to their high surface-area-to-volume ratio that allows for a high concentration of particle loading. Additionally, after a functionalization process, CNTs have increased solubility and decreased toxicity in the body: an important consideration for biological applications. Now, it should be mentioned that the majority of the studies involving CNT-based targeted drug delivery are performed heavily from a chemistry, biology, and experimental points of view. Researchers studying this topic from a dynamics and vibrations of view are often overlooking the points of view of these other researchers and thus are developing models for non-physical systems with unrealistic assumptions. Therefore, one of the highlights of this research will be the identification of realistic representations of the CNT-based system at different stages of the drug delivery process. This can include, but is not limited to, identifying the effective properties before and after functionalization and loading and developing nonlinear reduced-order models to characterize the static and dynamic stability of the system as it travels through the bloodstream and reaches the injection site. In particular, a focus will be placed on modeling the surrounding viscoelastic medium with respect to the CNT at the point of drug release in the body. Primarily, we will focus on modeling the CNT-based system using beam theory that accounts for attached or encapsulated particles and size dependent phenomena using Eringen's nonlocal elasticity. We consider this is a considerable contribution to the field, especially for those that have previously studied these types of systems from a mechanics, dynamics, and vibrations point of view that have been making non-physical assumptions. After deriving the governing equations for the system, we will analyze what types of thermal or magnetic loading can be used to release the particles from the CNT once reaching the target site when the CNT is surrounded by the viscoelastic medium, such as the blood or tissues in the body. In analyzing the results for this system, we will be able to share our points of view with experimentalists, chemists, and biologists to advance this growing field more quickly and effectively.

B12

Adsorption of Dibenzothiophene in Model diesel by Amarula wastes biomass as a low cost adsorbent.

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Keywords: Adsorption, Model diesel, Dibenzothiophene, Biomass, Kinetics, Isotherms, Thermodynamics

This study focused on mitigating the issue of waste management and land pollution by using the Amarula waste biomass which is a low cost adsorbent that is obtained from industrial waste by product.

The Amarula waste biomass was divided into three parts: Amarula fruit waste, Amarula seed wastes, and Amarula shell wastes. Each waste was used to reduce sulphur content in dibenzothiophene (DBT) model diesel using a batch reactor for 180minutes at 25°C ±2°C. The Amarula shell wastes were found to have higher adsorption efficiency of 35% as compared to the Amarula seed wastes and the Amarula fruit wastes which had 22% and 8% respectively. The effect of adsorption temperature was carried out. It was found that the Amarula wastes biomass performed better at lower temperatures. The effect of biomass quantity was performed at room temperature using Amarula shell wastes biomass and the adsorption capacity was found to decrease with increasing quantity of biomass. Both the kinetic models and the Adsorption Isotherms were applied to the experimental data. Thermodynamic parameters were also studied to determine the spontainity of the adsorption processs. Characterisation of both the fresh and used Amarula wastes biomass was analysed using Elemental analysis, FTIR, SEM-EDS, BET and TGA.

B13

Microbial Reduction of Iodate by Community 31 at the Hanford Site

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This research aims to develop methods for in situ microbial reduction of radioactive iodate (I129) from radioactive waste contaminated groundwater at the Hanford Nuclear Site in Washington State. A microbial community, named “Community 31”, was isolated from the Hanford site. The community has yet to be characterized but was suspected by researchers at the Pacific Northwest National Laboratory (PNNL) to be capable of reducing iodate to iodide. This type of reduction is called dissimilatory microbial reduction and, in this case, iodate (oxidation state of +5) was targeted to be reduced to Iodide (oxidation state -1). Community 31 was cultivated in a specially designed minimal media that allowed for analysis of iodate concentration with a colorimetric assay and UV spectrophotometry. Batch cultures of the microbial community were exposed to an initial concentration of 100µM of iodate and incubated at 30 °C, shaken at 130 RPM in aerobic and anaerobic conditions at. Samples were taken every 8 hours for measuring iodate concentration and microbial growth. Approximately 36.3% reduction in aerobic conditions and 9.9% in anaerobic conditions iodate was recorded after 24 hours. This could have significant environmental implications as it suggests an in-situ approach for remediation of iodate contaminated groundwater at the Hanford site.

B14

Nanopatterning of Cr thin films using low energy ion beam for selective solar absorber application

Zebib Yenus

Nanopatterned chromium (Cr) solar absorber coatings were deposited onto glass substrate using MBE technique at room temperature. Subsequently, the prepared samples were sputtered at 50°, 60° and 70° angle of incidence using low energy Ar+ ion beam. XRD analysis confirmed that the as-grown Cr films showed highly crystalline bcc Cr (110) orientation, whereas the sputtered films showed a decrease in intensity and widening of the peak, which is typical of materials with small grain size. RBS analysis confirmed that the thickness of the Cr films was monotonically decreased with increasing the sputtered angle, which is due to removal of particles from the surface using ion beam. AFM indicated that uniform distribution of micropeaks and microgrooves with well-defined nanopattern structures were achieved for Cr films sputtered at 70° angle of incidence. High solar absorptance of 0.94 in the solar spectrum region and low thermal emittance of 0.16 was achieved for the Cr film sputtered at 70°, which is due to appropriate ratios of mean height deviations and the autocorrelation distance to the wavelength as indicated from AFM

B15

Controlling lithium-ion solvation for improved lithium metal deposition

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Abstract

Lithium-ion batteries have enabled the portable electronic revolution of the past decade. However, before transportation and electricity generation can be revolutionized by electric vehicles and renewable energy technologies respectively, batteries with much higher energy densities must be developed. The next generation batteries currently being explored (e.g., lithium-sulfur and lithium-air) depend on lithium metal as the anode because lithium has a high gravimetric capacity. Unfortunately, lithium is quite reactive, and it continuously reacts with the electrolyte leading to poor cycle life. To control electrolyte degradation, we explored an unreactive nonpolar alkane as part of the electrolyte mixture to control the electrode-electrolyte interface. We observe that the nonpolar alkane modifies the lithium solvation structure within the electrolyte, changes the lithium deposition morphology, decreases the overpotentials required for deposition and stripping, and more importantly improves cycle life. Our work provides insight into the ion solvation structure and how reactions at the electrode-electrolyte interface can be tuned through careful understanding of ion solvation.

B16

Potential of Nano -Engineered Thermal-to-Electricity Energy Conversion Systems in South Africa

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South Africa and the African continent offers an abundance of thermal energy as originating from solar irradiation. Utilizing solar incident thermal energy in the infrared region offer substantially more solar energy than is available in the visible and ultraviolet regions of the solar spectrum. Black thermal absorbers have almost a 100% absorbance for solar incident thermal irradiation, while photovoltaic technology only, at best, converts only about 10 % of available energy in the visible region, which again is only about 25 % of the energy as available in the whole solar irradiation spectrum. The utilization of thermal energy systems are clean, require often no moving mechanical parts. have exceptional long lifetimes and produce no harmful gases as by-products. It is hence absolutely clean The efficiency and cost structures of Seebeck effect thermal to electricity conversion cells that are available on the international market are currently quite expensive. Peltier conversion cells that are normally used for cooling purposes, and that are freely available in supply stores in SA, are suitable to be utilized to convert thermal energy to electricity, but their conversion efficiency is very low, of the order of 1 %. We have succeeded in developing an innovative electronic control system that can be used to increase the extraction of electrical charge from Peltier Cells, and improve the conversion efficiency to electricity to 10 %. This technology has recently been extensively patented in SA and internationally by UNISA. In the presentation, some aspects of this system are revealed. Deeper research of efficiency of Seebeck Cells as currently internationally developed depends on the ratio of the thermoelectricity power, S, or thermoelectric EMF, to the thermal

conduction o of materials. Current prices to import these cells are very high and range from 100$ to 300 $ per Watt capacity of conversion. Most of these cells use an np series semiconductor materials stack configuration and use complex materials compounds such as PbTe and Pb Sb in order to increase thermoelectric powers as compared to thermal conduction in the materials. The cost of energy of such systems as currently developed at UNISA CSET is compared with existing international imported technology, and the cost aspects of developed local solar energy conversion systems is compared with grid electricity prices when water is used as an energy storage medium. No expensive battery technology is used to store energy. Combining the developed systems with large area Black Body and Reflector Plate absorber systems at CSET UNISA, tentatively reveal a cost structure of only 0.5 ZAR/kWh, while Solar Geyser systems and Solar cell (PV) systems, respectively reveal 1.5ZAR/kWh and 15ZAR/kWh over ten years capital outlay. Implementation of the proposed new production routes in SA could reduce the cost of future systems further while exploiting and adding value to SA's rich mineral resources, and creating numerous new job opportunities in SA. Keywords: Solar Energy, Thermal Energy, Photovoltaic Technology, Electronic control systems

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B17

Magnetic Nanostructured Materials for permanent magnets and data storage applications

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Magnetic nanostructured materials (MNMs) are involved in all the advanced technology nowadays. While you are reading this abstract maybe few minutes ago you have checked your phone, or you may even be reading this chapter on your tablet or laptop. It is curious that while you try to learn about MNMs, you are surrounded by them. MNMs are used in a wide variety of devices including electronic devices, motors and generators, hard disk drives, magnetic refrigeration and even in general home appliances (e.g. washing machines). Therefore, small is beautiful and powerful. Magnetic nanoparticles can be classified to soft or hard magnetic materials. Soft magnetic materials such as Fe, Co, Ni or their alloys can be used for magnetocaloric effect for magnetic refrigeration as well as medical applications. The other type of the magnetic nanoparticles, which is the focus of this talk, is hard magnetic materials. Co_xC, Mn_xGa, and $CoFe_xC$ nanoparticles are good examples of hard magnets, which have the property of storing magnetic energy even after removing the magnetic field. Such property are commonly used for fabrication of permanent magnets. The main advantage of such particles is due to the higher magnetic anisotropy which can act as good candidate for new generation of magnetic data storage. Magnetic characterization of the novel carbide phase (CoFe2C) revealed thermal stability up to 790 K for particles with a domain size as small as 5 nm and have giant MCE of 4.6×10^6 J/m^3 , which is ten times larger than that of Co nanoparticles. Such colossal anisotropy leads to a thermally stable long-range magnetic order.
Therefore, the talk focusses on the synthesis of CoxC, MnxGa, CoFexC magnetic nanoparticles and their potential for permanent magnets and data storage applications.

B18

Atomistic Molecular Simulations of Polyamide Membrane in Desalination at Equilibrium and Nonequilibrium States

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Subnanoporous reverse osmosis (RO) of cross-linked aromatic polyamide (PA) membrane is one of the most promising techniques for water desalination. Fundamental understanding of PA RO membranes at the atomistic level is critical to the enhancement of their separation capabilities, leading to significant societal and commercial benefits. Atomistic molecular dynamics simulations were performed to investigate the relationship between PA membrane microscopic structure and membrane performance, including water permeation, water-ion separation and surface biofouling. A realistic model of cross-linked membrane has been developed by employing in-house developed hierarchical cross-linking procedure. Our results demonstrate that three structural components (parallel stacked benzene rings, T-shaped benzene rings and linearly bonded neighboring rings) as the result of benzene rings' short-range π−π stacked interactions and chemical bonding mainly contribute to the membrane's porosity. Water heterogeneous diffusive dynamics presents as a result of heterogeneous microscopic membrane structure. The membrane's interfacial roughness is crucial to protein attachment and biofouling leads to a decrease of water flux. The pore size distribution with the majority of the pore radiuses around 0.20 nm, gives rise to the membrane's water-ion selectivity. The feasibility of water-ion separation through such subnanopores is indeed controlled by the strength of the ions' dehydration free energy in addition to the size of a hydration cluster. Water molecules in the formation of water chains in less crosslinked area facilitates their transfer through the PA membrane subnanopores. The water flux linearly increases with the increase of the applied pressure drop (5-30 MPa), indicating that the membrane internal overall structure remains unchanged.

B19

dMIST: Data-driven Management for Interdependent Stormwater and Transportation Systems

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