

# SNO letter

NEWSLETTER OF THE SUSTAINABLE NANOTECHNOLOGY ORGANIZATION



**Sustainable  
Nanotechnology  
Organization**

Research | Education | Responsibility

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### SNO Newsletter Submissions

Please send news, conference announcements, job postings, letters to the editor, and other contributions to the newsletter to Drs. Sadik or Karn  
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The next newsletter will be released in February 2015.

Edited by:  
**Kyle Doudrick**  
[kdoudrick@nd.edu](mailto:kdoudrick@nd.edu)

Greetings SNO Members,

## The 2014 SNO CONFERENCE IS JUST AROUND THE CORNER

The 3<sup>rd</sup> annual conference of the Sustainable Nanotechnology Organization (SNO) is just around the corner. The conference will be held at the *Boston Hyatt Regency, Boston, MA*, from November 2 - 4, 2014. The conference co-chairs, Drs. Jackie Isaacs of Northeastern University and Philip Demokritou of Harvard University, as well as the conference committee had put together an outstanding technical program. SNO will also hold its 3<sup>rd</sup> workshop on November 1<sup>st</sup> at the same location. "NanoEHS: Fundamental Science Needs," which is co-sponsored by the National Science Foundation and SNO, will be co-chaired by Professors Vicki Grassian and Amanda Haes.

Information for the 2014 SNO meeting in Boston is now available on [www.susnano.org](http://www.susnano.org). The final tally of conference attendees is yet to be finalized but we are expecting about 200 participants. We have invited seven (7) eminent scientists and engineers as plenary speakers. We will again have Dr. Mike Roco as a plenary speaker along with Dr. Clayton Teague, former director of the National Nanotechnology Coordination Office. We have invited Professors George Whitesides from Harvard University & Mark R. Wiesner of Duke University. Others include Dr. David Rejeski, Director of the Wilson Center Project on Emerging Nanotechnologies; Ms. Lynn Bergeson, Bergeson & Campbell, P. C., and Dr. John Warner, Warner Babcock Institute for Green Chemistry, LLC.

The SNO annual conference is a place where the new community of sustainable nanotechnologists is being formed and advanced. In addition to the excellent talks, the conference program is built around providing plenty of time for networking and social interactions. This includes the Sunday evening welcome reception and banquet, thus making the welcome dinner the SNO business meeting and a very special evening. The 2014 event will honor winners of the Graduate Student Awards, give the RSC award to Professor Vicki Grassian, present the SNO awards for 2013 and 2014, and award the first SNO Young Investigator Award sponsored by RSC. A \$500 prize will be given to each of the 20 students awardees based on their resumes and the relevance of their research to sustainability and nanotechnology.

In this edition of the SNO Newsletter, we are pleased to include previews of conference abstracts and interviews from Professors Vicki Grassian and Robert Yokel. Young SNO members and women in STEM who are just beginning their journey can also read the advice from Professor Vicki Grassian. The interview with Professor Yokel provides readers with the reason why SNO is an excellent venue to address the real divide on the benefits and risks of nanotechnology. The SNO meeting is small enough to provide meaningful discussions and yet a neutral ground, with both beneficial and toxicologists researchers attending. Hope you enjoy this edition, and see you in Boston.

Wunmi Sadik, SNO President

## SNO Q &amp; A SESSION



**DR. VICKI GRASSIAN**  
*Professor, University of Iowa*

**(Doudrick) What drew you to participate in SNO?**

**(Grassian)** For the past ten years, I have been interested in using nanomaterials for environmental remediation

applications as well as the implications of nanoscience and nanotechnology. Some of our research is focused on fundamental aspects, but we like to collaborate on some of the more applied aspects, like nanotoxicity. So, naturally SNO is of great interest to me because of its unique focus on all aspects sustainable nanotechnology. Based on my past experience at SNO meetings, I think the interactions between the different camps are key. In addition to the excellent talks on a broad range of topics, the meeting is small enough so that you get a chance to meet up with everyone that is there.

**(Doudrick) Now that ES: Nano has been in print for nearly a year would you say the published articles are representative of what you'd define as sustainable nanotechnology?**

**(Grassian)** The journal is doing well in terms of publishing very high quality articles on the many different aspects of sustainable nanotechnology. As the journal continues into its second year, I would like to see more studies published on biological systems, nanotoxicity and some of the social science aspects of sustainable nanotechnology. I would also like to see more perspectives defining new research areas. But overall, I am very pleased with the quality of the research articles that we are publishing in ES: Nano and I think the Associate Editors of the journal, Greg Lowry, Jim Hutchison and Kristin Schirmer, along with Vice Editor-in-Chief Christy Haynes are doing a great job.

**(Doudrick) For the upcoming NSF/SNO workshop on fundamental needs in NanoEHS - can you elaborate on the importance/purpose of this workshop for directing the future of nanoEHS research? And do you see the understanding of these fundamentals as the next logical step to gaining a better understanding of EHS effects?**

**(Grassian)** There are gaps in our approach and knowledge that I see related to fundamental science needs. For example, an implication study might only focus on one nanoparticle size, arbitrarily chosen, relating its toxicity to all sizes, whereas for application studies there is typically a range of sizes studied and then it is determined what size actually key to see a desired outcome and to further understand why that size gives that outcome. So, what are the gaps between the different approaches and how do we bridge them? I am co-chairing the workshop with Professor Amanda Haes (Iowa), and our main goal for this workshop is to provide a framework for these needs so that it helps move forward the field of sustainable nanotechnology.

**(Doudrick) You have a lot of experience in surface chemistry of natural and engineered particles in air and water. How important would you say knowledge of what is happening at these interfaces is to understanding the risks of nanomaterials?**

**(Grassian)** We want to contribute to understanding the behavior of nanoparticles in environmental and biological systems by translating what we know about surface chemistry and surface science to nanomaterials in more complex environments. This knowledge is very important as the properties of the surface will dictate the behavior of nanomaterials in these systems. So, we focus our attention on this particular area, and I think there is more that needs to be done. Nanomaterial behavior in these systems is complicated though, and we are still in need of assessment tools. But, we are slowly learning and

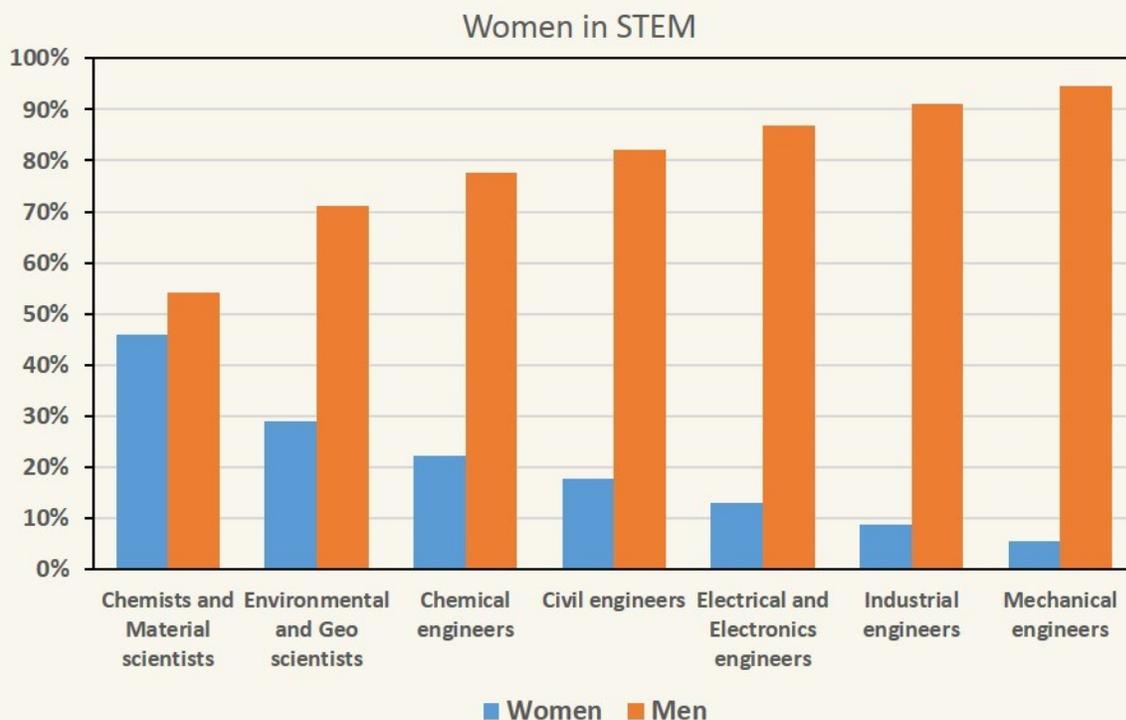
## SNO Q &amp; A SESSION

that's good, and we should not apologize for the complexity, as "yes" or "no" or "good" or "bad" sometimes isn't an appropriate answer.

**(Doudrick) What advice can you give young scientists beginning their journey in sustainable nano research? Do you have particular advice for women in STEM?**

**(Grassian)** For new researchers in general, I suggest you identify areas of research that are important and underexplored, where data are sorely needed. The bottom line is that if you can figure an area that is not well understood (where words like we "assume" or "think" are used as opposed to "it has been shown"), those are areas that need research, and usually, more often than not, assumptions that have not been proven are wrong. If you are successful at this you can make a nice career. Just be sure to define your research goals clearly so that others can understand.

For women in STEM, the social science research clearly shows that women are not given the same opportunities as men. My advice is that if you are affected by this don't let these biases or slights define or derail your research or career path. Instead, use the social science findings that show biases are occurring to empower you, as it shows that you are not alone. Continue to excel, and your efforts will eventually be recognized. Awareness is key, and there has been recent measures taken to push back against implicit assumptions and implicit biases by making people aware of them. There are more women in the field than when I started, so that's good and has helped, but there is more to do on this front.



Data adapted from:  
<http://www.ngcproject.org/statistics>

## SNO Q &amp; A SESSION



**DR. ROBERT YOKEL**  
*Professor, University of Kentucky*

**(Doudrick) Why did you choose SNO as a venue for your nanoceria workshop last year?**

**(Yokel)** There seemed to be a real divide in the views of the benefits and risks of nanoceria among researchers, such as myself, working on the “dark” side that were reporting adverse effects and those working on the “light” side that were reporting the beneficial applications. There wasn’t much, if any, communication between those two camps. The big question was – why are we seeing these two very different effects? We wanted to determine why there was such a great divide between the two. We chose SNO as an excellent venue to address this question for its neutral ground, with both beneficial and toxicologist researchers attending. We also liked that we could tie in the workshop with a larger meeting and many of our targeted invitees were already attending the conference. From this workshop came a series of critical reviews that are being published in a themed collection of Environmental Science: Nano.

**(Doudrick) Your research group deals primarily with neurotoxic metals. Why did you become interested in nanoceria, and how does it relate to this category?**

**(Yokel)** I ignored nanoscience for many years until our VP for Research was putting together a team to respond to a NIH funding opportunity. They wanted someone with a CNS focus, so I was invited to participate. We put together a research team and decided to look at nanoalumina, which has abundant applications. However, aluminum is ubiquitous, making the detection and quantitation of aluminum from nanoalumina difficult to distinguish from endoge-

nous aluminum. It is not electron dense, so electron microscopy could not be used to easily follow its distribution. So we looked at nanoceria which is easy to detect with ICP-MS, because background levels are very low and it is electron dense. It is also an extensively used metal-based nanomaterial. This made it an ideal candidate as a model nanomaterial, or more specifically a model insoluble nanomaterial. From a pharmacokinetics standpoint, this type of nanomaterial is important, as they tend to persist for a long time compared to soluble nanomaterials. The University of Kentucky funded our preliminary work, which enabled us to submit an application to pursue nanoceria. It was funded by the US EPA because of their interest in nanoceria for its use as a fuel additive. Interestingly, we observed adverse effects in the brain even though nanoceria wasn’t crossing the normal blood-brain barrier. Rather, high concentration areas were the spleen, liver, and bone marrow. We believe that nanoceria is causing something to be released that is crossing the blood-brain barrier resulting in these adverse effects. That is speculation at this time.

**(Doudrick) Given the current knowledge on nanoceria toxicity, how do the benefits measure up to the potential risks?**

**(Yokel)** In our nanoceria research we were finding ceria persistence in areas such as the liver with correlating adverse effects. But, we were looking at relatively high exposures, as one often does in toxicology studies. We found that nanoceria partly breaks down over time, and some recrystallization occurs forming a “new” 1-3 nm ceria with difference surface properties and surface chemistry having more ceria (III), which is anti-oxidative and has been shown to be beneficial. Interestingly, a majority of the beneficial applications of nanoceria use 5-7 nm

## SNO Q &amp; A SESSION

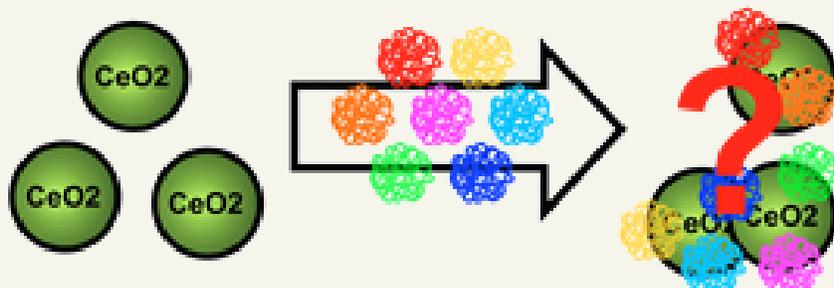
particles, so perhaps the body has the capability to break down larger nanoceria particles into something more beneficial. Toxicology is basically the high end of the dose-response curve, and when you go down to lower concentrations you don't often see these adverse effects. So, some of the differences between the good reported by others and the bad we are seeing could just be due to dose and concentration. Another explanation could be how the nanoceria is made, the physico-chemical characteristics, surface covering, and contaminants for example. In this sense, I think nanoceria certainly has therapeutic potential as a "drug," though these things need to be sorted out. We know that nothing is totally safe, and nothing produces only one effect. This was an important topic of discussion in our workshop. We need better data to make these decisions, and a follow-up workshop is needed to discuss how we've addressed the research questions we presented.

**(Doudrick) You mentioned that one explanation to account for the differing effects could be the way the material is made. How important then is a thorough materials characterization for obtaining accurate toxicity results?**

**(Yokel)** I think it is absolutely essential. Simply put, if you don't know what you're working with, then you can't anchor the toxicity effects to the material. In this regard, science is too independent sometimes, and nanoceria is a great example of that. This is where collaborations and consortiums are useful in order to relate effects to the same material used by all parties. More international collaborations would be useful as well.

**(Doudrick) Where is the future of nanotoxicity heading?**

**(Yokel)** Like all new technologies, people start to advance it first and discover all of these neat applications. Then temporally later we start to think about this dark side, these adverse effects. So nanotox has really come in only about ten years ago while nanoscale technologies are more like twenty or more years ago. So, it's behind. I think one of the key things driving government funding are these projects demonstrating the benefits of nanoscale materials, but if the public will not accept the benefits of nanoscale materials that it will all go down the drain. Like GMOs in Europe, which are basically not accepted, so the potential benefit will not be realized. And we are starting to see this same trend in the US, because the public is leery of potential bad things and that leads them to be less open-minded to the benefits. This is a concern I have about speaking out too much about adverse effects of nanoceria. Everything has potential adverse effects, but it also has beneficial effects and we have to define both. So I think nanotox will continue to be important. One of the big challenges is doing a thorough nanotox assessment on all these materials. It is just too expensive. One approach is to find materials that are similar enough that you can extrapolate the toxicology from a few model compounds.



## 3<sup>rd</sup> SNO CONFERENCE PREVIEW

### PLENARY SPEAKERS

Dr. Clayton Teague, Pixelligent Technologies Advisory Board  
 Ms. Lynn Bergeson, Bergeson & Campbell, P.C.  
 Dr. Mihail (Mike) Roco, US National Science and Technology Council  
 Dr. George Whitesides, Harvard University  
 Dr. John C. Warner, Warner Babcock Institute for Green Chemistry, LLC  
 Dr. Mark Wiesner, Duke University  
 Mr. David Rejeski, Woodrow Wilson Center



### STUDENT AWARD WINNERS

Congratulations to this year's student award winners! Students had to write a short essay describing how their work related to SNO and why it was important for sustainable nanotechnology.

Student	University	Student	University
Catherine Anders	Boise State University	Sanghamitra Majumdar	UTEP
Matthew Chan	Virginia Tech	Megan O'Connor	Duke University
Yingqing Deng	Umass Amherst	Francis Osonga	Binghamton University
Jingjing Fan	University of Houston	Jared Schoepf	Arizona State University
Yuxiong Huang	UCSB	Brian Sim*	UMass Amherst
Camilla Jensen	Arizona State University	Adel Soroush	Concordia College
Victor Kariuki	Binghamton university	Natalia von Reitzenstein	Arizona State University
Andrew Lake	SUNY Binghamton	Kaitlin Vortherms	Arizona State University
Xitong Liu	Johns Hopkins University	Ben Wender	Arizona State University
Sharlee Mahoney	University of Pittsburgh	Nubia Zuverza	UT El Paso

\*Undergraduate student

## ABSTRACT PREVIEW

### Accumulation of engineered nanoparticles in plant foods: Nutritional bioaccessibility and dietary exposure risks

Stephen Ebbs, Southern Illinois University

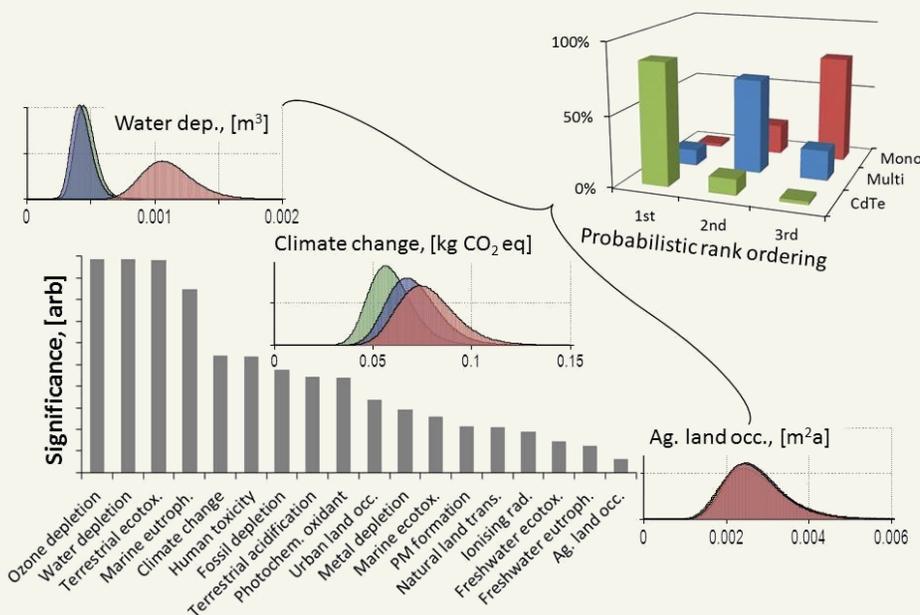


The release of engineered nanomaterials (ENMs) into the environment has raised serious concerns about their potential risks to food safety and human health. There is a particular need to determine the extent of ENM uptake into plant foods. Belowground vegetables that grow in direct contact with the soil are the foods which will likely accumulate the highest concentration of ENMs and present the most significant risk to human health. Ongoing studies funded by USDA-NIFA are using species such as carrot and sweet potato to examine accumulation of ENMs in edible tissues. Results from carrot and parsnip have shown that for the outer layers of the vegetable, the peels typically removed prior to consumption, effectively screen ENMs preventing their accumulation but not free ions. Dietary intake models are being developed to relate the accumulation of the metals from metallic nanomaterials to the potential impact resulting from

consumption of those plant tissues. Currently, a physiologically-based extraction test is being applied to assess the extent to which these metals are released during the gastric phase of simulated digestion. The goal of these efforts is to provide a comprehensive picture of the food safety risk posed by these ENMs in these vegetables.

### Anticipatory LCA for Responsible Innovation of Nanotechnology

Ben Wender, Arizona State University



Current research policy and strategy documents recommend applying life cycle assessment (LCA) early in research and development (R&D) to guide emerging technologies toward decreased environmental burden. However, existing LCA practices are ill-suited to support these recommendations. Barriers related to data availability, rapid technology change, and isolation of environmental from technical research inhibit application of LCA to developing technologies. Overcoming these challenges requires methodological advances that help identify environmental opportunities prior to large R&D investments. Such an anticipatory approach to LCA requires synthesis of social, environmental, and technical knowledge beyond the capabilities of current practices. This paper presents a novel framework for anticipatory

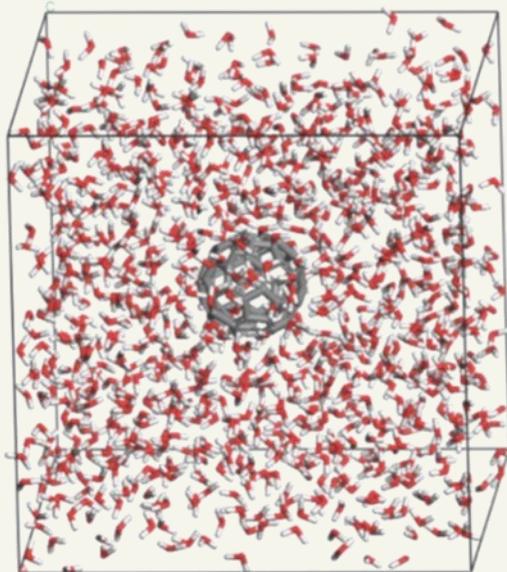
LCA that incorporates technology forecasting, risk research, social engagement, and comparative impact assessment in a way that promotes integration of environmental criteria early in innovation. Components of this framework are illustrated using carbon nanotubes (CNTs) and suggest that uncertainty in toxicity data and potential improvements in manufacturing efficiency drive uncertainty in LCA results. These results indicate that an anticipatory approach to LCA can prioritize research questions to help guide environmentally responsible innovation of emerging technologies.

## ABSTRACT PREVIEW

### Functionalized Fullerenes in Water: A Closer Look

Jae-Hong Kim, Yale University

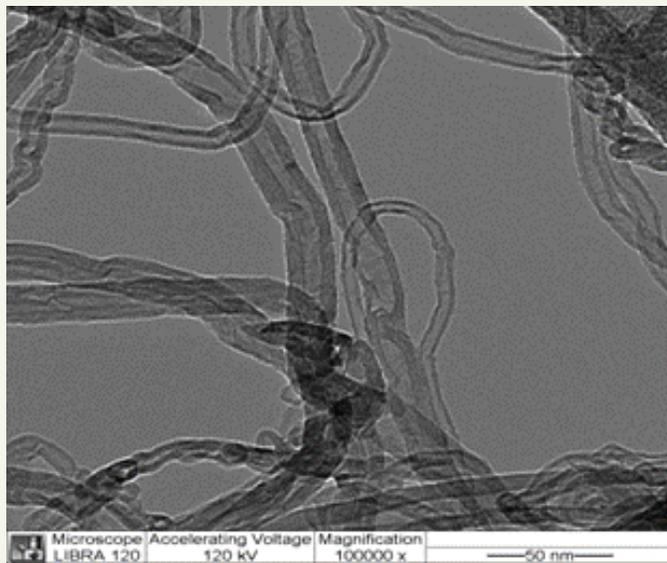
The excellent photophysical properties of  $C_{60}$  fullerenes have spurred much research on their application to aqueous systems for biological and environmental applications. Spontaneous aggregation of  $C_{60}$  in water and the consequent diminution of photoactivity present a significant challenge to aqueous applications. The mechanisms driving the reduction of photoactivity



in fullerene aggregates and the effects of functionalization on these processes, however, are not well understood. By examining and characterizing several series of functionalized fullerenes, we take a closer look at the surface and molecular phenomena involved in photosensitization. Complementary theoretical (computer simulation) and experimental tools are used to probe the underlying mechanisms of fullerene aggregate photoactivity. Molecular dynamics (MD) simulations of fullerenes with water, oxygen, and neighboring fullerene molecules were performed to investigate time-evolved interactions in systems containing 1,000 water molecules. High resolution transmission electron microscopy complimented the simulated fullerene-fullerene interactions by providing physical evidence of fullerene interaction characteristics. Raman spectroscopy was employed to provide supplementary evidence for the highly-ordered water structures predicted by the molecular simulations. Photoactive fullerene aggregates had weaker fullerene-fullerene and fullerene- $O_2$  interactions, suggesting that photoactivity may be reduced by strong fullerene-fullerene interactions promoting self-quenching pathways and strong fullerene- $O_2$  interactions that interfere with the sensitization process.

### Analysis of cardiac repolarization as a tool for the noninvasive assessment of cardiovascular system exposure to carbon and metallic nanotubes

Joseph Starobin, University of North Carolina at Greensboro



Recent experimental studies demonstrated that just a moderate pulmonary exposure to carbon nanotubes may trigger an oxidative vascular damage which, in turn, may significantly accelerate the formation of atherosclerosis and atherosclerotic plaques.

Although these findings conclusively demonstrated the importance of biochemical and immunological markers for identifying nanotube induced oxidative stress and vascular damage, the association of such exposure with noninvasive electrophysiological factors was not understood.

In this study we investigate the dynamics of cardiac repolarization, in particular QT and RR intervals, during an intensity-controlled dobutamine exercise stress test for the conscious mice after pulmonary exposure to single/multiple-wall carbon (CNT) and  $TiO_2$  nanotubes.

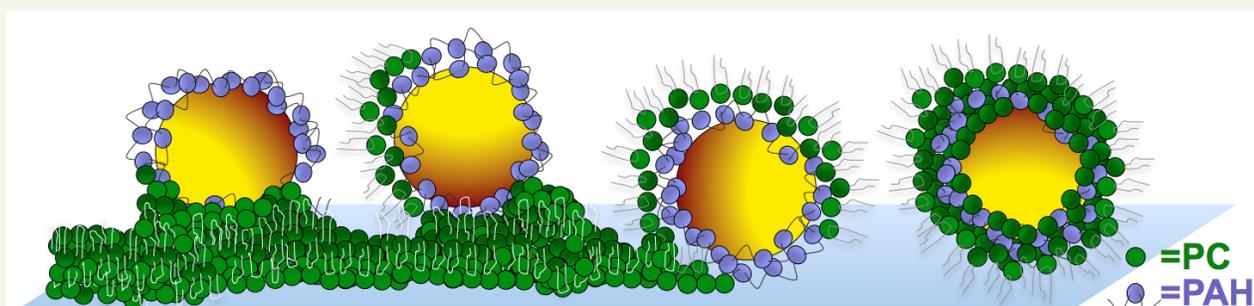
We demonstrate that the association of toxic outcomes of pulmonary exposure to different nanotubes using QT and RR intervals is comparable with toxic responses determined using major bio- and immunochemical markers. Our results suggest

that the analysis of cardiac repolarization can be utilized for the noninvasive systemic evaluation of cardiovascular nanotoxicity.

## ABSTRACT PREVIEW

**Direct Views of the Nano-Bio Interface***Franz Geiger, Northwestern University*

This work presents a comprehensive, multi-probe molecular-level investigation of the nano-bio interface that focuses on the lipids of a supported lipid bilayer, the core of engineered nanoparticles, and the role of molecular structure, electrostatics, and ionic strength in mediating the interactions between bilayers and nanoparticles. Interfacial charge densities and potentials are determined for silica-supported phospholipid bilayers formed from lipids having zwitterionic, negatively charged, and positively charged headgroups. Quartz crystal microbalance with dissipation monitoring (QCM-D), fluorescence recovery after photobleaching (FRAP), and atomic force microscopy demonstrate the presence of well-formed supported lipid bilayers, which, as probed by vibrational sum frequency generation (SFG), undergo negligible structural changes along their alkyl chains when NaCl concentration is raised from 0.001 to 0.1 M. From second harmonic generation (SHG) measurements we estimate that each zwitterionic headgroup of the bilayer formed from pure DOPC is associated with an apparent charge of  $-0.028(+0.008/-0.007)\times 10^{-19}$  C, corresponding to  $1.8 \pm 0.5$  % of an elementary negative charge. Moreover, we show that a supported lipid bilayer carrying an apparent negative interfacial potential may interact with not just positively charged 4-nm diameter gold nanoparticles but also with negatively charged gold nanoparticles. In this latter case, charge-charge repulsion does not appear to inhibit particle-bilayer interactions and is likely overcome by multivalent interactions that are estimated to involve three to five hydrogen-bond equivalents, or, alternatively, hydrophobic interactions between, for instance, 30 to 35 methylene groups of the bilayer lipids and the particle ligands. FRAP, QCM-D, and SFG measurements indicate that the bilayers remain intact under the conditions of the experiments. SHG charge screening experiments are consistent with a charge density ranging between  $-0.06$  and  $+0.02$  C/m<sup>2</sup> when positively charged gold nanoparticles attach to a supported lipid bilayer, and  $-0.05$  and  $-0.01$  C/m<sup>2</sup> when negatively charged gold nanoparticles attach to the same bilayer, which includes the interfacial charge density of the bilayer of  $-0.015 \pm 0.007$  C/m<sup>2</sup> that we estimate from our experimental data. The positively charged PAH-coated particles were shown by QCM-D to be present at surface coverages of roughly  $6 \times 10^{12}$  particles attached per cm<sup>2</sup>. Using well-justified assumptions regarding particle surface coverage from QCM-D measurements, the total charge density per PAH-coated particle attached to the supported lipid bilayer is estimated from Gouy-Chapman model fits to be between  $-7.5 \times 10^{-19}$  C and  $+5.8 \times 10^{-19}$  C. The surface coverage of the MPA-coated particles was too small to be detected by QCM-D. With a limit of detection of  $\sim 7$  ng/cm<sup>2</sup>, we estimate that the upper bound for the charge density per MPA-coated particle attached to the supported lipid bilayer ranges from  $-3.5 \times 10^{-16}$  to  $0.5 \times 10^{-16}$  C/particle. The quantitative thermodynamic, spectroscopic, and electrostatic data presented here serve to benchmark experimental and computational studies of the nano-bio interface.



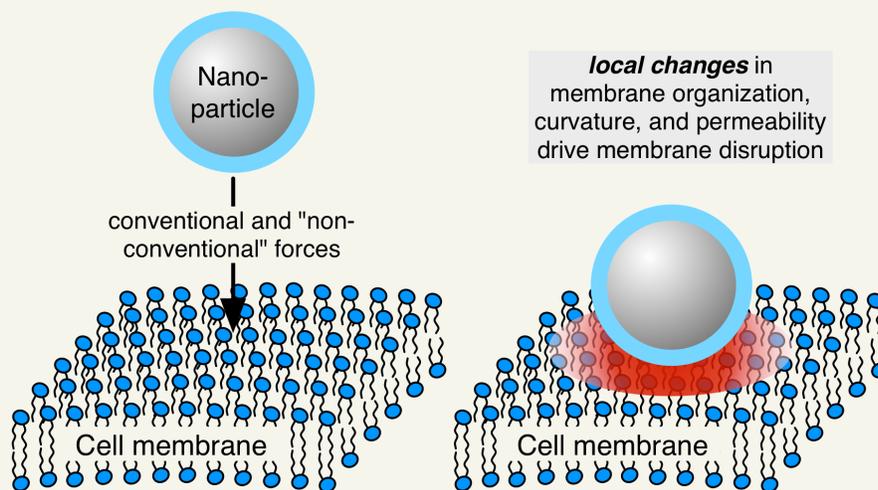
Research at the NSF Center for Sustainable Nanotechnology shows polyallylamine hydrochloride-coated nanoparticles destroy DMPC-rich bilayers by lipid corona formation

## ABSTRACT PREVIEW

**Beyond binding: The complexity of nanoparticle-biomembrane interactions**

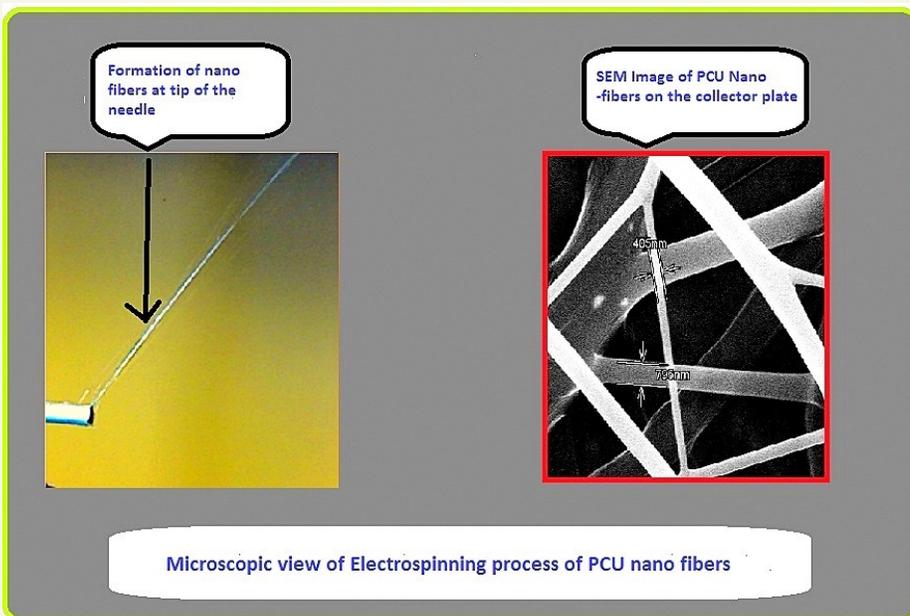
Geoffrey D. Bothun, University of Rhode Island

This presentation will address the complexity of nanoparticle-biomembrane (i.e. cellular membrane) interactions that derives from the biochemical and biophysical diversity of biomembranes, the chemical and physical diversity in natural and biological environments, and environmental transformations of engineered nanoparticles (ENPs). Most studies of ENP-biomembrane interactions, ours included, have utilized model homogeneous biomembranes in order to obtain fundamental insight into ENP-biomembrane binding and membrane disruption. However, establishing firm links between these interactions and the degree of inhibition or toxicity caused by an ENP requires "realistic" biomembrane models that can reflect the inherent dynamic and heterogeneous response to ENP binding, and strategies for decoupling ENP-biomembrane interactions that arise during environmental transformation processes.

**Environmental Impact Analysis of Electrospun PCU Nano fibers**

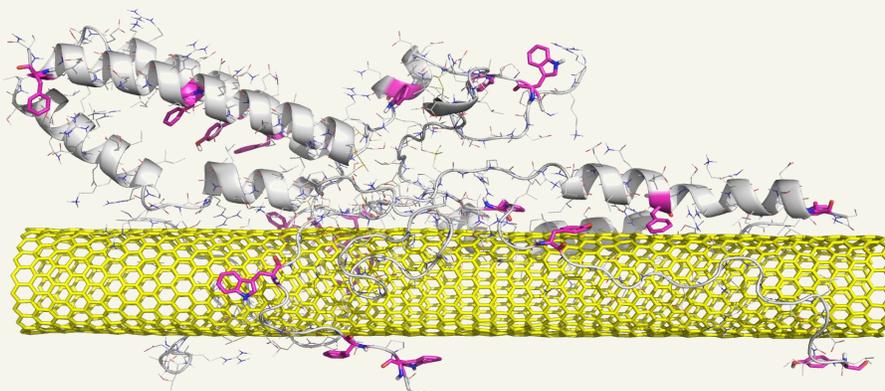
Hruday chand Katakam, University of South Florida

It is very important to evaluate the environmental impacts of synthesis, process, or products associated with an emerging technology like Nanotechnology. Life cycle assessment (LCA) is one of the recognized reliable techniques used to assess sustainability impacts. This study includes the comparative LCA of the production of Polyurethane carbonate (PCU) nano fibers using N,N-Dimethylformamide (DMF) and Tetrahydrofuran (THF) solvent mixtures (1:0, 0:1, 1:1, 3:7, 7:3). The aim of this study is to analyze the impact of solvents for the fabrication of PCU nanofibers and plan for the use of more environmentally friendly solvent to produce sustainable nano fibers. The stages considered for LCA analysis are materials, processes used for preparation of polymer solution, and power consumption used in electrospinning the nano fibers. The comparisons are made on equal mass basis i.e. materials, processes used to fabricate 1 gram of PCU nano fibers (functional unit). The entire inventory is compiled from open literature. LCA software version Simapro 7 is used. IMPACT 2002+ Life Cycle Impact Assessment (LCIA) tool is used to evaluate the environmental impacts. The preliminary results of this study reveals PCU nano fibers fabricated through DMF alone has less environmental impact in terms of all impact indices when compared to rest.



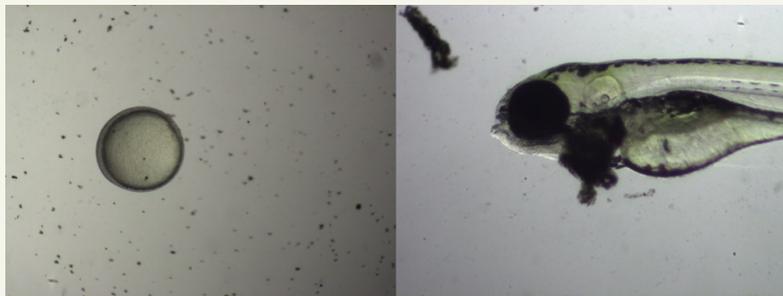
The stages considered for LCA analysis are materials, processes used for preparation of polymer solution, and power consumption used in electrospinning the nano fibers. The comparisons are made on equal mass basis i.e. materials, processes used to fabricate 1 gram of PCU nano fibers (functional unit). The entire inventory is compiled from open literature. LCA software version Simapro 7 is used. IMPACT 2002+ Life Cycle Impact Assessment (LCIA) tool is used to evaluate the environmental impacts. The preliminary results of this study reveals PCU nano fibers fabricated through DMF alone has less environmental impact in terms of all impact indices when compared to rest.

## ABSTRACT PREVIEW

**Multiscale study of the structure and dynamics of nanoparticle corona***Feng Ding, Clemson University*

Upon entering biological environments, nanomaterials readily absorb biomolecules onto their surfaces and assume the form of “bio-coronae” that dictate their biological identities. Interactions with nanoparticles can also alter the structure, dynamics, and functions of the bound biomolecules. Therefore, understanding of structure and dynamics of bio-coronae is essential for our understanding of their biological and pathological functions. By offering not only molecular insight of experimental observations but also experimentally testa-

ble hypothesis, computational modeling can be used together with experimental studies to uncover the structure, dynamics, and function inter-relationship of coronae. The major challenges in the computational modeling of nanoparticle bio-coronas include the large system size and the long timescales associated with corona formation. We apply state-of-the-art multiscale molecular dynamics simulations to study the structure and dynamics of bio-coronae at the nano-bio interface, including the formation of protein-silver nanoparticle corona, the competitive binding of natural organic material with graphene, and the effect of surface chemistry on protein-nanoparticle interactions, and etc. With the continuous development of computational and experimental methodologies in characterizing the nano-bio interactions, we hope to more accurately evaluate the adverse or beneficial effects of engineered nanoparticles, which allows the design of more biocompatible nanomedicine or nanoproducts.

**Towards the Development of a Model that Informs Safer Carbon Nanotube Design: Using Zebrafish Mortality to Evaluate Carbon Nanotube Ecotoxicity Potential**
*Leanne Gilbertson*

Release of carbon nanotubes (CNTs) to the environment will increase significantly with rising production volumes and advancement of applications to market. Yet, the magnitude and mechanism of CNT hazard remains unresolved. The aim of this study is to advance our understanding of potential CNT environmental impacts through the development of a statistical model intended to both correlate specific CNT physicochemical properties with *Danio rerio* (zebrafish) toxicity endpoints and serve

as the foundation of a predictive toxicity paradigm. Zebrafish are considered the gold standard for assessing environmental toxicity impacts and are ideal candidates for high throughput toxicity screening. Multi-walled carbon nanotubes (MWNTs) were investigated due to their large production volumes, utilization in high concentration applications, and enhanced dispersion compared to SWNTs. Furthermore, our previous work shows that MWNTs exhibit variable cytotoxicity depending on the extent and type of surface oxygen functionalization. Thus, MWNTs were differentially treated to systematically alter their physicochemical properties, including dispersity (aggregate size and morphology), surface charge, electrochemical activity, and percent oxygen, which have been identified as key properties that can influence CNT toxicity. Our statistical analysis of the combined results determined that surface charge is the most significant single predictor of embryonic mortality at 24 and 120 hpf and when combined with dispersed aggregate properties, comprise the most significant multivariate regression model.

## ABSTRACT PREVIEW

**Advancing sustainable nanomaterials solutions through greener design and synthesis***James E. Hutchison, University of Oregon*

Nanotechnology offers new materials and applications that promise numerous benefits to society and the environment, yet there is growing concern about the potential health and environmental impacts of production and use of nanoscale products. Because nanotechnology is still in the “discovery” phase, the design and production of materials have yet to be optimized. For example, the synthetic methods used to produce nanomaterials are often inefficient or require the use of hazardous reactants. To advance beneficial applications of nanomaterials and minimize harm, we need to understand how nanomaterials interact with the environment and the causes of their biological impacts, and we need to develop new methods of production that address the limitations of discovery scale approaches. Green chemistry is an approach to the design of materials, processes and applications that has the potential to reduce hazards at each stage of the life cycle. I will describe how green chemistry applied to nanoscience - greener nanoscience – can advance safer, more efficient nanosyntheses and provide design rules for safer nanomaterials. I will provide examples from our research on the synthesis, functionalization and application of metal nanoparticles and metal oxide nanocrystals.

**Explosive thermal reduction of graphene oxide-based materials: Safety implications for production and storage***Yang Qiu, Brown University*

Nanotechnology risk is not solely associated with material toxicity, but may also extend to manufacturing safety, since some nanomaterials are capable of energetic chemical reactions leading to heat release and overpressure when processed in large quantities. Thermal reduction of graphene oxide or graphite oxide (GO) is an important processing step in the fabrication of many graphene-based materials and devices. Here we show that some bulk solid GO samples can undergo explosive decomposition when slowly in inert gas environments, while others do not. These micro-explosions can occur for samples as small as few milligrams and are sufficiently energetic to cause laboratory equipment damage. Thermochemical analysis methods are used to understand the factors that lead to the explosive reduction mode. The studies show that the explosive mode of reduction is caused by the exothermicity of GO reduction coupled with a threshold sample mass/size that causes heat and mass transfer limitations leading to local temperature rise, pressure build-up and even a thermal runaway reaction. The explosive mode of reduction is not caused or promoted by interstitial water but its onset temperature of exothermic reduction can be lowered by metal hydroxide impurities or reducing agents. By allowing early release of internal gas pressure, the explosive mode reduces the extent of surface area development in GO exfoliation from an optimum value of 1470 m<sup>2</sup>/g obtained under non-explosive reduction conditions. Explosive reduction of bulk GO may poses an industrial safety hazards during large-scale storage, handling, and processing.

**Development and Application of Crumpled Graphene Oxide-Based Nanocomposites as a Platform Material for Advanced Water Treatment***John Fortner, Washington University in St. Louis*

This presentation highlights the potential for crumpled graphene-based nanocomposites in water treatment technologies, both as a high performance photocatalyst and self-assembling component(s) of reactive membrane assemblies. Recent material advances with combined TiO<sub>2</sub>-carbon nanomaterial based photocatalysts, such as graphene, have demonstrated superior physical and chemical properties compared to traditional analogues. However, in water, flat graphene (or reduced graphene oxide, rGO)-TiO<sub>2</sub> nanocomposites restack due to strong  $\pi$ - $\pi$  attraction, leading to significant decay of photocatalytic performance. Here, I will present recent work on aggregation resistant crumpled graphene oxide (GGO)-TiO<sub>2</sub> nanocomposites, which have been developed and demonstrated to be superior aqueous photocatalysts. The as-synthesized quasi-spherical, core-shell nanostructured composites, with controllable size and functionality (including magnetic susceptibility), show significantly enhanced photocatalytic activity compared to bare TiO<sub>2</sub> due to increased lifetime of photo-induced holes and electrons – leading to significant oxidative and reductive reaction pathways, which can be directed. In addition, porous, CGO-based nanocomposite films which are highly water-permeable, photo-reactive, antimicrobial and even subject to magnetic manipulation, will be described, including performance regimes for: thin film nanocomposite (CGO embedded) membranes, (2) CGO surface functionalized - commercial UF/NF/RO membranes, as well as (3) self-assemblies of CGO nanocomposites.

## ABSTRACT PREVIEW

**Concurrent plant uptake of pharmaceuticals and nanomaterials in hydroponic and soil environments***Yingqing Deng, University of Massachusetts Amherst*

Pre-existing pharmaceutical residues in agricultural soils may interact with nanomaterials. The accumulation of nanomaterials in the environment poses risks to food safety and nanotechnology sustainability. In this study, the addition of pristine or carboxyl-functionalized carbon nanotubes (CNTs) was tested on the uptake of the pharmaceutical residue carbamazepine by collards (*Brassica oleracea*) under hydroponic and soil-grown conditions. Pristine CNTs alleviated collard stress from carbamazepine exposure by reducing observable leaf injury, but the plants biomass was significantly compromised by concurrent exposure of CNTs and carbamazepine. Collard roots accumulated carbamazepine and effectively translocated it to shoot in hydroponics (transfer factor, TF=25.9), but amendment with pristine and carboxyl-functionalized CNTs dramatically lowered TF to 2.5 and 3.5, respectively. When added to soil, both CNTs similarly reduced overall carbamazepine accumulation in collard. Notably, 80% of the carbamazepine associated with the root could be washed off by sodium dodecylbenzenesulfonate under sonication. The results show that CNTs significantly affect the bioavailability and translocation of carbamazepine in collards and in soil, resulted in greater contaminant binding and exclusion of the contaminant outside of the plant. The interactions among nanomaterials, plants and pharmaceuticals is of critical importance to assess the implications of nanotechnology for the environment and for agriculture.

**Inactivation of foodborne microorganisms using Engineered Water Nanostructures (EWNS)***Georgios Pyrgiotakis, Harvard School of Public Health*

Food borne diseases caused by the consumption of fruits and vegetables contaminated with pathogenic microorganisms or their toxins have serious economic and public health implications. We explored the effectiveness of a recently developed novel, nanotechnology-based, intervention method for the inactivation of microorganisms on fresh produce and food production surfaces. This method utilizes Engineered Water Nanostructures (EWNS) produced by electro-spraying of water. EWNS possess unique physico-chemical and biological properties. They have an average diameter of 25 nm, are highly charged (10 electrons/structure), have extended lifetime in the air (in the order of hours) and are loaded with Reactive Oxygen Species (ROS). We investigated the efficacy of EWNS in inactivating pathogens of importance to the food industry such as *Escherichia coli*, *Salmonella enterica* and *Listeria innocua*. The delivery of the EWNS to the fresh produce/surfaces was also optimized using two exposure approaches: 1) EWNS were introduced in a chamber and deposited on surfaces by diffusion; 2) a "draw through" Electrostatic Precipitator Exposure System (EPES) was developed and characterized and used to increase EWNS deposition on surfaces by utilizing their high electric charge. When inoculated bacteria on stainless steel surfaces were exposed to an EWNS aerosol concentration level of 24,000 particles/cc for 90 minutes, using the diffusion exposure approach, the bacterial concentration was reduced by 0.7 – 1.8 log, as compared to the non exposed (control). Inactivation was also found to be bacteria dependent. Similarly, for bacteria inoculated organic tomatoes, using the same exposure approach and aerosol concentration levels, bacterial concentration was reduced by 0.5 – 0.9 log, as compared to the control. The EPES exposure approach increased the delivery of EWNS to the fresh produce/surfaces and was found that at EWNS aerosol at concentration of 50,000 particles/cc and a 90 minute exposure time, resulted in a 1.4 log reduction of *E.coli*, as compared to the control. These preliminary results indicate that this environmental nanotechnology based approach is a very promising approach in the battle against foodborne diseases.

**Recycling of Waste Tires for Supercapacitor Electrodes***Nianqiang (Nick) Wu, West Virginia University*

About 27 million waste tires are disposed annually. Only a small percentage of waste tires are recycled to low-value commercial products such as the ground cover and the activated carbon as the environmental adsorbent. On the other hand, the carbon materials used for commercial supercapacitor electrodes are mainly synthesized with fossil materials as the precursors. In order to address develop sustainable materials for supercapacitors, this study presents the recycling of waste tires for supercapacitor electrodes. A synthetic route has been developed to carbonize the scrap tires and to active the resulting carbon product. In addition, the pore structure of the resulting carbon product has been tailored. The experimental and statistical analysis results show that the micropores and mesopores in the active carbon have significant effect on the electrochemical performance of supercapacitor electrodes.

**Precious metal recovery from nanowaste for sustainable nanotechnology: Current challenges and life cycle considera-**

## ABSTRACT PREVIEW

**tions***Paramjeet Pati, Virginia Tech*

The increasing use of nanomaterials poses new challenges for their disposal and waste management. Moreover, several nanotechnologies employ resource-limited materials, such as precious metals and rare earth elements. It is therefore essential to develop strategies to recover and recycle these materials from nanowaste, and thus make nanotechnology more sustainable. However, at present, neither well-established protocols nor federal regulations exist for nanowaste management and precious metal recovery from nanowaste. To address this issue, we developed laboratory-scale methods to recover gold from nanowaste. For our initial experiments, we used potassium tetrabromoaurate and citrate-coated gold nanoparticles (AuNPs) as simulated waste. Alpha-cyclodextrin was used to recover gold via selective complexation, followed by downstream treatments to form chloroauric acid. Finally, the chloroauric acid from recovered gold was used to make new AuNPs. Besides developing new methods for recovering and recycling gold from nanowaste, we are also conducting life cycle assessment to compare scenarios of gold production with and without recycling. Our research can provide new insights into the chemistries involved in gold recovery, as well as into the life cycle considerations in nanowaste recycling. This research also has the potential to improve current waste management practices and inform future nanowaste management policies.

**Nanotechnology for the Photocatalytic Degradation of Cyanobacterial Toxins and Contaminants of Emerging Concern***Changseok Han, University of Cincinnati*

Water contaminants of emerging concern such as cyanobacterial toxins, pharmaceuticals, pesticides, and personal care products, showing either high toxicity or adverse effects on humans and animals' health has been frequently found around the world.

For an appropriate treatment of the water contaminants, nanostructured titanium dioxide (n-TiO<sub>2</sub>)-based advanced oxidation processes have been extensively studied due to the low-toxicity, thermal and chemical stability, and relatively high photocatalytic activity of n-TiO<sub>2</sub>. Despite of its excellent properties, much effort for a modification of the optical and morphological properties of n-TiO<sub>2</sub> is still needed to enhance the efficacy of photocatalytic degradation of the contaminants and to improve its solar energy utilization.

In this direction, different methods for the modification of optical and morphological properties of n-TiO<sub>2</sub> to use visible light (~45% of whole solar spectrum) and to enhance the efficacy of the treatment were explored. The modified n-TiO<sub>2</sub> was thoroughly characterized with X-ray diffraction, scanning electron microscopy, transmission electron microscopy (TEM), high resolution-TEM, X-ray photoelectron spectroscopy, and porosimetry analysis. Moreover, the photocatalytic activity for decomposing the contaminants was evaluated and the degradation pathways were scrutinized. In this presentation, results on the modification, characterization, and evaluation of photocatalytic activity of n-TiO<sub>2</sub> will be discussed in detail.

**Attachment and Interactions of Graphene Oxide with Model Biological Membranes: Implications for Nanotoxicity***Kai Loon Chen, Johns Hopkins University*

Graphene oxide (GO) is a two-dimensional, carbon-based nanomaterial with unique electrical, mechanical, and thermal properties. Recently, several studies have shown that GO can exhibit toxicity toward human and bacterial cells and that GO can damage cell membranes. The detailed mechanisms for the damage of cell membranes by GO, however, are still not well understood. The objective of this study is to investigate the interactions between GO and model biological membranes in order to better understand the mechanisms for the cytotoxicity of GO. In this study, supported lipid bilayers (SLBs) composed of zwitterionic 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), as well as DOPC vesicles, are used as model cell membranes. The deposition rates of GO on SLBs are measured with a quartz crystal microbalance with dissipation monitoring (QCM-D). The deposition kinetics increased with increasing salt (NaCl or CaCl<sub>2</sub>) concentrations under neutral pH conditions, indicating that electrostatic interactions are likely to play a critical role in controlling the attachment of GO to cell membranes. When GO comes into contact with DOPC vesicles, no significant damage to the vesicles is observed. Further investigation will be conducted with the use of a fluorescent dye to evaluate the integrity of vesicles when GO attaches to the biological membranes.

**A Recent History of Federal Involvement in the Regulation of Nanotechnology Research: A Potential Model for Fu-**

## ABSTRACT PREVIEW

### ture Scientific Research

*Brandi L. Schottel, National Science Foundation*

While scientific breakthroughs promise a better quality of life for humanity, they have often inadvertently caused health and environmental harm. The ethics of scientific discovery, more recently couched in terms of intellectual property issues, have traditionally sought to create breakthroughs without damage. However, many have come with negative repercussions. Within this background, several key players in the federal government contributed to a revolutionary approach in the development of the game-changing field of nanotechnology. This emerging technology of materials which measure 100 nm or less has led to an explosion of advances in all science and engineering fields such as electronics, medicine, materials, food, agricultural, and environmental applications. However, nanotechnology could come with a heavy price with regard to human and environmental health. In order to stem harmful consequences from what should be a remarkable tool for societal progress, federal government programs ensured that investigations of possible health and environmental impacts paralleled commercial advances. This paper will present a recent history of proactive environment, health, and safety (EHS) research programs in the federal government which complement research in advancements of nanotechnology. This more recent approach to research represents a potential shift in how scientific investigations will be approached in the future.

### Straw Man System for Defining "Good" and "Bad" Nano

*Richard Reibstein, Massachusetts Office of Technical Assistance*

Scientific, medical, legal, engineering and policy specialists are capable of diving into the enormously complex aspects of nanotechnology, and it cannot be expected that a "Sustainable" nanotechnology can be created or maintained without some measure of mastery of what may be termed a "complex of complexities". But the general public may think of nano in very simple terms, of "good" or "bad" nano. Although from the point of view of those willing to grasp complexities it may seem overly reductive and in some ways dangerous to think in this way, if it is done well it could be helpful in generating consensus on policy directions, and therefore a reasonable accommodation to the tendency to reduce the issue to simple moral terms may be desirable. The body of experts concerned with this issue could include in their deliberations how very simple discernments may properly be made, along with the very complex analyses in which they are engaged. If those inclined to understand the relevant matters as deeply as they can do not take the lead in devising simple, useable concepts that the public can apply, default judgments will likely be used, and the risks of their being overbroad or unfair - the risks of sloppily reductive thinking - will likely be increased as a result. Experts should weigh in on what is good and bad, before the public places those labels on the new classes of materials that are being developed.

### Recent developments in occupational exposure assessment

*Derk Brouwer, TNO*



Over the last five years the number of published studies on occupational exposure to nanomaterials have increased substantially, documenting relevant developments with respect to release and exposure assessment, exposure modelling, and harmonization and standardization issues. Partly due to lack of harmonization

## See you there!

with respect to measurement strategy and data interpretation and reporting, meta-analysis of exposure data is not feasible yet, however, some indications of scenarios with potential for relatively high release and eventually exposure can be observed which enables preliminary mapping of exposure 'hot

## ANNOUNCEMENTS

**SNO Workshop III—NanoEHS: Fundamental Science Needs**

A WORKSHOP SPONSORED BY  
THE NATIONAL SCIENCE FOUNDATION AND SNO  
SATURDAY, NOVEMBER 1, 2014

**Vicki H. Grassian**, Workshop Chair  
**Amanda J. Haes**, Workshop Co-Chair

The development of NanoEHS and the field of sustainable nanotechnology must be backed by solid scientific underpinnings. One grand challenge includes a greater understanding of the size and shape dependent properties of nanomaterials from a fundamental chemistry and physics perspective and then applying this understanding to environmental health and safety issues associated with nanomaterials. A National Science Foundation Sponsored Workshop focused on identifying and highlighting fundamental science needs in NanoEHS research will be held in association with the 2014 SNO annual meeting. See [www.susnano.org](http://www.susnano.org) for more information.

**SUN-SNO-GUIDENANO Conference**  
**March 9-11, 2015 in Venice, Italy**

More info at <http://www.susnano.org/conferenceOverview2015SNO-SUN-GN.html>

**Annual SNO Meeting**  
**November 1-3, 2015****WANTED: Good ideas for SNO**

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