

SYMPOSIUM BI01/ET14/NM04

TUTORIAL: Life Cycle Analysis from an Industrial Perspective
November 25 - November 25, 2018

* Invited Paper

TUTORIAL Life Cycle Analysis from an Industrial Perspective

Sunday Afternoon, November 25, 2018
Hynes, Level 2, Room 200

Environmental issues keep steadily increasing, thus there is a strong urge to discuss how materials scientists could more rapidly respond to the worldwide concerns. This joint tutorial effort would be organized by the three symposia together. To ensure the success of such synergistic efforts it is also urged a close dialogue with society so to establish guidelines for policymakers, thus this tutorial will incorporate both the societal and the engineering aspects of life cycle analysis (LCA) would be covered. The main objective of this tutorial is to explore communications pathways between companies and materials researchers that further elevate the profile and challenges of sustainability that represents a societal necessity and a viable and critical topic for research.

1:30 PM

Societal Aspect of LCA Jean-Pierre Birat; ArcelorMittal

Materials are not simply the product of an engineering discipline, Materials Science, but also "social constructs" that have entertained a close relationship with society all through the historical timeline and remain a core element of our modern world, what is called a Key Enabling Technology. How this can be analyzed by parallel approaches of hard and soft sciences will be explained in the class as well as the tryptic of economic, environmental and social values of materials. Examples reported in the 13 past SAM conferences will be used as examples.

2:45 PM BREAK

3:15 PM

Engineering Aspect of LCA Alan Rae; IncubatorWorks

The instructor will provide an overview on all the aspects considered in a life cycle analysis aimed to the engineering design of an industrial process. A part of the tutorial will involve the interaction with the audience in order to apply some of the concepts described in the first part of the tutorials to common objects.

4:15 PM Sustainability Challenge

The symposia organizers will divide the participants into groups and a sustainability challenge will integrate the concepts presented by the instructors so to review and facilitate networking among participants and instructors

4:45 PM

Final Remarks

SYMPOSIUM BI01

Sustainable Development in Materials Science and Related Societal Aspects
November 26 - November 28, 2018

Symposium Organizers

Jean Gaumet, University of Lorraine
Margrit Hanbücken, Université Aix-Marseille

* Invited Paper

SESSION BI01.01: Education and Society I
Session Chairs: Joelle Lighezzolo-Alnot and Ashley White
Monday Morning, November 26, 2018
Sheraton, 3rd Floor, Hampton

8:15 AM BI01.01.00

Eigenprot—A Musical Instrument Based on the Molecular Vibrations of Over 100,000 Protein Structures Zhao Qin and Markus Buehler; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

We developed a high-throughput method that enables to automatically compute the vibrational spectra of more than 100,000 proteins available in the Protein Data Bank in a consistent manner, and then use the resulting eigenvalue of the first 70 normal modes of protein to generate audible sound by overlaying the molecular vibrations in a desirable pattern and translating them to the audible frequency range. The method, implemented as a Max audio device, provides unparalleled insights into the rich vibrational signatures of protein structures, and offers new ways for creative musical expression by using it as a modern musical instrument, and serves as an interactive educational tool for broader outreach. This musical instrument, named Eigenprot, is fully defined by the vibrational feature of almost all known protein structures, making it fundamentally different from all the traditional instruments that are limited by the material properties of conventional engineering materials.

8:30 AM *BI01.01.01

Key Concepts and Educational Approaches for Engaging Public Audiences in Learning About Materials Science and Sustainability Rae Ostman and Karyn Perdue; Arizona State University, Tempe, Arizona, United States.

Over the past several decades, sustainability scientists and informal educators have developed a number of ways to engage multiple and diverse public audiences in learning about—and acting on—sustainability concepts related to materials science and related fields. Meanwhile, scientific professional societies such as MRS are seeking to integrate sustainable development in materials science and engineering and to enhance communication among scientists, engineers, and the public for the greater good.

Science museums are trusted public institutions and a perfect venue to engage the world's citizens to learn about and address solutions to global challenges we face. Arizona State University's Sustainability in Science Museums initiative supports science museums around the world in their efforts to expand their sustainability programming. The program is building a global network of science centers and museums that have a shared goal of increasing public understanding and interest in sustainability action, and offers content-rich trainings, hands-on activity kits, and other resources for partners museums.

This paper will introduce key concepts, approaches, and resources for engaging the public in sustainability science and practice, with a specific emphasis on materials science and engineering. Presenters will outline key concepts from the field of sustainability science and best practices from the field of informal STEM education that provide a foundation for engaging public audiences in learning about sustainability. Presenters will also share examples of trainings and hands-on activities designed for use in public outreach in settings such as museums. Attendees will gain access to a variety of resources developed through the initiative.

9:00 AM *BI01.01.02

What Means a Benefits/Risks Approach in the "Imperative of Precaution" Framework? Conditions for a Reasoned Development of Nanotechnologies Patrick Chaskiel^{1,2,3}; ¹CERTOP, Toulouse, France; ²Université Paul Sabatier, Toulouse, France; ³CNRS, Toulouse, France.

Since the beginning of the nanotechnology ambitious policies, i.e. since the early 2000's, controversies on their risks have spread in many countries. Facing these disputes, scientific or political institutions have classically proposed to improve communication between stakeholders according to the famous "deficit model of communication", which has not worked since we can observe that the controversies have not stopped. They also have insisted on the necessity of adopting a benefits/risks approach to show that nanotechnologies could bring some "progress" to "people".

However, *to be sustainable*, this approach should be somewhat theorized.

The purpose of this presentation is to examine the reasons why the notion of "benefits from nanotechnologies" appears to be much more complex than generally supposed. In a perspective, notably in France, framed by "the imperative of precaution", researches on nanos are confronted to the necessity (and the difficulty) of defining what a benefit is. In a classical benefits/risks approach, benefits are often considered in a very technical way: professional experts are supposed to understand what should be understood. But benefits (or risks) of nanos could be differently assessed, according to professional experts or citizens points of views.

In particular, the benefits of a (nano)technology cannot be assessed only in accordance to its technical properties because properties are only part of the problem. As we can learn from the thematization process of risks, any innovation must be submitted to a validity test, which supposes taking into account social norms, notably that, progressively shaped by public debates, relating to the environment and health topics.

Based on a social sciences research dealing with a medical nanotechnology and supported by the French CNRS and the Occitanie Region, we will show that a *reasoned development of nanotechnologies* must rely on, and combine two criteria: technical efficacy and some kind of legitimation by civil society representations, namely associations.

This implies to combine two ways of reasoning: the "properties" and "validity" ones which are self-referential and cannot immediately match or even fit. Thus we have to examine the conditions in which an outcome could be built linking these two issues.

9:30 AM BI01.01.03

The Implementation and Role of Automation and Materials Acceleration Platforms (MAPs) in Material Science Jamie Thompson^{2,1}, Gregory Whiting³ and Camille Petit⁴; ¹NASA Ames Research Ctr, Mountain View, California, United States; ²Materials, Imperial College London, London, United Kingdom; ³Mechanical, University of Colorado Boulder, Boulder, Colorado, United States; ⁴Chemical Engineering, Imperial College London, London, United Kingdom.

In the age of automation and cloud computing, scientific research has a huge opportunity to reassess its evolved methodology and reinforce some of its core values. Through the implementation of simplistic hardware, data acquisition systems, cloud-based data storage and non-traditional data analysis methods, a mostly automated scientific system is well within reach of most research laboratories.

Aside from the obvious advantages of not having to manually operate an experimental apparatus, as well as increasing potential human error in the collected data, there are several key advantages to automating many day-to-day lab tasks. Topics around these concepts are discussed, and preliminary prototype systems for large-scale lab automation and collaboration are presented.

Using a materials laboratory as a testbed and assessing the processes by which we interact with our experiments, the modern scientific process is studied and critiqued. The question of where innovations during the experimental process occur is asked in order to more accurately predict what the role of humans in a rapidly accelerated form of science will be in the near and distant future.

9:45 AM BI01.01.04

A Bright Tomorrow—Design: STEM Teaching and Learning Through the Integration of Design, Material Science and Synthetic Biology Raymond Oliver; Northumbria University, Newcastle upon Tyne, United Kingdom.

Fashion and creative design are a window on how we have and how we will live. By 2099, we will understand how to design and fabricate materials at the molecular and biomolecular level. In between, the development of 3 and 4D bio-nano hybrid materials with functionalities similar or superior to Silicon will allow the evolution of 'soft' machines and programmable surfaces and interfaces with intelligence through associated informatics, VR, AR and AI providing tangible materials 2 materiality 2 material experiences. Putting these together, you create a powerful Design:STEM Interactive platform that can significantly influence and enhance both the fabrication and function of novel products and devices that can significantly effect everyone's Future Ways of Living.

The work described in this paper examines some of the ways in which creative design can guide and interact with materials science and material fabrication leading towards programmable material systems through integrated informatics that leads to innovation in 'calm technology' that is burdenless for the user. We will present evidence based examples drawn from our ongoing work as follows:

- a) Ambient assisted living for both individuals and communities
- b) Sensors, sensing and sentient behaviour for anticipatory healthcare and real time monitoring
- c) The development of responsive surfaces and interfaces that serve as real time polyvalent interactive skins for 'smart' interior environments
- d) Sustainable consumer product packaging through the replacement of synthetic polymers with polysaccharide based natural materials

In addition, we will provide Design:STEM insights from our work on the current research and teaching landscape within the School of Design at Northumbria. Finally, the three axes of Design, Materials and Biology are shown to be a very powerful way to address and collaborate with industry to solve identified compelling human centric needs that can significantly benefit everyday life through direct, multidisciplinary Studio, Lab and workplace learning.

Within the School of Design at Northumbria University, we are implementing new MRes masters courses that bring creative designers, material scientists and synthetic biologists together in a common research and teaching environment to accelerate teaching and making practice to address Design led, Needs driven, Materials anchored and solutions focussed Design:STEM Integration.

10:00 AM BREAK

10:30 AM *BI01.01.05

Research, Teaching and Outreach as Examples of Helping to Go Towards a More Sustainable Future Ivana Aguiar¹, Maria E. Perez Barthaburu², Mauricio Rodríguez Chialanza² and Laura Fornaro²; ¹Grupo de Desarrollo de Materiales y Estudios Ambientales, Área Radioquímica, Facultad de Química, Universidad de la República, Montevideo, Uruguay; ²Grupo de Desarrollo de Materiales y Estudios Ambientales, Departamento de Desarrollo Tecnológico, Centro Universitario Regional del Este, Universidad de la República, Rocha, Uruguay.

We are a research group devoted to materials science research since 2000, and we work in the three aspects of Uruguayan University teaching profession: research, teaching and outreach. We started working on ionizing radiation detectors, but through the years our work has evolved to adapt ourselves to our country's reality. In 2011, 44% Uruguayan electricity came from fossil fuels, with a strong dependence on foreign countries. Today, we are self-sufficient and 95% of our production comes from renewable sources, mainly wind and hydroelectrical. Our group aligns with this policy, developing semiconductor nanostructures for hybrid polymeric-inorganic solar cells. Another remarkable aspect of our country is that water is a resource widely available, but in the last years the quality of our water has aggravated mainly due to bad agricultural practices. In this line, we develop semiconductor nanoparticles for tertiary treatment of water.

We put a lot of effort, not only in research to develop a more sustainable country, but also in teaching and outreach that helps to create consciousness in the population about new technologies and also to give them tools to create their own opinion. Regarding to teaching, in the last year we embarked on a challenging project to change the traditional lecturing courses, in our Introduction to Nanotechnology course. We decided to introduce the Problem Based Learning approach together with collaborative work with emphasis in sustainability issues, to anchor the assessment in performances directly related to the discipline. Moreover, the course design included face-to-face and virtual activities. At the end, the students increased their commitment and showed a deeper understanding of the topics.

Regarding to outreach, we have been working to bring materials science activities to schools and high schools for over 10 years. We started this path with small steps, performing isolated activities in the Science and Technology Week frame. Afterwards, we carried out different outreach projects, such as "Materials that surround us" and "Materials in our home". In all our activities, we always carry out hands-on activities and try to emphasize how materials have had a major role in human kind development.

Although the availability of funding has been irregular and there are difficulties to sort out, we believe that the best way of improving materials science in our country and to contribute to a sustainable development is through the education of young students, therefore, we plan on continuing this kind of activities in 2019 and beyond.

11:00 AM *BI01.01.06

Teaching Sustainability—Engineering Possibility Meets Business Case John R. Abelson; University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

To promote sustainable development, we must thoroughly understand the landscape ourselves. The *Energy and Sustainability Engineering* program at the University of Illinois (EaSE.illinois.edu) was launched with a considerable focus on the possibilities for, and fundamental limitations on, improved efficiency in energy conversion and materials use from a life cycle perspective. We have found, however, that the major challenge faced by our graduate students is not technical understanding, but how to articulate problems and potential solutions in the "big picture" context of development and deployment.

The recent books by M. F. Ashby (*Materials and the Environment, Materials and Sustainable Development*) are among the resources that provide a clear conceptual framework and specific approaches for analysis.

We therefore challenge our students to define the following aspects of any proposal intended to improve sustainability. (i) What are the different objectives at play and the constraints on each one? (ii) What is the quantitative scale of the proposal in terms of technology to be deployed, spatial region and time scale? What does this imply in terms of the materials supply chain? (iii) Does the proposal depend on cost reductions as the technology matures? If so, what is reasonable to expect? (iv) What are the inevitable tradeoffs between the objectives – as well as the unintended consequences – and how should those tradeoffs be valued? (v) Who are the important stakeholders, and how should they be engaged? (vi) What are the demands for financial investment and the probable return on investment? How are these influenced by the hidden cost of externalities (which tends to favor investment in sustainability) and by economic discounting (which emphasizes short-term gains over lifecycle impact)?

In summary: we find that to advance sustainability, scientifically trained professionals need to *construct and articulate a comprehensive and compelling business case around the technical possibilities made possible by engineering*. I will provide key examples of the above challenges, the ways we attempt to provide insight, and welcome discussion with the audience.

11:30 AM BI01.01.07

Can Materials Science Save Us (From Ourselves)? [Mark A. Miodownik](#); University College London, London, United Kingdom.

Despite the long history of materials development, materials science as a distinct discipline is relatively new. It only came of age in the 20th century, brought into existence by necessity, as a result two developments. Firstly, industry needed it to understand the complex materials, on which it and society, was becoming ever more dependent such as the silicon chip, jet engine alloys, polymer composites, optical fibres, medical implants, etc. Secondly, it became increasingly clear that materials could not be understood by the study of engineering, physics, chemistry or biology alone. So, as the 20th century progressed, so did materials science as a discipline.

We now live in the 21st century and the power of materials science is immense. It is making possible a world where buildings harvest their own energy, bridges heal themselves, clothes monitor a person's health, and biomaterials increase the average life expectancy to 100 years of age. This all sounds thrilling, but many alternative realities await us, each driven by different cultural, economic and political forces. In these alternative realities, we could find ourselves in the grip of mass migrations, with declining life expectancy, dealing with global pollution and energy blackouts, to name but a few potential scenarios. Which future will we choose?

In this talk, I argue that much hinges on a deeper understanding by materials scientists of all parts of society. To achieve this, public engagement is not enough, the core of the discipline needs to move beyond its current limits in the physical sciences, to a more people-focused approach to materials design and manufacturing. From an educational perspective, this will require understanding of, or at least an acknowledgment of, the importance of psychology, economics, politics and materials culture. I use a case study of the development of self-repairing cities to illustrate the necessity of such changes to materials science as a discipline.

11:45 AM BI01.01.08

Engineering Major Students' Perceptions of Nanotechnology [Haci H. Yolcu](#); Kafkas Univ, Kars, Turkey.

Nanotechnology will be among the most needed workforce areas in the near future. It is also a creative and highly dynamic field of innovative research areas that displays numerous open fields for future graduates. The central thesis of this paper is to better understand undergraduate engineering students' awareness, exposure, and motivation towards nanotechnology, how those constructs correlate with each other, and whether there are differences by gender or year of study. This exploratory study used mixed methods to answer the research question. Results revealed that engineering students have more motivation to pursue further nanotechnology knowledge or study than they have exposure or awareness about nanotechnology. The results showed that male students have more awareness about nanotechnology than female students. Educational implications are that it is necessary to provide students with more opportunities to learn about and study nanotechnology during their undergraduate experience. While students are interested in learning more, their current levels of awareness and exposure may hold them back in pursuing nanotechnology-related careers.

SESSION BI01.02: Education and Society II
Session Chairs: Ivana Aguiar and Jean Gaumet
Monday Afternoon, November 26, 2018
Sheraton, 3rd Floor, Hampton

1:30 PM *BI01.02.01

How Understanding Materials Risk Helps Materials and Engineering Students Learn About Circularity, Eco Design and Sustainability [Marc Fry](#)¹, [Hannah Melia](#)¹ and [Michael F. Ashby](#)²; ¹Granta Design Ltd, Cambridge, United Kingdom; ²University of Cambridge, Cambridge, United Kingdom.

Material choice affects the performance of products and their impact on the environment and society. Although damage to the environment and society is not usually priced into products, companies are increasingly interested in minimizing risk; to their reputations, and to their supply chains. Engineers of the future need to learn how to approach complex trade-offs of price, performance, risk and impact in their material selections. This talk will illustrate data, tools, methodologies and teaching resources that can be used to help Materials and Engineering students gain knowledge and skills in this area.

The Granta Eco Audit Tool [1] supports the introduction of the concepts of circular economy and is widely used in teaching materials and engineering courses, as well as in capstone project work. Its methodology is particularly useful at the conceptual design stage and is comparable with a streamlined life-cycle inventory. The Eco Audit Tool enables the running of scenarios with different feedstock, processing, and end-of-life options (including reuse). The Eco Audit analyses draw on the data on materials and processes available in the software and on the bill of materials from users. The visual outputs present estimated energy use, CO2 equivalent emissions and cost at each stage of the product life. Warning indicators for toxic substances and critical materials help in the process of material selection for product design projects.

The Sustainable development 5-step methodology [2] developed by Prof. Michael F. Ashby and Dr. Didac Ferrer, which helps students structure their analyses of the sustainability of a technological development will also be presented. Drawing on data in CES EduPack [1] the methodology encourages

students to identify the scope of a development and the stakeholders involved, before fact finding on different aspects and pulling together the newly gained knowledge into a considered opinion.

Alongside the materials selection tools that are a standard part of CES EduPack and can illustrate trade-offs in price and performance, these tools and methodologies help students see the bigger picture around their material decisions.

2:00 PM *BI01.02.02

Focusing on Sustainability—Raising Awareness of the Materials–Sustainability Nexus [Ashley White](#)¹, Ivana Aguiar², Jonathan Cullen³, Martin L. Green⁴, Anthony Ku⁵, Elizabeth Kupp⁶, Alan Rae⁷, Julie M. Schoenung⁸, Richard Souza⁹ and Margeaux Wallace¹⁰; ¹Lawrence Berkeley National Laboratory, Berkeley, California, United States; ²Universidad de República, Montevideo, Uruguay; ³University of Cambridge, Cambridge, United Kingdom; ⁴National Institute of Standards and Technology, Gaithersburg, Maryland, United States; ⁵National Institute of Clean-and-Low-Carbon Energy, Mountain View, California, United States; ⁶The Pennsylvania State University, University Park, Pennsylvania, United States; ⁷IncubatorWorks, Painted Post, New York, United States; ⁸University of California, Irvine, Irvine, California, United States; ⁹Materials Research Society, Warrendale, Pennsylvania, United States; ¹⁰GE Global Research, Niskayuna, New York, United States.

As technology enablers, materials play a pivotal role in solving the key challenges our society will continue to face, such as carbon dioxide mitigation, access to clean energy and water, and a dependable supply of raw and recycled materials for infrastructure, devices, and consumables. Meeting these challenges will require new approaches to materials science as well as expertise from related fields, including other scientific and engineering disciplines, sociology, economics, and policy. In recognition of the complexity of tackling sustainable development issues and the importance of materials to enabling solutions, the Materials Research Society (MRS) Board of Directors approved the creation of the Focus on Sustainability Subcommittee of the Public Outreach Committee. The subcommittee's formation was an important step in the evolution of MRS's sustainability-related programming and other activities.

This talk will cover the history and evolution of sustainability efforts within MRS, concentrating on the recent impacts of the Focus on Sustainability subcommittee. Its activities have included professional development seminars and workshops, symposia and tutorials, a dedicated booth at MRS meetings, industry panel discussions, hands-on activities, poster sessions, and a series of high-profile panel events organized in collaboration with the *MRS Energy & Sustainability* journal entitled "Materials for Energy Sustainability by 2050."

Moving forward, the challenge for us as sustainability enthusiasts is to engage and integrate with the broader materials science community and other related disciplines. Towards that goal, this talk will discuss newer efforts to involve the broader MRS membership in our sustainability activities, raise awareness of the materials–sustainability nexus, and bring a higher level of understanding of the role different materials sub-disciplines play in sustainable development—the defining challenge of our time.

2:30 PM OPEN DISCUSSION

2:45 PM BI01.02.04

PodQESST—A Case Study for a New Form of Science Communication [Sebastian Husein](#), Joseph Karas, Michelle Jordan and Mariana I. Bertoni; Arizona State University, Tempe, Arizona, United States.

This talk will showcase a form of communication severely under-utilized in the scientific community—namely, podcasts. Podcasts are an audio file made digitally available on the internet, typically accessible to anyone by computer or mobile. While early forms of this communication medium have been available since the 1980s, modern podcasts have grown rapidly in popularity since 2004 [1]. Reports estimate over 44% of the U.S. population over the age of 12 has listened to a podcast, with 80% of listeners following an average of 7 podcasts per week [1]. Podcasts are therefore rapidly becoming one of the largest information dissemination methods. Scientific communities must begin engaging at the intersection of podcasting and social media networks, which have become essential in circulating information [2].

Currently, scientific research is often locked away in niche websites and academic journals, with much of the research process (i.e., development of experiments, analysis of collected data, and peer review) obscured by technical jargon and complex topics. While some scientific achievements may spread into popular culture and news, most Americans receive science news by "happenstance rather than intentionally" with only ~17% both actively and frequently seeking it out [3]. To maximize positive societal impact, the scientific community must actively pursue new forms of science communication to both inform the general public and open dialogue between researchers and those potentially impacted by the research.

Through podcasts, collection and dissemination of scientific knowledge can follow a story-telling format. Our podcast, PodQESST, hosted by two Ph.D. students, examines the research process by following the human experience. Rather than discussing complex scientific concepts, this podcast interviews graduate students and research professors about how their work evolved, from conception to process, and in some cases, to real-world implementation and influence. By using this story-telling format, research work and scientific advancements can become relatable to audiences with little to no scientific background. Additionally, communities of current graduate student are potentially strengthened through this shared experience and may impact retention rates in STEM, enhancing workforce development. The impact of this podcast on perception of science and interest in STEM careers is currently being tracked among pre-university students and university students from 8 U.S. institutions partnered through the Quantum Engineering and Sustainable Solar Technology (QESST) Engineering Research Center.

References:

[1]: The Infinite Dial © 2017, "The podcast consumer 2018", Edison Research and Triton Digital, 2018.

[2]: P. Luarn, J. C. Yang, Y. P. Chiu, "The network effect on information dissemination on social network sites", *Computers in Human Behavior*, 37, 2014.

[3]: C. Funk, J. Gottfried, A. Mitchell, "Science News and Information Today," Pew Research Center, 2017.

3:00 PM BREAK

3:30 PM *BI01.02.05

How Can Sustainability Become Tangible? Serious Games and Digital Tools Help Learners Develop Sustainability Competences [Vasiliki Kioupi](#); Imperial College London, London, United Kingdom.

Sustainable development is a complex concept, but it is also powerful and transformative. In order for students to make sense of its holistic, interdisciplinary and participatory nature they should become engaged in meaningful educational activities that reveal interconnections between social, economic and environmental aspects, take into account stakeholder viewpoints and at the same time assist them to develop sustainability competences. Serious games and digital tools for sustainability help shape students attitudes when making important decisions regarding sustainability and also think systematically and critically about taking courses of action and evaluating them. In contrast to games designed predominantly as free-time activities taken up for leisure or competition, serious games may be played seriously or casually, but are not intended to be played primarily for amusement. This definition of

serious games embraces both digital and analog games whose focus is on a “serious” goal, be it education, skill training, self-development or increased work motivation, etc. Game-based and experiential learning are fun and creative, giving the opportunity to participants to experience real-world situations but in a safe and controlled environment where they can test their ideas, express their opinions, develop strategies and check the outcomes. Also, the focus is on engagement, interaction with peers and reflection on the results and processes. Digital tools help students develop their own questions and hypotheses related to sustainability issues, investigate their current state, understand stakeholder involvement, select alternative courses of action, develop criteria for evaluation and weigh different scenarios in terms of their sustainability capacity to produce viable solutions. Through these educational activities, students develop important knowledge and skills that are required in order to achieve the vision of a sustainable society as it is articulated by the Sustainable Development Goals (SDGs). Those include systems thinking, anticipatory, normative, strategic, collaboration, critical thinking, self-awareness and integrated problem-solving competences.

4:00 PM *BI01.02.06

Responsible Research and Innovation—Some Societal and Ethical Issues Joelle Lighezzolo-Alnot; Univ of Lorraine, Nancy, France.

Today, the concept of “responsible research and “responsible innovation” (RRI) is one of the main preoccupations in in the field of science and technology studies. If nanomaterials and nanotechnologies have of course opened hope for a better quality of life in our societies with a lot of progress and applications, they are not without asking some questions regarding their potential effects, toxicity, and by the way, some ethical issues. Recurring debates shake not only the scientific community, but also citizens, leading sometimes to controversial and contradictory positions. The traditional balance cost-benefit, and the classic “precautionary principle”, gave way to an “uncertainty principle”, and the necessity of considering differently nowadays the question of risk and safety. In fact, if we want to avoid a gap between researchers and citizens, science and society should not be regarded as two distinct spheres, and the way for that is rather to establishing a better and more trustful relationship between science and society. In order to achieve this objective, one of the outcomes could then consist in promoting an interdisciplinary dialogue. In the European Union (UE), responsible research and innovation is becoming an increasingly part of policies, particularly throughout the EU’s Horizon 2020 research work program “Science with and for society” (2018-2020): the challenge is, facing to the evolution of science and society and the open science context, to develop innovative ways connecting science to society, through an inclusive

4:30 PM BI01.02.07

Pathway Toward Sustainable Development of Next Generation Photovoltaics—A Detailed Study on Research Trends Through Social Network Analysis Jun-Seok Yeo and Yeseul Jeong; Korea Institute of S&T Evaluation and Planning (KISTEP), Seoul, Korea (the Republic of).

Organic-inorganic hybrid perovskite solar cells (PeSCs) have attracted great attention as next-generation photovoltaics due to their high efficiency, low manufacturing cost, facile solution-processability, light weight, and mechanical flexibility. Since the advent of the PeSCs, the researchers have devoted a lot of efforts to improve the PeSC-performance, boosting the progress in the power conversion efficiency (PCE) of over 20%. This progress has gradually shifted the focus of the PeSC research to study of reliability and cost-effectiveness of the PeSCs. In this study, we systemically investigate these research trends of the PeSCs for their sustainable development and market entry by using ‘Social Network Analysis (SNA)’. For SNA data, SCI(E) papers on PeSCs published from 2009 to 2017 are collected, and classified into two categories (research fields and commercialization factors). Next, we conduct respective networks visualization, networks topological analysis, and node centrality analysis. With the aid of SNA, the technology and knowledge networks (flows) for PeSC research fields are investigated in terms of countries, research institutions, research fields, and commercialization factors.

4:45 PM SYMPOSIUM WRAP-UP DISCUSSION

SESSION BI01.03: Sustainability in Industry and Agriculture
Session Chairs: Jean-Pierre Birat and Khosrow Ghavami
Tuesday Morning, November 27, 2018
Sheraton, 3rd Floor, Hampton

8:00 AM BI01.03.01

Self-Healing Polymers Using Reversible Supramolecular Metal-Ligand Interactions Ulrich S. Schubert, Stefan Zechel, Marcel Enke, Stefan Götz and Martin D. Hager; Friedrich-Schiller-University Jena, Jena, Germany.

Metallo-supramolecular polymers are an interesting class of polymeric materials since they combine the typical character of metals and polymers leading to novel and outstanding features. Furthermore, metal-ligand interaction can feature a reversibility of the binding enabling the design of novel self-healing materials.[1]

For this purpose, terpyridine moieties were incorporated into the side chain of different copolymers using the RAFT polymerization technique.[2,3] Subsequently, metallo-supramolecular polymer networks were prepared by the addition of different metal salts.[4] The healing of the metallopolymers strongly depends on the chosen metal salt. In particular, the metal as well as the counter ion has a strong impact on the healing behavior.[3] Interestingly, the crosslinking with manganese(II) chloride resulted in the best scratch healing ability (**Figure 1**). Furthermore, the metallopolymers were studied by temperature-dependent rheological measurements and the supramolecular bond life-time (τ_b) was determined by the crossover of G' and G'' . A correlation between the presence of the crossover as well as the ability to close cracks could be revealed. Thus, the mechanical properties could be correlated with the self-healing performance of supramolecular networks.[3]

[1] M. Enke, D. Döhler, S. Bode, W. H. Binder, M. D. Hager, U. S. Schubert, *Adv. Polym. Sci.* **2016**, 273, 59-112.

[2] M. Enke, R. K. Bose, S. Bode, J. Vitz, F. H. Schacher, S. J. Garcia, S. van der Zwaag, M. D. Hager, U. S. Schubert, *Macromolecules* **2016**, 49, 8418-8429.

[3] S. Bode, M. Enke, R. K. Bose, F. H. Schacher, S. J. Garcia, S. van der Zwaag, M. D. Hager, U. S. Schubert, *J. Mater. Chem. A* **2015**, 3, 22145-22153.

[4] S. Götz, M. Abend, S. Zechel, M. D. Hager, U. S. Schubert, *submitted*.

8:15 AM BI01.03.02

The Biomaterial Age Javier Gomez Fernandez; SUTD, Singapore, Singapore.

The history of humanity can be summarized in different periods dominated by the use of a new material bringing a new paradigm and a revolution in engineering, becoming in a short time the engine of development of that historical period. The ages of stone, bronze and iron are clear examples of how certain materials have transformed society and its economy. Nowadays the equivalent to these materials is plastic. Driven initially by a continuous demand from the WWII, the production of plastic began a vertiginous development, finally surpassing in production to all the rest of materials used outside the field of construction in the decade of the 60s.

The first voices of alarm about the impact of plastic on the environment occurred also in the 60s, with the first observations of the accumulation of plastic waste in nests of seabirds. While these early studies were anecdotal and remote for most, today virtually no one is unaware of a problem in continuous growth. We are in a difficult situation; as a society we have developed a greater awareness of the impact of our actions on the environment in general, and the impact of plastic in particular. Moreover, unlike other environmental problems, the problem of plastic is indisputably anthropogenic and easily observable. However, the production of plastic it is accelerating. If in the 50s, we were producing half a million tons of plastic a year, now we are close to the five hundred million tons. At the current rate in 2050 we will double that amount, requiring one fifth of the world's oil production to produce plastic. The apparent failure to produce feasible solutions, both by scientists and legislators, is mainly because the solutions being considered implicitly assume that humanity has reached a kind of technology summit with the invention of plastic and its methods of manufacturing. As legislators we fail because, in the absence of alternatives, we can only limit very specific uses of plastic. As scientists we are failing because we are trying to find materials that replace plastic to make objects that have been designed to be made with plastic. Moreover, not only the objects, in our search for solutions we also impose the mode of manufacture of the plastic and that is the basis of our industrial system. We mistakenly assume that necessity is the motor of development, but the question we should be asking ourselves is not how can we change an economy and society molded around plastic to get rid of our addiction to it. The question should be: What comes after the plastic and what kind of society will it bring?

In this talk we will explore the role that biomaterials will play in the future of manufacturing and the emergence of new economic models, giving rise to what we have called "the biomaterial age". The role of bio-inspired engineering, 3D printing, or new models of organic waste processing will be covered as key pieces in this transition.

8:30 AM *BI01.03.03

IMERYS—Sustainable Development for Innovative Mineral Based Solutions [Claire M. Theron](#); External Innovation, IMERYS, Suwanee, Georgia, United States.

Imerys is the world leader in mineral-based specialties for consumer goods, industrial equipment and construction. Its Corporate Social Responsibility is central to the Group's long-term strategy, supporting growth and underpinning long-term relationships with all stakeholders.

While Imerys operates on a global level, the group is committed to play a role in society, to meet its obligations to the countries and communities within which it does business by empowering our people, caring for our planet and building for the future together with our stakeholders. Through these commitments the Group contributes to sustainable development and foster positive changes including regional projects covering education, sanitation, health and diversity, renewable energy, and biodiversity such eradication of invasive plants, preservation of protected species.

Following main international standards, in-house Sustainable Development (SD) Challenges have yielded 847 projects during the last 13 years. Those projects are aligned with Imerys high priority areas, such as diversity and inclusion, education, environment management, climate change and relation with communities. The group's commitments in Imerys Code of Ethics and Business Conduct and CSR Charter are available to all detailed in policies, procedures and protocols gathered on Imerys intranet.

An example of Imerys contribution includes lightweighting of vehicles by delivering functional additives (High Aspect Ratio talcs) to polymers industry. The 3G HAR® product enables weight reduction of the automotive plastic injection-molded parts while its production uses 63% less electricity than previously.

Imerys is also active in cosmetics, offering its ImerCare® range is P-Scrub, product using 100% natural minerals designed as an eco-friendly alternative to plastic microbeads.

In agriculture, Imerys Mechanical Insecticides offer three natural mineral solutions, based on diatomaceous earth or kaolin (DiaFil® 610, Celite® 610 and IMERGARD™) which provide effective environmentally friendly solutions.

Building on existing systems and initiatives and going beyond compliance, a program fully aligned with the United Nations' Global Compact and Sustainable Development Goals is being implemented. The ambition is clear: anchoring sustainable development at the heart of the Group's overall strategy and mobilizing employees at every level to achieve Corporate Social Responsibility targets.

9:00 AM *BI01.03.04

Sustainable Construction Materials for XXI Century [Khosrow Ghavami](#); Pontificia Universidade Catolica de Rio de Janeiro, Rio de Janeiro, Brazil.

New constructions are being erected scraping the skies with nearly 1000m high. And still in spite of all the advances a large percentage of people of the world live in misery without the minimum of nourishment, clean drinking water and decent housing. Industries are demanding more and more raw materials, existing now mainly in developing countries and creating havoc on earth searching for and exploiting the lands holding these needed raw materials. Nature is responding with climate changes, freak storms and other disasters. The big centralized industries are not able or rather not willing to stop polluting our environment by reducing carbon emissions. Their ambition is to be the owners of the Earth, and do what they think is good for their bottom line, and not the working people of the planet. Now, sustainability goes together with moderation, meeting basic needs and a general well-being of the population. Sustainability of our environment makes possible that a greater part of the population can follow up a life's dream or at least ability to have a decent meaningful life through preserving remaining natural resources available for the future generations. In schools and universities, yet, only the industrial non-renewable materials such as cement, concrete, steel and recently composites made of polymers research and application. The study of Non-Conventional Materials and Technologies, NOCMAT, has been started in the years of the seventies of the last century. A new line of research has been initiated to investigate local renewable materials such as bamboo, vegetable fibers, soil composite, which is called Kah-gel in Persian language. These materials have been used as construction materials for thousands years, recycled materials, such as rice husk and sugar cane ash among others. This paper will present the recent results of research on NOCMAT and their application in practice. To improve the durability of the studied materials, nano-particles applied in kah-gel and also impregnated into bamboo culm. To achieve the final objective to tune a fine nanocoating of vascular bundles' of bamboo, internal wall has been done through the interfacial compatibility, based on self-assembling interactions, between the NFs-surface and the lignin-cellulose walls of bamboo vessels.

9:30 AM BI01.03.05

Closed Loop Recycling of Electric Vehicle Batteries to Enable Ultra-High Quality Cathode Powder [Mengyuan Chen](#), Xiaotu Ma and Yan Wang; Worcester Polytechnic Institute, Worcester, Massachusetts, United States.

The lithium-ion battery (LIB) recycling market is becoming increasingly important because of the widespread use of LIBs in every aspect of our lives. Mobile devices and electric cars represent the largest application areas for LIBs. Vigorous innovation in these sectors is spurring continuous deployment of LIB powered devices, and consequently more and more LIBs will become waste as they approach end of life. Considering the significant economic and environmental impacts, recycling is not only necessary, but also urgent. The WPI group has successfully developed a closed-loop recycling process, and has previously demonstrated it on a relatively small scale 1kg spent batteries per experiment. Here, we show that the closed-loop recycling process can be successfully scaled up to 30kg of spent LIBs from electric vehicle recycling streams, and the recovered cathode powder shows similar (or better) performance to equivalent commercial powder when evaluated in both coin cells and single layer pouch cells. All of these results demonstrate the closed-loop recycling process has great adaptability and can be further developed into industrial scale.

9:45 AM BI01.03.06

Reclaiming Sb Metal from Lead Alloy with Electrochemical Method Qiang Wang; Worcester Polytechnic Institute, Worcester, Massachusetts, United States.

Antimony is a widely used element in human's daily life. For example, Sb_2O_3 plays role as flame retardant in plastics, coatings, and electronics; functioning as a hardener, 2wt % to 7wt % of antimony metal is added into lead metal to fabricate electrode for lead-acid battery; and antimony can work as catalyst for synthesizing chemicals. In 2016, antimony mine production in the world was 130,000 t, and China, the leading producer, accounted for about 76.9 % of the production. The strong dependence of antimony industry on the import of Chinese antimony drives USA and Europe to seek solution of reclaiming and recovering antimony from secondary resource. Herein, an innovative method composed of electrochemical and chemical reactions is presented to purify antimony from lead alloy, which is treated as anode in an "H" shape electrolytic cell. Stainless steel sheet works as cathode, and potassium hydroxide solution is applied as electrolyte. O_2 is purged into the cathode at the beginning, and the electrolytic cell works in the principle of metal- O_2 battery, when voltage is applied on the two electrodes. Lead, antimony, and other metals dissolve into the electrolyte as ions at the first stage. When the ions inside the electrolyte accumulated to a certain amount, O_2 is switched off without interference of the electrolysis. At this second stage, lead alloy of the anode dissolve into electrolyte successively, but lead metal deposits on cathode side simultaneously. Lead ions concentration stops increasing, and antimony ions concentration keeps on rising. When antimony concentration is high enough, the electrolysis is stopped, and Na_2S is added into the electrolyte to precipitate lead ions in the stage 3. Almost all the lead can be removed from electrolyte, leaving antimony inside, by taking advantage of the low value of K_{sp} (PbS). At the last step, antimony can be extracted from the electrolyte at low potential of -1.25 V (vs Hg/HgO), leaving other impurity, such as As, Sn, Al inside with low concentration under 50 ppm. The electrolyte can be re-used for the next circle. This flow sheet can purify lead and antimony metals from lead alloy, with lead purity of 99.2 wt% and antimony purity of 92 wt%, and antimony recovery efficiency is ~ 82%. Because the electrolyte can be used repeatedly, no waste is generated in the whole process.

Stage 1. Cathode: $\text{O}_2 + 4\text{e}^- + 2\text{H}_2\text{O} \rightarrow 4\text{OH}^-$ (1)

Anode: $\text{Pb} + 4\text{OH}^- - 2\text{e}^- \rightarrow \text{PbO}_2^{2-} + 2\text{H}_2\text{O}$ (the main oxidation reaction) (2)

$\text{Sb} + 4\text{OH}^- - 3\text{e}^- \rightarrow \text{SbO}_2^- + 2\text{H}_2\text{O}$ (3)

Stage 2. Cathode: $\text{PbO}_2^{2-} + 2\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{Pb} + 4\text{OH}^-$ (4)

Anode: $\text{Pb} + 4\text{OH}^- - 2\text{e}^- \rightarrow \text{PbO}_2^{2-} + 2\text{H}_2\text{O}$ (the main oxidation reaction) (5)

$\text{Sb} + 4\text{OH}^- - 3\text{e}^- \rightarrow \text{SbO}_2^- + 2\text{H}_2\text{O}$ (6)

Stage 3. $\text{Pb}^{2+} + \text{S}^{2-} \rightarrow \text{PbS}\downarrow$ (7)

Stage 4. Cathode: $4\text{OH}^- - 4\text{e}^- \rightarrow \text{O}_2 + 2\text{H}_2\text{O}$ (8)

Anode: $\text{SbO}_2^- + 2\text{H}_2\text{O} + 3\text{e}^- \rightarrow \text{Sb} + 4\text{OH}^-$ (9)

10:00 AM BREAK

10:30 AM BI01.03.07

Cellulose Nanomaterials in 3D Printing and Aerogels—High-Performance Nanocomposites Rigoberto C. Advincula; Case Western Reserve University, Cleveland, Ohio, United States.

Sustainable and renewable materials start with the use of biobased feedstocks or derived raw materials for direct utilization (little conversion or synthetic procedures). The preparation of nanocellulose materials from a variety of sources include agricultural, non-agricultural, and can vary in properties depending on the method of preparation and high fiber source. Cellulose nanocrystals (CNC) and cellulose nanofibers (CNF) have various uses for the fabrication of polymer nanocomposites, making them useful as an additive for improving thermo-mechanical properties and perhaps improving processability. In this talk, we will focus on the use of CNC derived from various sources, Abaca, coconut fibers, miscanthus grass, mango seeds, etc. The mode of raw materials can be from processed pulp or directly from the agriculture or plant source. These nanofiller materials have been utilized in two types of applications: nanofiller materials for 3D printed parts via SLA, FDM, or VSP and the preparation of smart aerogels with nanoclay. The former enabled strengthening of the thermo-mechanical properties of the 3D printed object and the latter results in a highly porous lightweight media useful also for oil-water separation and clean-up. The talk will discuss the methods of synthesis, fabrication, and characterization for their intended application and a pathway of high value adding from sustainable materials and its societal and technopreneurship impact.

10:45 AM BI01.03.08

A Green Process for Electrochemical Recycling of Lead Using Deep Eutectic Solvents A.K. Ola Hekselman and David J. Payne; Department of Materials, Imperial College London, London, United Kingdom.

There were approx. 1.2 billion motor vehicles in the world in 2015 and industrial forecasts predict the number of cars may reach 2 billion cars globally by 2035.^[1] Even with an increasing development of Li-ion technology, lead-acid batteries (LABs) remain the most popular power supply for automotive industry and there are no signs of decline in this market as LABs are also present in state-of-art hybrid and fully electric vehicles.^[2] A major challenge facing the lead-acid technology is, however, its toxicity and the environmental impact of lead.

To address these issues, we need to develop novel processes to recover lead from spent lead-acid batteries. It is critically important to develop more sustainable methods with a minimal pollution and low energy consumption in comparison with the traditional smelting and hydrometallurgical routes. We propose a process where Pb-containing battery waste is dissolved into deep eutectic solvents (DES), followed by an electrochemical recovery of metallic lead to provide a low-energy, low-temperature and an environmentally friendly alternative to recycling of spent batteries.^[3] In our work, cyclic voltammetry and chronoamperometry were used to determine the mechanism and electrodeposition behaviour of lead, while ICP-OES and EXAFS provided insight into speciation of lead in DESs, and SEM and XPS were used to characterise the lead electrodeposits.

[1] International Organization of Motor Vehicle Manufacturers, *World Vehicles in use 2005-2015*

[2] P. T. Moseley, D. A. J. Rand and J. Garche in *Lead-acid batteries for future automobiles: Status and prospects*, Elsevier, Amsterdam, 2017, pp. 601-618.

[3] A. D. Ballantyne, J. P. Hallett, D. J. Riley, N. Shah and D. J. Payne, *Royal Society Open Science* **2018**, *5*.

11:00 AM BI01.03.09

Nb₂O₅/CuO Nano-Heterostructures Photocatalysts for Reductive Reactions—Towards an Efficient Material for Artificial Photosynthesis [Andre E. Nogueira](#)², [Caue Ribeiro de Oliveira](#)¹, [Gelson Tiago d. da Silva](#)¹ and [Osmando F. Lopes](#)¹; ¹EMBRAPA, São Carlos, Brazil; ² Brazilian Nanotechnology National Laboratory (LNNano), Brazilian Center for Research in Energy and Materials (CNPEM), Campinas, Brazil.

The reform of CO₂ through photocatalytic processes to obtain products with high energy value and compatible with the current energy infrastructure, is a compelling strategy to minimize the emission of CO₂ at atmosphere, one of the main greenhouse gases. However, practical application of such a photocatalytic system requires significant efforts for improved CO₂ photoreduction performance and product selectivity. Thus, in the present work, CuO nanoparticles were combined with Nb₂O₅ in order to improve the photocatalytic properties of these semiconductors in the CO₂ photoreduction process. The Nb₂O₅/CuO heterojunctions were prepared via solvothermal treatment method, while that experimental tools, such as FESEM, HRTEM, and DRS were employed to evaluate the microstructural and electronic properties. The physicochemical properties of the Nb₂O₅/CuO heterostructures were characterized and evaluated in the ability of the CO₂ photoreduction with different electrolytes (pure water, sodium oxalate, and KBrO₃) under ultraviolet radiation (UVC). The use of these electrolytes besides conducting the formation of a certain product enables the elucidation of the mechanisms of the CO₂ photoreduction process. Further, the Nb₂O₅/CuO heterostructures was active also to CO reduction in CH₄, HCOOH and CH₃COOH, besides this result demonstrated that CO is intermediate in the CO₂ reduction to all products. The synthesized heterostructures showed photocatalytic activities superior to the pure Nb₂O₅ and the TiO₂ (P25). This improvement could be attributed to the formation of junctions between CuO and Nb₂O₅, which facilitated charge transfer, and suppressed the recombination of electron/hole pairs. The FESEM and HRTEM analyzes show that CuO nanoparticles were uniformly distributed on the surface of Nb₂O₅, showing the formation of a junction between the oxides.

Acknowledgments

The authors are grateful to FAPESP (grants n° 2014/09014-7 and 2013/11821-5), CAPES and FINEP for the financial support.

11:15 AM *BI01.03.10

Why Non-Conventional Materials are Answers for Sustainable Agriculture [Caue Ribeiro de Oliveira](#); Brazilian Agricultural Res Corp, Sao Carlos, Brazil.

Fertilizers undoubtedly are key factors for agricultural productivity, but their widespread use is continuously impacting the farmers' economic balance and, indirectly, being associated to many environmental impacts – such as volatilization or lixiviation. These impacts might be significantly reduced if the nutrients could be supplied in constant, controllable rates – as controlled release systems – however any technological alternative should be capable to offer affordable prices and large production scales, since these are often applied in hundreds of kgs per hectare. Therefore we have proposed a strategy to produce composite fertilizers where the matrix is composed by nutrients, i.e., all the constituents play a nutritional role for plants. This strategy allows, for instance, the controlled delivery of phosphate from hydroxyapatite nanoparticles dispersed in a nitrogen-rich matrix (even urea or partially polymerized urea). Recently, we noticed that similar strategies are applicable to sulfur (S), often neglected about its importance as nutrient. The production of S-rich polymeric matrices, using elemental S and biopolymers, provide means for multiple nutrient administrations, by integrating these nutrient matrices to mineral phosphates as dispersed nanoparticles as composites. This structure was shown as very adequate for microorganism colonization (e.g. *A. niger*), which accelerates the S oxidation to sulfates (which are properly absorbed by plants) while imposes a local acidification solubilizing the mineral phosphates to absorbable species. This complex system can be extend to other structures, keeping very high total nutrient contents (higher than 30% wt) and easy processing steps, since these features allows the fertilizer production by high-output techniques such as extrusion.

Acknowledgements: FAPESP; CAPES; CNPq; FINEP; National System of Nanotechnology Laboratories – SISNANO/MCTI; Rede Agronano/Embrapa

11:45 AM BI01.03.11

Sustainable Crop Protection Management in Sub-Saharan Africa Through Biodegradable Seed Wraps [Tahira Pirzada](#) and [Saad A. Khan](#); Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, North Carolina, United States.

Plant parasitic nematodes are one of the major constraints on yield and production of food crops throughout the world. While abamectin has broad nematicidal activity, its poor mobility in soils compromises its efficiency against nematode infestation. Using abamectin as a model pesticide, we present an innovative and cost effective approach for crop protection from plant parasitic nematodes, using a lignocellulosic matrix 'wrap and plant' methodology. In our 'wrap and plant' approach, we have used abamectin loaded matrices as wraps for seeds to be planted in the soil. To better understand the effect of various processing parameters and nature of the pulp on final properties of the matrix, we have produced lignocellulose matrices using pulp refined at various time intervals. Resulting hand sheets are characterized by the controlled release of abamectin which is incorporated into the matrices through sorption. Pulp refining time as well as various physical and chemical properties of the matrix are found to affect its tendency to let the germinating roots penetrate it and also the release rate of abamectin. We perceive that by varying refining time of the pulp, we can obtain matrices that facilitate in slow and sustained release of abamectin which results in long term nematicide protection to the growing plant roots. We have used these results to develop pilot scale paper rolls which are currently used in field trials in various regions of Africa and initial field trials demonstrate promising results regarding better crop protection in nematode infested soils in Benin and Kenya.

SESSION BI01.04: Circular Economy and Recycling Applications
Session Chairs: Marc Fry and William Olson
Tuesday Afternoon, November 27, 2018
Sheraton, 3rd Floor, Hampton

1:30 PM *BI01.04.01

Creating a Circular Economy for Hard Disk Drives—A Shared Vision [Carol A. Handwerker](#)¹, [William Olson](#)² and [Mark Schaffer](#)³; ¹Purdue University, West Lafayette, Indiana, United States; ²Seagate, Technology, Bloomington, Minnesota, United States; ³International Electronics Manufacturing Initiative iNEMI, Austin, Texas, United States.

The iNEMI project on Value Recovery from Used Hard Disk Drives (HDDs) is an industry-academia-government lab-NGO partnership whose vision is

icreating a global, circular economy for HDDs. Hard disk drives have a special role in electronics: they are ubiquitous, having been designed to be replaceable and interchangeable in products as diverse as computers, servers, and sensor/monitoring equipment. In Phase 1 of the project, an iNEMI multi-stakeholder team developed the groundwork and created momentum for a Phase 2 collaborative project to build an integrated, sustainable, adaptive CE system for end-of-use HDDs. The project framework has been modeled after sustainable management of common pool resources on which many people rely for their livelihoods. Dr. Elinor Ostrom (2009 Nobel Laureate in Economics) laid out a framework for how people and organizations develop voluntary, community-based solutions involving adaptive, self-governing systems that effectively manage common pool resources without the need for government regulations or privatization. We have applied this framework explicitly to HDDs, as a first demonstration. Phase 1 was built on stakeholders identifying decision pathways for HDD refurbishment, component reuse, and material recovery, incorporating economic and resource recovery analyses, and identifying how and why stakeholders make decisions that limit value recovery. The Phase 1 findings showed the existing barriers to value recovery based on these decisions and established the basis for a more effective, implementable system. The Phase 2 team included a broad cross-section of electronics stakeholders necessary for a working CE supply chain: HDD designers and manufacturers, different types of users/owners (and discarders) of HDDs, IT asset managers, technology developers, reuse and recycling companies that do both pre-processing and final processing, standards development organizations, and R&D organizations that can fill critical technology and materials gaps to increase value recovery and make the circular economy a reality. The US Department of Energy's Critical Materials Institute is playing an important role by creating new technologies for rare earth metal resource recovery, as well as by using this analysis to propose specific recommendations to strengthen the US manufacturing base. The iNEMI team designed and completed Demonstration Projects that showed new, technologically and economically viable pathways for value recovery that enable creation of a Circular Economy.

2:00 PM BI01.04.02

Recovery of Electronics Waste to be Converting into Functional Devices [Roberto Baca](#); Inst Politecnico National, Distrito Federal, Mexico.

Today, processing technologies have generated negative environmental impact as emission of toxic gases and degradation of the earth when certain products are placement in landfills leading to environmental pollution and several biological risks, which damage societies to sustain the planet for future generations. As electronics waste, grain-oriented iron foils, graphite films, and Mn-Zn ferrites has been identified as interesting candidates. Then, uncommon physical properties from such materials are available when it is converting technologically. A strategy such as Life-Cycle Assessment (LCA) is employed here to take into account all stages of the life cycle of electronics waste, including processing technology, manufacturing processes, use phase, and end-of-life routes to quantify the recycling performance as a function of the physical parameters that will characterize these to operability into a functional device. Hence, structure and conduction properties in waste materials are exploring by using X-ray diffraction, Raman spectroscopy and electrical characterization techniques with emphasis on knowledge of their physical behavior. Researching waste materials will provide theoretical basis for open-loop recycling, where trends related to green engineering should be attained with material recycling for adaptive structures as functional devices using different performance principles compared to those used with silicon devices.

2:15 PM BI01.04.03

Eumelanin's Biodegradability—Not to be Taken for Granted [Eduardo Di Mauro](#)¹, Denis Rho² and Clara Santato¹; ¹Polytechnique Montreal, Montreal, Quebec, Canada; ²Aquatic and Crop Resource Development, Canadian National Research Council, Montreal, Quebec, Canada.

The exploitation of natural materials has been identified as a valuable route towards the achievement of green (sustainable) electronics, whose development would reduce concerns related to conventional electronics, such as the depletion of natural resources and the increase of waste electrical and electronic equipment [1]. Biodegradability, "the metabolic breakdown of materials into simpler components by living organisms" [2] in a certain time frame compatible with the disposal route, is among the key characteristics of materials for green electronics [1]. Eumelanins are a dark-brown subclass of the melanin pigments, biopolymers abundant in flora and fauna [3]. They feature metal-ion chelation, photoprotection [3], biocompatibility [4], and mixed ionic-electronic conduction [5]. Because of this vast set of properties, eumelanin has been studied as a possible candidate material in the context of green electronics [6]. In addition, eumelanin has been assessed as an additive for plastic polymers to enhance their absorption in the UV and to stabilize them against photodegradation and thermal degradation [7]. Significant efforts have been made in the last decades towards sustainability, not only of the plastics themselves but also of their additives [8]. In both the fields of potential application of eumelanin, its biodegradability is paramount. Eumelanin is usually defined biodegradable by material scientists and physicists referring to a work where only its bioresorbability had been studied [4]. In the microbiology community, the biopigment has been reported to be resistant to biodegradation in some studies [9] and biodegradable in others [10]. Our work is the first to evaluate the biodegradability of eumelanin extracted from the ink sac of a cuttlefish (Sepia Melanin). The biodegradability was studied both at room temperature and at 58°C (composting conditions following ASTM D5338-2015). Conclusions are drawn considering the biopigment's hygroscopicity, molecular structure and super molecular assembly. We thus provide further insights into the environmental impact of such biopigment in the possible end-of-life scenarios, additive for packaging polymers or electroactive material for packaging sensors.[1] M.Irimia-Vladu, Chem. Soc. Rev., 43,2, 588–610,2014[2] M. Falkiewicz-Dulik et al., Elsevier, 2015[3] M. d'Ischia et al., Pigment Cell Melanoma Res., 26, 5, 616–633, 2013[4]C. J. Bettinger et al., Biomaterials,30,17, pp. 3050–3057, 2009[5]S. Rienecker et al., J. Phys. Chem. B, 119, 48, 14994–15000, 2015[6] M. d'Ischia et al., Angew. Chemie - Int. Ed., 48, 22, 3914–3921, 2009[7] Y. Wang et al.,ACS Sustain. Chem. Eng.,4,4,2252–2258,2016[8] E. Castro-Aguirre, Polym. Degrad. Stab., 137, 251–271, 2017[9] M. Blois, Academic Press, Inc., 1965[10] J.P. Luther, H. Lipke, Appl. Environ. Microbiol. 40,1980,145–155

2:30 PM BI01.04.04

Photonic Devices with Reduced In, Ga and Sb Content [Thierry Baron](#)¹, Marie-Leonor Touraton^{2, 1,3}, Tiphaine Cerba^{1,3}, Mickael Martin¹, Jérémy Moeyaert¹, Sylvain David¹, Virginie Loup³, Franck Bassani¹, Bassem Salem¹, Karine Samuel⁴, Blandine Ageron⁴, Thomas Ernst³, Didier Dutartre² and Christophe Jany³; ¹Univ. Grenoble Alpes, CNRS, CEA/Leti Minatex, LTM, F-38054 Grenoble, France; ²STMicroelectronics, Crolles, France; ³Univ. Grenoble Alpes, CEA, LETI, Grenoble, France; ⁴Univ. Grenoble Alpes, CERAG, Grenoble, France.

The access to raw materials is an economic and major geopolitical stake for the 21st century. Some key elements considered today in the emerging devices for the Internet of Things (IoT) must be substituted or saved (by orders of decades) in a drastic way in the near future. Since tens Billions electronics objects are then being disseminated all over the world in homes, buildings, cars, roads, etc., it is obviously a major concern to revisit the economic, technological, and societal models to develop a sustainable electronic industry that will care about its impact right from the conception of these objects. III-V semiconductors present interesting properties and are already used in electronics, lightening and photonic devices. More particularly alloys containing Ga, In and Sb are increasingly used by the semiconductors industry for high frequency operation, WIFI technology, high power devices, lasers for communications, sensors... This sector accounts for about 90% of world consumption of gallium for example. With the huge increase of IoT devices there is a real challenge to be able to minimize the consumption of these elements or substitute them but more abundant one to fulfill the same function. In this contribution, we will show routes to develop processes either to save or substitute In, Ga and Sb to realize specific functions such as light emission and detection, and sensors with technologies compatible with large-scale integration. An important aspect of the work will be devoted to synthesis on large area namely 300 mm wafers, with the concern for compatibility with CMOS processes. We will show that bulk material (InP, GaAs and GaSb substrates) could be substituted by thin layers elaborated on a standard Si(100) microelectronic substrates. Selective deposition will also be considered to put the materials only at the place where it is needed. The physical properties of In, Ga, Sb containing semiconductors elaborated on a silicon platform will be

shown and compared with those elaborated on III-V substrates. Demonstration of LEDs emitting in the visible and infra-red region will be shown. As an ultimate solution, 2D materials elaborated on large scale 300 mm Si substrates will be presented and their physical properties will be exposed.

ACKNOWLEDGMENTS

This work was supported by the French government managed by ANR under the Investissements d'avenir economic stimulus package, with reference IRT Nanoelec ANR-10-IRT-05, ANR-15-IDEX-02 and LabEx Mimos ANR-10-LABX-55-01

2:45 PM BI01.04.05

Synthesizing Pr³⁺/Dy³⁺ Doped Nd₂O₃ Nanoparticles from Nd-Fe-B Magnets Sourced from E-Waste Samane Maroufi, Rasoul Khayyam Nekouei and Veena Sahajwalla; UNSW, Sydney, New South Wales, Australia.

The global supply of rare earth elements (REEs), is under considerable strain. As many countries have no suitable ore deposits within their territories, and deposits elsewhere are both limited and finite, the recovery of REEs through recycling is essential. Currently, less than one percent of REEs are recovered via recycling. Nd-Fe-B permanent magnets are now one of the most widely used type of rare-earth magnets which are implemented in a variety of applications such as electric power generation (computer and laptop hard drive) and transportation (hybrid and electrical vehicles). Given the growing demands for lightweight products with high magnetic strength to support the miniaturization of equipment in many existing and emerging applications, demand for Nd-Fe-B magnets is, likewise, expected to continue to rise, particular for the clean energy/transport sectors.

In this study oxidation-reduction process was used for the recovery of rare earth elements (REEs) (i.e. Nd, Pr, and Dy) from Nd-Fe-B permanent magnets. Nd-Fe-B permanent magnets collected from e-waste were subjected to an oxidation process at 1000°C for 60 minutes followed by carbothermal reduction at 1450°C for 90 minutes using waste tyre rubber-derived carbon (WTR-DC) as a reducing agent. Fe-based metal and rare earth oxides (REO) phases were successfully separated from the original magnets. The distribution of elements (i.e., Nd, Dy, Pr, Fe, B, Al, and C) between the Fe-based metal and oxide phases were investigated via *Inductively Coupled Plasma (ICP)*, Energy-Dispersive X-ray Spectroscopy EDS/Electron Probe Microanalysis (EPMA) elemental mapping. REEs were confirmed as the main components of the oxide phase and it was shown that the REEs did not remain in the Fe-based metal phase. The oxide phase mainly contained REEs (i.e., Nd, Dy and Pr) and a minor amount of B and Al.

Using REEs (i.e., Nd, Pr and Dy) derived from Nd-Fe-B magnets we applied a low temperature urea-based homogeneous precipitation method and synthesized crystallized RE (i.e., Nd, Pr and Dy) OHCO₃ nanoparticles with diameters of 40-50 nm and high specific surface area of 60 m².g⁻¹. The synthesized REOHCO₃ was used as a precursor for the synthesis of REO nanoparticles through a thermal degradation process at 700°C. FE-SEM images revealed that the synthesized REO nanoparticles inherited their parent's morphology. X-ray diffraction spectrum of the synthesized REO nanoparticles showed cubic phase of Nd₂O₃ with no additional peak corresponding to the secondary phases of Pr and Dy. High resolution TEM (HRTEM) micrographs and electron diffraction of the selected area (SAED) of the as-synthesized REO nanoparticles exhibited the deformation in crystalline structure, shrinkage of the crystalline size and decrease in interplanar distance value indicating that Nd³⁺ in Nd₂O₃ host lattice were replaced with dopants of Pr³⁺ and Dy³⁺.

3:00 PM BREAK

3:30 PM *BI01.04.06

Nanoparticles from the Gas-Phase—A Technical, Ecological and Economical Answer for Stainable Future Energy Applications? Sophie M. Schnurre and Tim Huelsner; Institute of Energy and Environmental Technology e.V., Duisburg, Germany.

Sustainability should be the objective of every future technology. Especially nanotechnology has shown that worries and concerns of consumers may hamper the development of nanomaterials. Therefore, it is indispensable for a sustainable fabrication of products containing engineered nanoparticles (ENP) to have no adverse effects on the environment. In the face of the conflict between immediate marketing of innovative products containing engineered nanoparticles and precautionary assessments with regard to potential environmental and human risks, a multi-disciplinary approach to work out functional, social and economic effects was established. Within this approach, first, the design and synthesis of sustainable nanomaterials on the pilot plant scale and, second, different aspects along the value chain are considered. Here, political regulations, social and economic chances, technical and social risk potential as well as barriers to economic growth are crucial from the synthesis to the implementation into applications.

For ceria nanoparticles (pure as well as doped), an enormous marketing potential is expected due to their presumed low toxicity and multiple application possibilities. We present methods (e.g. doping particles with Europium) to tune particle morphology, which allows to identify particles in biological systems and enhance low temperature catalytic properties. Results of end of life cycle assessment using new models of nanoparticle distribution scenarios are displayed.

As another application oriented material, we chose silicon nanoparticles, since this material is a candidate for anode material in lithium batteries because of its high storage capacity, good availability of raw material, cost-efficient production method and its sufficient long-term stability.

We demonstrate the formation of silicon nanomaterial by homogeneous gas-phase reactions as a direct and highly economic way to produce the required high-purity raw material for battery applications. We developed a value chain for lithium ion battery materials with respect to market, patent and literature analyses as well as the innovation potential. Here, the synthesis process, the manufacturing, the utilization phase and the end of life phase are taken into account.

These tools will form the basis of a "value chain" regulatory process, which allows NM to be assessed for different applications on the basis of available data and the specific exposure and life cycle concerns for that application. To determine the technology readiness level (TRL) of a technology a scheme has been worked out, which shows a timeline that is divided into laboratory-, pilot plant- and industrial-scale from today to 2030. Technology related topics such as material, processing, component development, assembly and the final product are integrated into scheme. Technology options like social and economic chances as well as limitations like risk potential, social risks and barriers to economic growth are considered.

4:00 PM BI01.04.07

Massive Production of Energy Materials from Fe-P Waste Slag with Novel Technics for Sustainable Development Guixin Wang, Yun Wei, Yujia Peng, Fei Xu, Yao Cai, Shunxing Wang and Yangping Yan; College of Chemical Engineering, Sichuan University, Chengdu, China.

Recycling solid waste slag as functional materials at low energy consumption and low environmental impact still faces challenges for sustainable development. A novel and green route has been proposed for the synthesis of energy materials like LiFePO₄, FePO₄, Fe₃(PO₄)₄(OH)₃ using Fe-P waste slag with a melting point of 1400 °C via a hydrothermal reaction at no more than 200°C, and the by-product is only water. A 2L autoclave was utilized to synthesize these materials by stirring to further decrease reaction temperature and shorten reaction time. FePO₄ or Fe₃(PO₄)₄(OH)₃ can be obtained by changing the mass ratio between Fe_{1.44}P slag, H₃PO₄ and H₂O₂, while LiFePO₄ can be obtained by using the raw materials of Fe_{1.44}P slag, LiOH H₂O, H₃PO₄ and H₂O₂. As the autoclave was cooled to room temperature, a solution with solid particles appears. After being washed, filtered and dried in air, fine product powders were obtained. The reaction process was investigated with thermodynamic calculation and thermogravimetric analysis. The as-obtained solution and powders were characterized with various techniques, and key factors affecting the synthesis were discussed. The as-obtained FePO₄ or Fe₃(PO₄)₄(OH)₃ can be further used to synthesize LiFePO₄. The electrochemical performance of the as-synthesized LiFePO₄ samples was evaluated with galvanostatic charge/discharge tests, cyclic voltammetry and electrochemical impedance spectroscopy. The LiFePO₄ samples obtained with one step or two steps all have specific electrochemical activity, and the specific capacity can reach 110 mAh/g at 1.0C current rate. In order to improve the

electrochemical performance of the samples, glucose was adopted to supply carbons to improve conductivity via calcining at 300 °C and 700 °C in a quartz tube furnace full of Ar. The emissions from the tube furnace were inlet an ammonia water to form a NH_4HCO_3 solution. The effects of H_3PO_4 and H_2O_2 on the composition and electrochemical performance of the samples were investigated in detail. After carbon modification, the discharge capacity of the LiFePO_4 samples can reach 150 mA/g at 1.0C current rate, and the capacity fade after 100 cycles is only 1%, which is comparable to the commercial LiFePO_4 synthesized with expensive raw materials. The successful conversion of alloy with a high melting point into energy materials at low temperature can be used for other alloys, which decreases energy consumption and waste emissions, shortens the traditional reaction process, as well as improves resource utilization efficiency.

4:15 PM BI01.04.08

A Novel Closed-Loop Process for Recycling LiFePO_4 and Graphite Xiaotu Ma, Mengyuan Chen and Yan Wang; Worcester Polytechnic Institute, Worcester, Massachusetts, United States.

With the rapid consumption of fossil fuel, lithium-ion batteries (LIBs) are widely used in an ever-growing list of consumer electronics, electric cars, energy storage, and other applications. Although LIBs have reduced environmental problems caused by fossil fuel, the spent LIBs waste has become another big problem. Moreover, the shortage of the supply of materials will be a potential risk for LIBs. Therefore, in order to protect the environment and ensure industry sustainability, it is necessary to develop technologies to recover and recycle spent LIBs efficiently and economically. A novel closed-loop hydrometallurgical process for recycling spent LIBs has been developed in our group. The advantages of this technology include no sorting, high-quality recovered battery materials, high efficiency, and applicability to any size and shape of spent LIBs. Here we show the method for recycling cathode, olivine structured lithium iron phosphate, LiFePO_4 (LFP), and anode, graphite. LFP, with high power capability, low cost, non-toxicity, excellent thermal safety, and high reversibility, has been commercialized as cathode materials. After leaching various spent LIBs and filtration, the mixture of FePO_4 , graphite and other impurities can be extracted from the remainder. Then the remainder is leached in a HCl solution and FePO_4 is dissolved as FeCl_3 and H_3PO_4 solution. The mixture solution is used to precipitate FePO_4 by adjusting the pH as the precursor to recover LFP. Similarly, graphite and other impurities remain after filtration. The mixture is washed and dried. Then, the mixture is heated at different temperatures in air to remove impurities and crystallize the graphite. The results show good electrochemical performances of recycled cathode and anode materials. Also, this will reduce the production cost, mitigate the shortage of resources and solve environmental problems.

4:30 PM BI01.04.09

Development of Integrated Technologies for Conversion of Industrial Waste CO_2 to MeOH and Other Value-Added Chemicals via Thermochemical Route Sebastian Chirambatte Peter and Soumyabrata Roy; Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India.

Two most imminent scientific and technological problems that the mankind is facing now, is that of energy and climate. The energy production and utilization in modern society is mostly based on the combustion of carbonaceous fuels like coal, petroleum and natural gas the combustion of which produces CO_2 , which alters earth's carbon cycle. 30 billion of tons of CO_2 per year get emitted globally as waste from the carbonaceous fuel burning and industrial sector, which if converted to valuable chemicals have the potential to change the economy of the world. We, in our lab are trying to address both issues and are keen upon translating our innovative technologies from the lab to the industrial and commercial scale. The CO_2 conversion technology is in the developmental stage for commercialization. We are capturing CO_2 from industrial flue stream (of any composition) and thermo-catalytically converting it to value added chemicals/fuels methanol, carbon-monoxide, methane, dimethyl ether, C2-C5 & C5-C11 gasoline hydrocarbons. The end to end technology comprises innovations in catalyst synthesis, reactor designs, hydrogen generation and product purification. MeOH is one of the most attractive conversion product in the thermo-catalytic pathway which could not be commercially realized yet due to problems of low catalytic conversion, limited conversion, energy efficiency of the technology and most importantly high cost of hydrogen. We at JNCASR, are working towards solving these bottlenecks of the overall technology through synthesis of efficient catalysts and designing more energy efficient reactor systems. Catalyst design is at the heart of all these technologies and we are developing customized catalysts and reactor systems for targeted product conversions as per the need of different industries. The catalysts have been synthesized through extensive structure property relation study corroborating with 1st Principle DFT calculations. Advanced CFD calculations are used to design energy efficient reactor systems. Nano structuring in the group 13 element doped CZZ systems showed highly enhanced conversion and methanol selectivity. At present we are scaling up the end-to-end process, the success of which might lead to opening of new directions in CO_2 conversion technology. We are in the process of taking our technology to the pilot plant scale during the course of which we are running for the 20 million-dollar NRG Carbon Cosia XPRIZE, which is a global competition for promoting commercially viable novel technologies for solving CO_2 and climate change issues.

SESSION BI01.06: Poster Session: Sustainable Development in Materials Science and Related Societal Aspects

Session Chairs: Jean Gaumet and Geoffrey Strouse

Tuesday Afternoon, November 27, 2018

8:00 PM - 10:00 PM

Hynes, Level 1, Hall B

BI01.06.01

Use of Inverse Vulcanization for the Production of Multifunctional Sulfur Fertilizers Stella F. Valle^{2,1}, Amanda S. Giroto^{2,1}, Rodrigo Klaiç^{3,1} and Caue Ribeiro de Oliveira¹; ¹Embrapa Instrumentation, São Carlos, Brazil; ²Department of Chemistry, Universidade Federal de São Carlos, São Carlos, Brazil; ³Department of Chemical Engineering, Universidade Federal de São Carlos, São Carlos, Brazil.

Sulfur (S) has a vital agronomic role in vegetable development, yet it is often the most neglected macronutrient in current agronomic practices and agrochemical research. Over the past decades, sulfur deficiency in soils has become increasingly common worldwide, harming the quality of crops as well as their yields. Elemental sulfur (S_8) stands out among other sulfur-based fertilizers as the most concentrated source (~100%). Additionally, S_8 is not susceptible to leaching problems like sulfate fertilizers, and it is an abundant byproduct of petrochemical industry. Nevertheless, plant uptake is only possible after S_8 biological oxidation by soil microorganisms, a slow rate process strongly influenced by the fertilizer characteristics. Oxidation is, therefore, the most limiting factor for S_8 agronomic efficiency, with commercial pellets generally taking more than 3 years for a conversion of only 50% of the applied products. Considering the intense world population growth expected for the next decades, developing innovative strategies to enhance fertilizers efficacy is fundamental to meet future food demands in a sustainable way.

In the present work, we propose a novel S-fertilizer based on the chemical modification of S_8 cyclic structure into a linear amorphous form, more available to oxidizing microorganisms, as an approach to improve the oxidation rate. In order to design this type of material, we applied the recently developed inverse vulcanization technique, a simple copolymerization method that guarantees better processing control for sulfur and allows the formation of

functional sulfur-rich polymers. In addition, this technique involves some green chemistry principles, such as the lack of solvent use and excellent atom economy. Soybean oil was selected as comonomer for the reaction as a cheap, non-toxic and renewable feedstock. The S-oxidation achieved by the polysulfide products revealed to be more than 50% superior than S₈, and the soybean oil fraction of those materials displayed a role as carbon source for microorganism activity. Therefore, the results could support the sustainable development of a non-conventional S-fertilizer with enhanced efficiency and multifunctional properties.

BI01.06.02

Amino-Moiety Designed Novel Ionic Liquids for Highly Efficient and Selective Extraction of Platinum Group Metal from Hydrochloric Acid Solution Chisato Hanzawa, Atsushi Muramatsu and Kiyoshi Kanie; IMRAM, Tohoku University, Sendai, Japan.

Platinum group metals (PGMs) are of significant importance for modern technologies and advanced materials. However, the continuous high demand and scarcity of PGMs are critical issues. Correspondingly, we need to challenge recycling technologies to fill the gap between demand and supply. Conventional organic solvent extraction is widely applied to the practical recovery method of PGM ions. Recently, ionic liquids (ILs) are considered as an alternative green solvent for PGM extraction. In our previous study, we have reported a metal-selective deprotection-mediated Pd(II) extraction by use of ILs with tetrahydropyran-2H-yl-protected thiol moieties.¹⁾ Also, the functionalization of ILs, regarded as task-specific ILs (TSILs), is a promising technique to introduce PGM extraction ability into ILs. In the present work, we have designed and synthesized novel ILs with amino moieties²⁾ in order to develop the selective recovery method of Pt, Pd, and Rh ions for industrial use.

All TSILs **C_n** (**n** means alkyl chain length of dialkylamines) forming a pale-yellow IL state at room temperature were immiscible in water. We next investigated the PGM extraction ability of **C_n** for Pd(II), Pt(IV), and Rh(III) ions. The initial PGM ion concentrations in the aqueous solutions were adjusted to 100 ppm. Influence of HCl concentration on the extractability was examined in the range from 0.30 M to 4.0 M. The extraction experiments of the PGM ions into the **C_n**-based IL phases (400 mg) from the aqueous phase (2.0 mL) was carried out by mixture of the solution in a vial, followed by vigorous shaking. The extractability was evaluated through the difference of PGMs concentration in the aqueous phase before and after extraction with ICP-AES measurements.

Both dihexylamino-substituted **C6** and dioctylamino-substituted **C8** exhibited excellent extractability (> 80%) towards Pt(IV) and Pd(II) ions in HCl concentration range from 0.30 to 4.0 M. However, the extractability of dibutylamino-substituted **C4** was significantly decreased with an increase in HCl concentration, possibly because of the instability of **C4** at rather high HCl concentrations. The extractability to Rh ions reached at 73% at maximum for **C8** in 3.0 M HCl solution, which exceeded that for **C6**, 51%. We considered that the high extractability of **C8** was attributed to the high hydrophobicity. The extraction/back-extraction abilities of **C_n** were also investigated.

References

- 1) K. Funaki, S. Ma, S. Kawamura, A. Miyazaki, A. Sugie, A. Mori, A. Muramatsu, and K. Kanie, *Chem. Lett.*, **46**, 434-437 (2017).
- 2) S. Ma, K. Funaki, A. Miyazaki, A. Muramatsu, and K. Kanie, *Chem. Lett.*, **46**, 1422-1425 (2017).

BI01.06.03

Efficient Photothermal Water Evaporation from Inked Filtration Paper Zhiqiang Wang^{1,2} and Ming Su¹; ¹Northeastern University, Boston, Massachusetts, United States; ²Tianjin Normal University, Tianjin, China.

Water evaporation with natural solar energy attracts much attention due to its wide applications as well as energy saving. However, this heating process is very slow under 1 sun shining. So current technology, which needs a large surface, collects the solar irradiation as much as possible, and concentrates the heat to accelerate this process. For future technology, evaporation upon local heating at air-water interface can be facilitated with energy saving, because such locally temperature gradient in the air-water system, compared to the heating scheme of bulk water, can effectively increase the heat utilization. Apparently, the implementation of such emerged photo thermal desalination technique is highly dependent on exploration of excellent photo thermal materials to absorb and evaporate water efficiently. In this work, we reported a low cost and high efficient evaporating material. Such an evaporating system achieved an extremely high water production rate of 1.34 kg h⁻¹ m⁻² and 89.9 % energy efficiency under 1 sun radiation. The excellent performance is attributed to the combination of multiple properties simultaneously exhibited by this as-prepared material, including its intrinsic blackbody-like high absorption, extremely low thermal loss to environment (low evaporating temperature and 1D water transporting), and automatic water transportation to the evaporating surface by capillary force through the huge microchannels. We also found the general relationships, not limited in our materials but all solar evaporation materials, between evaporating rate, energy efficiency and evaporating surface temperature. Following this relationship, people may control the steam temperature and the evaporating rate for some purpose, respectively.

BI01.06.04

Improving the Efficiency of N Fertilizers Using Thermoplastic Starch-Modified with Molecules High N Levels Amanda S. Giroto¹, Caue Ribeiro de Oliveira¹ and Gelton G. Guimaraes²; ¹LNNA, EMBRAPA Instrumentation, São Carlos, Brazil; ²Epagri, Itajaí, Brazil.

Nitrogen (N) deficiency has been considered as the most important limiting factor for crop yield, explaining the high N fertilizer application worldwide. Among all the N-content molecules urea is the most used due to its high N content, however, its efficiency is limited by losses such as leaching and volatilization. For this reason, we propose the production of a fertilizer based in urea-melamine-thermoplastic starch using a one-step method aiming to control the nitrogen release as a nutrient. The extrusion process used has been showed to be a simple, continuous, high throughput method, capable to promote melamine incorporation, which was responsible to increase the interaction among urea and starch. The results reveal that melamine plays an important role as structure modifier, increasing the effective use of available N for plants in pot experiments. The characterization shows that this material is a polymeric blend, possible to be processed by continuous method (extrusion) leading a plastic granule, with high homogeneity and high nutrient contents. Pot trials (using maize) shown that this material increases the N efficiency (based in the actual available N) leading to a significant nutrient residual in soil useful for future cultures, confirming that this product might replace with advantages the conventional N fertilizers.

BI01.06.05

Investigating the Effects of Different Spun-Cast and Molded Polylactic Acid (PLA) and Polystyrene (PS) Composites on the Proliferation, Differentiation and Biomaterialization of Dental Pulp Stem Cells Kuan-Che Feng¹, Ethan Ho², Bhuvna Murthy³, Rushi Patel⁴, Antony Deluxe⁸, Wenqi Zhao⁵, Benjamin Chang⁶, Nicholas Zumba⁷, Chung-Chueh Chang¹, Marcia Simon¹ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Northfield Mount Hermon School, Gill, Massachusetts, United States; ³Huron High School, Ann Arbor, Michigan, United States; ⁴Herricks High School, New Hyde Park, New York, United States; ⁵Milton Academy, Milton, New York, United States; ⁶Woodbridge High School, Irvine, New York, United States; ⁷Columbia University, New York City, New York, United States; ⁸Wheatley High School, Old Westbury, New York, United States.

Polymers are known to be more combustible than other structural materials, and hence flame retardant formulations are frequently added. Recently it has been shown that many of these formulations, especially those containing halogenated compounds, are toxic and leach into surrounding water and soil. This concern is even more pressing when biodegradable polymers are used, where the degradation process facilitates the environmental release of the toxins. Here we report on a study of the toxicity of resorcinol diphosphate, RDP, a phosphorous based flame retardant additive. RDP is easily compounded into homopolymers or polymer blends when adsorbed onto clay, where it also facilitates compatibilization.

In this study, we show that when included into PLA, RDP appears to have no deleterious effects on cell adhesion, proliferation, and differentiation. When RDP-Clay is added to polystyrene, it has an advantageous influence. Cells do not adhere to PS, but when RDP Clay is added, cell plating efficiency and cell proliferation is drastically improved and the doubling time is comparable to that of the cells plated on PS. In contrast to the cells on PS, those on the PS-RDP-Clay and PLA-RDP-Clay scaffolds underwent differentiation, where large amounts of hydroxyapatite deposits were found. With the appearance of what is believed to be hydroxyapatite deposits (biomineralization), RAMAN spectroscopy will be used to determine any possible developments of an extracellular matrix on the PS-RDP-Clay and PLA-RDP-Clay scaffolds. Additionally, RT-PCR will be conducted on days 28 and 42 in order to evaluate the presence of all genes that may be associated with osteogenic or odontogenic differentiation. Even though further in-vivo testing is required, these results indicate that the probable toxicity of RDP is low, since RDP-Clay preserves both cellular proliferation and function.

BI01.06.06

Improved Dispersion of Asphaltenes in Heavy Oil by the Addition of Base and Either Acidic Copolymers or Aliphatic Compounds Terminated with Functional Groups Myong-Guen Jo, Kwang-Hwan Ko and Joon-Seop Kim; Chosun University, Gwangju, Korea (the Republic of).

Recently, we have been attempting to develop the dispersants for the improved dispersion of the asphaltenes that presented in heavy crude oil and became gel or precipitated upon the agglomeration. It has been known that effective dispersants for asphaltenes in heavy crude oil should have the following factors: a proper amount of aromatic and functional groups that can interact with those of the asphaltenes, low molecular weight ($MW < 10,000$) because of the better solubility to heavy crude oil, amphiphilicity for the improved dispersion because the asphaltenes have both polar and non-polar units, and alkyl chains of proper lengths for the better miscibility with heavy crude oil. Thus, in the course of the present work, we prepared two types of dispersants, analyzed their chemical structures, and determined the effects of the dispersants on the dispersion of the asphaltenes. The two types of the dispersants were low MW styrene copolymers and various aliphatic alcohol, carboxylic acid, or amine compounds. In the first part of the work, we compared the effects of the types of the functional groups of the oligomeric styrene copolymers on the asphaltene dispersion. It was found that the sulfonic acid groups were better than the carboxylic acid groups on the dispersion. In addition, it was also observed that the more carboxylic acid groups in the acidic unit enhanced the dispersion. Furthermore, as expected, with decreasing MW of oligomers, the dispersion behavior of the asphaltenes became more improved. In the second part of the work, we investigated the effects of the addition of the aliphatic alcohols on the asphaltene dispersion. It was found that when the types of functional groups and alkyl chain lengths of aliphatic compounds did not affect the asphaltene dispersion in the heavy oil significantly. However, it was observed that the addition of NaOH to the heavy oil containing aliphatic alcohol or carboxylic acid compounds enhanced the dispersion of asphaltenes strongly. Interestingly enough, even the addition of NaOH to the heavy oil also improved the asphaltene dispersion, at least to some extent. Furthermore, it was seen that the effect of the NaOH addition to the heavy oil containing aliphatic alcohols became more pronounced than that to the heavy oil containing aliphatic carboxylic acids. Especially, the NaOH addition improved the asphaltene dispersion more significantly in the heavy oil containing 2-ethylhexyl alcohol than normal alcohols, having shorter or longer alkyl chains. Thus, we have been trying to find the reason why the base, i.e. NaOH, influences the asphaltene dispersion; we will present our interpretation on the results.

BI01.06.07

Processing of Sulfur-Phosphate Composites—Use of Synergy to Improve the Fertilization Roles Gelton G. Guimaraes¹, Amanda S. Giroto², Rodrigo Klaiç² and Caue Ribeiro de Oliveira²; ¹EPAGRI-EEI, Empresa de Pesquisa Agropecuária e Extensão Rural de Santa Catarina, Itajaí, Brazil; ²Embrapa Instrumentação, Empresa Brasileira de Pesquisa Agropecuária, São Carlos, Brazil.

An environmentally-friendly alternative to phosphate fertilization is the supplementation of P from rock phosphates, however, these sources do not have P readily available to plants. In this sense, the reduction of particle size from grinding techniques have been studying to increase the solubility of the phosphate minerals. However, a difficulty presented during this process is the tendency of agglomeration of the particles, preventing them from maintaining nanometric dimension. Elemental sulfur (S^0) comes up as a dispersant potential that through the acidity generated by the S^0 oxidation to sulfate (SO_4^{2-}) can aid in the solubilization of mineral phosphates. The fungus *Aspergillus niger* has the ability to oxidize sulfur, besides to have a high production capacity of organic acids such as citric acid, oxalic acid, and gluconic acid that increased the solubilization of phosphorus. Thus, *A. niger* presents two mechanisms that may favour the solubilization of phosphates: first by natural acidification provide by oxidation of S^0 and the second by organic acids production. In this work, a composite was designed based on a matrix of S^0 prepared by low-temperature processing, reinforced by rock phosphate (P) particles acting as P fertilizer, and with encapsulation of *Aspergillus niger* as an oxidizing microorganism. The effects of dispersion of the phosphate particles on the elemental sulfur matrix and starch were evaluated, as well as the natural acidification provided by the oxidation of S^0 and the production of organic acids in the solubilization of P from the natural phosphate. In addition, after the release of P and SO_4^{2-} , from the composite-fertilizer incubated in the soil, the dynamics and interaction of P with the colloidal fraction of the soil were analyzed using P K-edge X-ray absorption near-edge structure (XANES). The inclusion of *A. niger* provided a means for improved S^0 oxidation and concomitant faster P release. The proposition of a granule fertilizer with a simultaneous dispersion of particles of phosphate rock, elemental sulfur, and *A. niger* spores can allow the reduction of pre-processing (e.g., for soluble fertilizer production) and reduces the indirect costs related to the conventional acid solubilization process and waste treatment. Soil incubation studies, probed by XANES, indicated that the composite structure played a role in nutrient fixation and immobilization, showing that nutrient dynamics was governed by the local pH. This fully integrated material (a smart fertilizer) is an innovative strategy for eco-friendly agronomic practices, providing high nutrient delivery with minimal source pre-processing.

BI01.06.08

Nanocomposites Fertilizers Biologically Activated for an Efficient Supply of Sulfur and Micronutrients to Plants Rodrigo Klaiç^{1,3}, Amanda S. Giroto¹, Gelton G. Guimaraes², Caue Ribeiro de Oliveira¹, Teresa C. Zangirolami² and Cristiane S. Farinas¹; ¹Embrapa Instrumentação, São Carlos, Brazil; ²EPAGRI-EEI, Empresa de Pesquisa Agropecuária e Extensão Rural de Santa Catarina, Itajaí, Brazil; ³Department of Chemical Engineering, Federal University of São Carlos, São Carlos, Brazil.

Many commercial fertilizers are based on the application of elemental sulfur (S^0) and oxides metallic to supply sulfate and micronutrients to plants. However, the soil ability to solubilize oxides and promote the S-oxidation is low, since it is dependent of the presence of microorganisms capable of carrying out such biological reactions. To overcome this limitation, different strategies have been explored to improve the availability of sources of nutrients of low solubility, such as oxides and S^0 . An interesting alternative is the application of microorganisms to promote the oxides solubilization and the S-oxidation in the field. The filamentous fungi *Aspergillus niger* has been applied to promote the phosphorus solubilization from phosphate minerals as well as bioremediation and bioleaching of metals from mining ores. Besides, previous studies also revealed that *A. niger* can promote the biological oxidation of S^0 as well as the oxides solubilization. However, the major challenge is to develop a material that would favor the integration of both oxides particles and microorganisms in a single granule to promote oxide solubilization that could be processed and stored, thus when applied in the field the

granule would be activated to allow microorganism growth to solubilize the oxide, this is an innovative concept of "bioreactor in granule". Herein, we proposed to produce a composite (granule) based on the dispersion of nanoparticles of S° and oxides in a polysaccharide matrix (polymeric gelatinized starch) with simultaneous encapsulation of *A. niger* spores. Three oxides model (ZnO, MnO and CuO) besides S° were used to produce different configurations of composites. The oxides were physical-chemical characterized as well as the composites produced. Experiments were performed to evaluate the effect of bio-activation of the composite by *A. niger* and consequent oxides solubilization and S-oxidation in a liquid medium and in soil. The results showed that all the different composites produced (St/Zn, St/Mn, St/Cu, St/Mix and St/Mix+S) increased solubility of the dispersed material. The effects of dispersion of the oxides and S° particles in starch matrix was analyzed using field emission gun scanning electron microscopy and X-ray microtomography, a high dispersion of the particulate materials was observed with low agglomerates formation. Nevertheless, the St/Mix+S show the best results for oxides solubilization, besides being a source of multi-nutrient (S, Zn, Mn and Cu). The St/Mix+S also showed considerable shelf time and when evaluated under greenhouse conditions, it showed an efficiency comparable to the experiment carried out with soluble commercial fertilizer for the cultivation of Italian ryegrass (*Lolium multiflorum* Lam.). This strategy opens a new route for development of smart fertilizer capable of making feasible the use of source of micronutrients of low solubility for plant nutrition.

BI01.06.09

Removal of Fluoride from Groundwater Using Alfu Metal Organic Framework (MOF) Impregnated Polyacrylonitrile Beads Sankha Karmakar, Debashis Roy and Sirshendu De; Indian Institute of Technology (IIT) Kharagpur, West Midnapore, India.

Novel mixed matrix hollow beads were prepared by phase inversion technique using polyacrylonitrile (PAN) as base polymer and aluminum fumarate (Alfu) metal organic framework (MOF) as additive. The beads were characterized in terms of surface morphology, surface charge, surface area and contact angle. With the incorporation of the hydrophilic Alfu MOF, contact angle of the corresponding beads decreases from 80° to 51° indicating an increase in hydrophilicity. The 10 wt% incorporated beads sustained upto 150 hours of operation with fluoride concentration of 10 mg/l at flow rate of 10 l/day. Regeneration study and leaching of aluminum were also investigated.

BI01.06.10

Exploring the Stability and Electronic Properties of Zn Doped Hematite Surfaces for Photoelectrochemical Water Splitting Joseph Simfukwe^{1,2}, Refilwe E. Mapasha¹, Artur Braun³ and Mmantsae Diale¹; ¹University of Pretoria, Gauteng, South Africa; ²Physics, Copperbelt University, Kitwe, Zambia; ³Empa–Swiss Federal Laboratories for Materials Science and Technology, Switzerland, Switzerland.

First principles studies of Zn doped {0001} and {012} surfaces of hematite for enhanced photoelectrochemical water splitting have been carried out. Doping was confined to planes in close proximity to the termination region, precisely from the top most layer to the third inner layer (plane P1, P2 and P3) of Fe atoms. The two surfaces and the three doped layers were found to be thermodynamically stable and would prefer exothermic formation under oxygen rich conditions. The analysis of electronic properties reveals that even with mono doping of Zn on the top most layer (P1) of the {0001} α -Fe₂O₃ surface, the band gap can be decreased without impurity states in the band gap which normally acts as recombination centres. The doping of Zn atom on P2 and P3 (second and third layer respectively) of the {012} surface narrowed the band gap from ~ 1.43 eV to ~ 1.0 eV for both systems, without any impurity states in the band gap. Furthermore, the conduction band minimum (CBM) of P2 and P3 of the {012} surface also become wavier and delocalised suggesting improved electron mobility of hematite, while the CBM of the {0001} surface shifted upward between ~ 0.05 eV and ~ 0.3 eV. The observed upward shift in the CBM is likely to enhance photoelectrochemical splitting of water with a smaller application of external bias. Analysis of the charge density difference plots showed concentration of charge mainly at the top of the surface, which is the termination region. This suggests facile transfer of charges to adsorbed water molecules due to the closeness of the charges to the adsorbate. The concentration of the charges at the surface, the decreased band gap and the absence of recombination centres within the band gap suggest improved photocatalytic activity of the Zn doped α -Fe₂O₃ surface.

BI01.06.11

Novel Fluorescent Polymer Sensor for Nitroaromatics Explosives Detection in Solution and Vapor Phase Vishal Kumar and Soumitra Satapathi; Indian Institute of Technology Roorkee, Roorkee, India.

The highly sensitive and reliable detection of explosives such as nitro substituted compounds (DNT, TNT and TNP) is of paramount importance for civilian and military security. NACs are also recognized as poisonous or carcinogenic explosive chemicals to the environment. Currently, explosive detection either relies on canines or highly sophisticated measurement techniques, such as mass spectrometry, gas chromatography, Raman spectroscopy, etc. High cost and/or complexity of these techniques limit their wide availability, especially in the field. Compared to those fluorescent polymers are particularly interesting for fluorescence based rapid detection as they exhibit large signal amplification due to the delocalization and rapid diffusion of excitons throughout the individual polymer chains¹. Moreover, the fluorescence polymers having high PL quantum efficiency, favorable redox potential and easy synthesis scheme need to be explored which can act as excellent electron donor for rapid electron transfer to NACs having electron-withdrawing nitro groups on the aromatic ring in order to make them as efficient optical sensor with ultra-high sensitivity².

Here, we report the synthesis and multimodal sensing applications of a highly emissive and electron-rich alanine based dansyl tagged copolymer P(MMA-co-Dansyl-Ala-HEMA) (DCP) which exhibited high sensitivity and selectivity towards DNT, TNT and TNP in solution at lower range of μ M level and also with saturated vapour of NACs. The high quantum yield of the co-polymer (77.3%) makes it an ideal candidate for sensing in solution as well as in vapor phase. In solution, the fluorescence signal from DCP co-polymer gets significantly quenched upon addition of aliquots of DNT, TNT, and TNP caused by photo-induced electron-transfer i.e. quantified by plotting Stern–Volmer plot ($K_{SV} = 1.1 \times 10^3 \text{ M}^{-1}$, $1.3 \times 10^3 \text{ M}^{-1}$ and $1.6 \times 10^4 \text{ M}^{-1}$ for DNT, TNT and TNP). The quenching mechanism was further established by time-resolved fluorescence and steady state absorption spectroscopy which was found to be predominantly dynamic in nature as lifetime of polymer (14.9 ns) is reduced to 13.9, 13.9 and 13.8 ns for DNT, TNT and TNP. The energetics of sensing process was calculated by Density Functional Theory(DFT) studies this is also in good agreement with the obtained result.

To explore the possibility of using the fluorescent co-polymer as sensor array, a prototype thin film polymer sensor was fabricated using drop-casted thin film of DCP which was able to detect saturated nitroaromatic vapor in real time with high selectivity. The initial fluorescence intensity of the 20 nm thin film of DCP was quenched to 19% for DNT, 13% for TNT and 4% for TNP in just 2 min.

In summary, this work opens up a novel approach for designing light weight and compact prototype sensor for field use as well as for environmental monitoring.

References

1. Sun, X. *et al. Chem. Soc. Rev.* **2015**,*44*,8019.
2. Rochat, S. *et al. ACS appl. mater. & interfaces* **2013**,*5* (11),4488.

Wednesday Morning, November 28, 2018
Sheraton, 3rd Floor, Hampton

8:00 AM *BI01.07.01

Thermally Stable and Sustainable Self-Assembled Ceramic-Metal Hybrid Metamaterials [Haiyan Wang](#); Purdue University, West Lafayette, Indiana, United States.

Nanoscale metamaterials exhibit extraordinary optical properties and have been proposed for various technological applications such as biosensing, superlenses, subwavelength optics, etc.. In this talk, our recent efforts in developing a new class of novel nanoscale 2-phase hybrid metamaterials in vertically aligned nanocomposite (VAN) form has been reviewed. Such hybrid systems are consist of transition metal nitrides and metals. Taking advantages of the long term stability and thermal stability of transition metal nitrides, we have demonstrated highly stable and mechanically strong metamaterials systems with tunable optical properties, including highly anisotropic reflectance, obvious non-linear optical properties indicating inversion symmetry breaking of the hybrid material, large permittivity tuning and negative permittivity response over a broad wave length range, and superior mechanical strength and ductility. The study demonstrates the novelty of the new hybrid plasmonic scheme with great potential in versatile material selection, and, tunable nanopillar spacing and dimension, all important steps towards future designable hybrid plasmonic materials.

Nanoscale Artificial Plasmonic Lattice in Self-Assembled Vertically Aligned Nitride-Metal Hybrid Metamaterials, *Advanced Sciences*, 1800416, 2018. DOI: 10.1002/advs.201800416.

8:30 AM BI01.07.02

Introducing Novel Hybrid Ion Exchange Membrane and ANAMMOX Bacteria to Improve Nitrogen Removal Efficacy of Microbial Fuel Cell [Gourav D. Bhowmik](#), Koushik Adhikary, Makarand M Ghangrekar and Arunabha Mitra; IIT Kharagpur, Kharagpur, India.

Emission of greenhouse gases due to the burning of fossil fuels led to climate changes drastically over the last few decades, which drives the researchers from all around the globe to seek for alternative renewable sources. On the other hand, high energy consuming wastewater treatment systems need to be replaced with less energy demanding or even energy harvesting treatment systems as wastewater is considered to be the reservoir of high energy content. Microbial fuel cell (MFC), a bio-electrochemical system (BES), can be a reliable alternative over the conventional wastewater treatment systems by simultaneously producing bio-energy through oxidising organic matter present in wastewater anaerobically using electrogenic bacteria as biocatalyst. In MFC, removal of nutrients from wastes have largely focused on exploiting nutrient cycle reactions, whereby reactive forms of nutrients are converted to unreactive simpler forms e.g. ammonia to inert nitrogen gas. To remove excess nitrogen present in wastewater, it is required to incorporate processes that primarily involves the elimination of NH_4^+ followed by reduction of NO_3^- . Hence establishment of suitable conditions to facilitate both nitrification and denitrification is necessary.

A hybrid membrane structure is developed to permit the exchange of both anions and cations in either way from anode to cathode of the MFC. The cation exchange part of the hybrid membrane was made of ceramic separator blended with 20% Montmorillonite as excellent cation exchanger and anion exchange part with poly(2,6-dimethyl-1,6-phenylene oxide) (PPO) via bromination and subsequent quaternization. Fish processing wastewater was used as target wastewater with chemical oxygen demand (COD) to nitrogen (N) ratio (C/N) of less than one g COD/g N for concurrent denitrification and ANAMMOX were assessed in two different MFCs with a working volume of two litre each. MFCs were fabricated one with only cation exchange membrane (CEM) and another one with as fabricated hybrid ion-exchange membrane (HEM) named as R1 and R2, respectively. The polarization study revealed the maximum power density of 252 and 163 mW/m^2 with the respective coulombic efficiency of $18.7 \pm 1.2\%$ and $14.8 \pm 1.4\%$ for R-1 and R-2. The marginally lesser power production of R-2 was because of the competition for electron donor (organic matter) inside the anodic chamber for concurrent denitrification and ANAMMOX process. The COD removal efficiency was observed to be $81 \pm 3\%$ and $86 \pm 4\%$, respectively for R-1 and R-2. The ammonium (NH_4^+) and total kjeldahl nitrogen (TKN) removal efficiency were found to be around 88% and 92% for R-2, which were almost two times higher than R-1 (46% and 50%, respectively) conforming hypothesis of introducing HEM with ANAMMOX bacteria for treating nitrogen rich fish processing wastewater with superlative efficacy compared to the existing treatment systems for real-life futuristic applications.

8:45 AM BI01.07.03

A Direct Z-Scheme Enhanced Photocatalytic CO_2 Reduction Over g- C_3N_4 Under Visible Light by Coupling of FeWO_4 [Reshma Bhosale](#)¹, Sharsti Jain¹, Santosh Kumar² and Satishchandra Ogale¹; ¹Indian Institute of Science Education and Research Pune, Pune, India; ²University of Bath, Bath, United Kingdom.

With increase in the energy demand and thereby the increased consumption of fossil fuels huge amount of anthropogenic CO_2 is released into the atmosphere leading to green-house effect and global warming. One approach which is being actively pursued to address this problem is CO_2 reduction to value added fuels using solar energy which is abundantly available. Many semiconductor materials are investigated for photocatalytic CO_2 conversion. Among them, a new and novel organic photocatalyst, namely graphitic carbon nitride (g- C_3N_4) has emerged as a sustainable, cost effective and environmental friendly semiconductor. It is a promising candidate which absorbs in the visible region (band gap of 2.7-2.8eV) and has favorable band alignment. Nevertheless, the photocatalytic efficiency is still moderate due to rapid recombination of photogenerated carriers before they could participate in surface reactions. Therefore, coupling of C_3N_4 with other semiconductor has proved to be an effective pathway to promote the activity through the spatial separation of excited electrons and holes across the interface.

In the present work, we introduce a new visible light photocatalyst material FeWO_4 (band gap 1.8-2.5eV) which belongs to the fascinating family of wolframite type system with monoclinic structure. To the best of our knowledge, FeWO_4 has not yet been investigated in the field of photocatalysis. In our work FeWO_4 was synthetically coupled with g- C_3N_4 by wet chemical method. The obtained composite exhibited direct Z scheme mechanism due to appropriate band matching of FeWO_4 with respect to C_3N_4 band edges as confirmed by Mott-Schottky plots and Diffuse Reflectance Spectroscopy. Such a Z-scheme without any mediator is a highly beneficial system in the photocatalysis context, as the electrons with high reduction ability in photosystem PS-I and holes with high oxidizing ability in PS-II are preserved and subsequently utilized for respective surface reactions. Therefore, the composite of FeWO_4 with g- C_3N_4 showed an impressive yield of 30 $\mu\text{mol/g}$ of CO , representing a six-fold increment in photocatalytic CO_2 reduction as compared to pristine C_3N_4 . Also, the composite was observed to be stable for CO evolution till 18 hours over which it was tested.

9:00 AM BI01.07.04

Direct Solar Desalination Using Nano/Micro-Porous Polymeric Membrane via Thin-Film Evaporation [Mona B. Bahman](#), Arwa A. Alshareif and Faisal Almarzooqi; Khalifa University, Abu Dhabi, Alabama, United States.

Evaporation from micro/nano structures is a ubiquitous phenomenon which plays an important role in nature and industrial applications, such as transpiration in plants, mammalian perspiration, electronic cooling and water desalination. Thin film evaporation from nanoporous membranes is a

promising thermal desalination approach because it utilizes the passive capillary pumping of liquid to the evaporating interface and allows for high heat transfer rates due to the large evaporating area in addition to the capillary pumping driving force. In this study, solar energy was used as a heat source to evaporate seawater through in-house fabricated polyvinylidene fluoride (PVDF) nano/micro-porous membranes. Compromising between the available area for evaporation via changing pore size and the available material for conductive transfer of heat to the liquid thin film is complicated. Since more porous membrane increases the evaporation surface area and at the same time this leads to having less conductive material for heat transfer which at the end will reduce the evaporation rate. The main objectives of this study are, firstly to investigate the pore size effect on the vapor flux by fabricating flat-sheet membranes via a phase inversion process with 12 wt% of PVDF and 500 µm thickness, and varying preparation parameters such as relative humidity and exposure time to achieve different pore sizes. Secondly to examine the thermal conductivity effect by blending different concentrations of fumed silica (1, 2, 3, 4, or 5 wt%) with the polymeric solution. The fabricated membranes were characterized by scanning electron microscopy (SEM), contact angle analyzer (CA), Fourier transform infrared spectroscopy (FTIR), capillary flow porometry (CFP), porosity and AFM, to further understand the observed thin film evaporation effects. The preliminary results showed, the mean flow pore diameter of the fabricated membranes are 117.2 nm, 123.3 nm and 206.6 nm and their porosity 28.4 %, 46% and 33% respectively. Also, the contact angle analyzer proved the hydrophobicity of these fabricated membranes since the contact angle was found to be above 95°.

Furthermore, this study is aiming to show that the polymeric membrane can be implemented as an alternative effective material in thin film evaporation applications with lower cost compared to commercial ceramic alumina anodiscs (AAO).

9:15 AM BI01.07.05

Development of Solar Absorbing Nanoporous Membranes for Direct Solar Seawater Desalination [Arwa A. Alsharief¹](#), Mona B. Bahman¹, Faisal Almarzooqi¹ and Evelyn N. Wang²; ¹Khalifa University, Abu Dhabi, United Arab Emirates; ²Massachusetts Institute of Technology, Boston, Massachusetts, United States.

In nature solar energy is the primary driving force for the formation of fresh water. Solar based desalination is an attractive technology to meet the ever-increasing water demand.

In this study we develop efficient and optimized nanoporous membranes for direct solar desalination of seawater. We developed black-body like membranes that maximize solar absorption via the structural design and coating. The structural design involves hierarchical shapes that increase roughness and hence forth increase surface area available for solar energy absorption. This is done via simple and low-cost phase inversion membrane fabrication, developed within our labs. The blackbody-like membranes we develop should pose high thermal conductivity, which is the other objective we focus on in this investigation.

To fabricate our envisioned solar absorbing membranes, we developed two distinct approaches, 1) flat-sheet membranes via phase inversion and 2) chemical vapor deposition. In the first, we use polyvinylidene fluoride as the active membrane material. We modified it to incorporate micro/nano particles which are known to have high surface area and good optical and thermal properties. These are graphene nanoplatelets and activated carbon. In the second, we use Anodised Aluminium Oxide (AAO) membranes as the base material and grown high absorbance blackbody like multilayered 3-dimensional graphene coating.

The absorbance of each membrane was measured using a UV(vis) spectrometer. The structures of the prepared membranes were characterized and observed by scanning electron microscopy (SEM) and Atomic Force Microscopy (AFM). The Meanflow Pore Size (MPS), Bubble Point Pore Size (BP) and Pore Size Distribution (PSD) were measured using a capillary flow porometer. Also, the porosity was calculated experimentally using a gravimetric method. Contact angle measurements were also performed to find out the hydrophobic/hydrophilic nature of the membranes.

All membranes are tested in a device fabricated specifically for the purpose of this study. The membranes are tested for their ability to evaporate seawater using direct sun light. Measurements of mass fluxes and temperatures are taken, and the overall efficiency of the device is calculated. This study aims at demonstrating these solar absorbing membranes as the core enablers for future direct solar desalination technologies.

The absorbance of the graphene coated AAO was measured using a UV(vis) spectrometer and was found to be 97%. The fabricated membrane with activated carbon (3.5,7g) were characterized and measured the porosity and were obtained to be 35.9%, 65.3%, and 56.8%. The MPS was measured at around 5.61, 6.95, and 2.88 µm for 3, 5 and 7g of activated carbon and also The BP was measured 14.72, 20.83 and 14.61 µm respectively. The complete set of results will be included in the full submission.

9:30 AM BI01.07.06

Application of Ion Exchange Membranes in Enhancing Algal Production Alongside Desalination of Saline Water in Microbial Fuel Cell [Neethu B. Pankaj Sarkar](#) and Makarand M Ghangrekar; Indian Institute of Technology Kharagpur, Kharagpur, India.

In the present world scenario where water scarcity around the world coincides with fresh water consumption, there is an increasing demand for a technology that can provide clean water. Microbial fuel cells (MFCs) can be used to treat wastewater along with generation of bioenergy in the form of electricity using microorganisms and natural biological processes. The demand for fresh water and clean energy is driving the need for converting an MFC into an algal-based Microbial desalination cell (MDC) that can support algal growth in addition to desalination of saline water. Ion exchange membranes (IEMs) are most commonly used for desalination of saline water and is a promising tool which, when oriented properly, can be applied in the MDC for algal production. In this study, a five-chambered MDC was designed by placing an alternating series of cation exchange membranes and anion exchange membranes between an anodic compartment (Synthetic wastewater) and cathodic compartment (*Chlorella Pyrenoidosa*). The middle compartment, either side of which constituted concentrated chamber, was fed with saline water with two different TDS concentrations, namely 2.5 g/L and 5.0 g/L. Algal-based MDC was analyzed for wastewater treatment efficiency, desalinating capacity, power generating efficiency and algal production and overall performance was compared with MDC without algae in catholyte. A maximum operating voltage of 125 mV was produced during the operation of algal-based MDC with TDS of 5 g/L in the middle chamber against 96 mV for TDS of 2.5 g/L due to change in internal resistance. Similarly, a better performance in terms of electricity generation and TDS removal was observed in MDC assisted with the algal cathode as compared to the one without algae in catholyte. The algal-based MDC with 5 g/L TDS in middle chamber exhibited the best results among all other combinations giving a maximum power density of 45.52 mW/m² and a desalination rate of 71 ± 2 %. The five-chamber MDC also demonstrated effective algal growth in the cathodic chamber and simultaneous TDS removal in desalination chamber along with energy recovery using photosynthetic oxygen, produced by microalgae, as the cathodic electron acceptor. Based on this experimental performance evaluation, it can be inferred that algal-based MDC can provide a promising and sustainable approach for wastewater treatment with the capability of simultaneous desalination, algal production, and electrical energy recovery.

9:45 AM BREAK

Wednesday Morning, November 28, 2018
Sheraton, 3rd Floor, Hampton

10:15 AM *BI01.08.01

Red Mud-Fly Ash-Based Geopolymer as an Alternative Construction Material Zhaotong Yang and Jianyu Liang; Worcester Polytechnic Institute, Worcester, Massachusetts, United States.

Today, the concrete industry is one of the largest producers of greenhouse gases, emitting 5% of the man-made CO₂ every year. To reduce this carbon footprint, geopolymers have attracted extensive interest as potential alternatives to Portland cement (OPC) the material traditionally used in structural concrete. Depending on the synthesis recipe of the geopolymer, the manufacturing process may be much less energy intensive and have a very small carbon footprint when compared with the OPC production process. Many different raw materials have been used to synthesize geopolymers, such as various natural minerals and industrial byproducts that are high in both amorphous silica (SiO₂) and alumina (Al₂O₃). A new synthesis method for geopolymer, sourced from two hazardous industrial wastes, red mud (RM) slurry and fly ash (FA) powder, has been developed in this study. Thermal properties including mechanical behavior, thermal shrinkage, weight loss, microstructure change, and crystallization of the RMFA geopolymers were investigated. After curing for fourteen days, RMFA geopolymers exhibited compressive strengths greater than 17MPa. Reaching this strength is significant, since the ACI (American Concrete Institute) building standards require a minimum of 17MPa for use in structural cement. It should also be noted that in geopolymer materials, as with OPC, the strength continues to increase over time. Thermal tests found the materials to be thermally stable up to 600°C, with the retention of mechanical strength. The synthesis process developed in this study provides significant advantages: the removal of the energy-intensive drying process and the repurposing of two overabundant industrial wastes.

10:45 AM BI01.08.02

A Novel Fire Retardant Solution to Mitigate the Onset of Wildfires Yuan Xue¹, Xianghao Zuo¹, Joshua Vilkas², Pik Hoi Lam³, Nicole Jacobsen⁴ and Miriam Rafailovich¹; ¹Stony Brook University, Stony Brook, New York, United States; ²Hebrew Academy of Nassau County High School, Uniondale, New York, United States; ³Wilson Area High School, Easton, Pennsylvania, United States; ⁴Plainedge High School, Massapequa, New York, United States.

The dangers of wildfires are brought to attention as they frequently ravage wooded areas like California and Greece. The current resolution is reactive rather than preventive, and involves dropping chemicals after the start and expansion of the fire. Additional concerns include the application of non-eco-friendly ingredients to quench the fires. The goal of this research is to engineer aqueous solutions that are sprayed onto leaves prior to the onset of fires to inhibit fires from spreading uncontrollably. Here we describe the results of a formulation that was used on the leaf species, *Cornus kousa*, a subspecies of the *Cornus*, or Dogwood family.

The experiments were conducted on three categories: fresh picked leaves, oven-dried leaves, and naturally fallen leaves. FTIR analysis of the leaves indicated that fresh leaves consisted of water (2/3 of the mass) while the dried leaves were predominantly of cellulose. Fresh leaves were coated with a thick waxy layer, while the drying process removed some of the surface wax. Different solutions were first formulated where contact angle goniometry was used to optimize the wetting properties for both dry and fresh leaves and viscometer was used to determine the optimal viscosity for spray applications. The solutions were then applied by spraying onto fresh leaves and piles of dried leaves. Burning tests were performed both on leaf piles, and individual leaves, using a propane torch. The flame was applied continuously for five seconds and then removed, and the time to self-extinguish was recorded together with the extend of the spread of the fire.

Results indicated that for fresh leaves, in the absence of the spray, the fire persisted till at least ¼ of the mass was consumed and for the dried leaves the entire mass was consumed before the fire was removed. With the addition of the spray, the fire self-extinguished immediately after the flame was removed, and the fire during the application of the flame consumed less than 25% of the mass. Similar results were obtained for both wet and dry leaves. FTIR and RAMAN spectroscopy was performed at each stage in the testing in order to determine the underlying mechanism leading to the flame retardant properties.

The toxicology of the solution and the individual components is being tested on grass and vegetable plants. Preliminary data, thus far, had not found any significant differences in root size or germination rate between the control plants culture and those watered with the undiluted solutions. The results of ongoing experiments regarding sequestration of the chemicals in the leaves and fruits will be presented.

11:00 AM BI01.08.03

3D Printing for a Sustainable Approach to Constructions Marco Stefancich¹, Berry Hendriks², Alessandro Zampieri¹ and Wadhah Alzhami¹; ¹Dubai Electricity and Water Authority, Dubai, United Arab Emirates; ²Cybe Constructions, Oss, Netherlands.

While 3D printing is having a large impact on many industrial sectors, its contribution in the constructions sector is still in its infancy. Construction is one of the bigger contributors to green-house gases and, thus, an increase in the efficiency of this process can have a significant societal and environmental impact.

However, dimensional scale factors, optimal printer and nozzle configurations, and, most importantly, the properties of the printable materials (e.g. cement) are still open questions ripe for developments and active research.

Moreover, societal acceptance of a completely novel concept for constructions, where delivery times and construction methodology are substantially different from a model that was substantially unchanged in the last several hundreds of years, is still uncertain.

From a technological point of view, the cement commonly used in construction has long setting times and rheological characteristics that make the direct 3D printing process complex. The use of specialty additives allows tweaking the relevant parameters, but the extrusion process of materials with paste-like rheology and the achievement of structural performances compatible with large scale buildings had been elusive for several years.

Harsh climatic conditions and the preference to print directly on site make things even more complicated due to the variability of environmental conditions affecting the material properties. The lack of established standards, due to the novelty of the approach, adds to the uncertainty level. However, the combination of novel materials combined with specific printing technology, opens the way to fascinating scenarios in a traditionally conservative sector.

From the social acceptance point of view, the revolutionary short building times, the strict adherence of the final product to the initial design and the substantial reduction of the construction crew are all aspects that need to be tested on the final clients.

We report here on the first example of a 100+ m² building for civil use, with complete regulatory authorities' certifications, successfully 3Dprinted *in situ*, in a total of 43 hours, in the harsh desert climate of the United Arab Emirates. The achieved structural properties, in relation with building code requirements and with overall building acceptance by its final users, are presented together with a discussion on the building technology and its overall capabilities to develop new structural concepts.

The potentials for use of different, non-cement based, materials for buildings with enhanced performances and reduced environmental impact (e.g. adobe) and the associated materials, technology and societal related challenges will, finally, be explored.

11:15 AM BI01.08.04

Closed-Loop Plastics Enabled by Reversible Polymer Chemistries [Brett A. Helms](#); Lawrence Berkeley National Lab, Berkeley, California, United States.

Networked polymeric materials that incorporate dynamic covalent bonds exhibit useful, reconfigurable character. Here I will describe our recent efforts in understanding and controlling the fundamental physiochemical aspects of such dynamic bonds, with a particular focus on new "clickable" dynamic covalent bonding motifs. Our polymer networks overcome many of the challenges in the field, particularly regarding activation barriers to bond exchange, accessible glass transition temperatures, and conditions required for chemical reprocessing (e.g., de-polymerization). Our work suggests that we are only at the beginning of a revolution in closed-loop polymers designed for both high performance, durability, and sustainability.

SESSION BI01.09: Sustainability in Biomedical and Environmental

Session Chairs: Margrit Hanbücken and Geoffrey Strouse

Wednesday Afternoon, November 28, 2018

Sheraton, 3rd Floor, Hampton

1:30 PM *BI01.09.01

Quantum Phenomena—Get Energized, Get Entangled [Andreas Holzenburg](#)¹ and Lisa Perez²; ¹Biomedical Sciences, School of Medicine, UTRGV, Harlingen, Texas, United States; ²Chemistry, Texas A&M University, College Station, Texas, United States.

Quantum phenomena are intrinsic to many living systems. A number of these phenomena will be explained conceptually including the biggest quantum machine in humans: the brain. The talk will allude to (i) brain hemispheres and their synchronization, (ii) entangled brain waves and related health benefits, (iii) the differentiation between the conscious and unconscious mind and its impact on self-transformation and well-being, (iv) the synchronous and asynchronous firing of neurons and how this relates to everyday problems as well as (v) pre-sentiment responses across the scales. Another fine example is the highly efficient quantum coherence-enabled energy-transfer processes employed by photosynthetic organisms. With regards to the latter, checking the truth of the underlying principles is challenging as the experimental measurements employed may perturb a quantum system into a classical one. This has been a concern with 2DES experiments employing ultrashort broadband laser pulses when probing the quantum processes of photosynthesis. Here we uncover the foundations of photosynthetic energy transfer as a role model for other biological quantum systems using an approach that extends experimental data into those realms where the use of a non-perturbing approach is critically required. To this end, this project uses quantum chemical calculations to three-dimensionally map the patterns of quantum and non-quantum effects observed in the highly effective energy transfer process of photosynthesis. Combining X-ray and electron tomographic data into an atomistic model as a starting point, we project to unravel the energy transfer patterns within the confinement of a single PSII component (intra-subunit) and then across the subunit boundaries (inter-subunit) to cover the entire complex. **Intra-subunit:** Investigations thus far have focused on UV-Vis spectra calculations to investigate the level of communication between chlorophyll chromophores in the LHCII subunit and the well-known strongly coupled special Chla/Chla pair (P680) in the D1/D2 subunit. **Inter-subunit:** This work will start with a refined all atom model fitted to an *in situ* tomographic data set. Based on the intra-subunit energy pathway peripheral chromophores delineating individual subunit-subunit contacts will be FRET-correlated to elucidate the most likely energy bridges between the two subunits in question. Eventually the full dielectric patterns of the energy transfer pathway between all PSII core and antennae components will be determined inching through the entire complex from one chromophore couple to the next.

Basing the analysis of energy transfer on a biological macromolecular complex, means any conclusions drawn are *a priori* based on a system derived from earth-abundant elements thus making this approach particularly attractive for next generation technologies such as quantum computing, organic photovoltaics or artificial intelligence.

2:00 PM BI01.09.02

Carbon Quantum Dots Deposited Chemically Modified β Cyclodextrin Based Biocompatible Thermoresponsive Composite Hydrogel for Transdermal Drug Delivery [Arpita Roy](#)^{1,2}, Sagar Pal¹ and Santanu Dhara¹; ¹Applied Chemistry, IIT (ISM), Dhanbad, Dhanbad, India; ²School of Medical Science and Technology, IIT Kharagpur, Jharkhand, India.

In this study, we have developed a novel thermoresponsive composite hydrogel material (cl β -CD/pVCL/CQDs) by free radical mechanism and *ex-situ* deposition of carbon quantum dots (CQDs) on chemically crosslinked β cyclodextrin polymeric network (*poly(N-vinyl caprolactam)* (pVCL) crosslinked with β cyclodextrin (cl β -CD/pVCL) in presence of crosslinker diethylene glycol dimethacrylate (DEGDMA)}. Here in also, we have explored the effect of carbon dots deposited polymeric matrix on transdermal drug delivery. The morphological assessment of synthesized hydrogel (cl β -CD/pVCL) has been assessed using FESEM analysis. The composite hydrogel (cl β -CD/pVCL/CQDs) have been characterized also by HR-TEM analysis which confirms the successful deposition of carbon quantum dots on hydrogel surface. Successful deposition of CQDs on the hydrogel surface has also been authenticated by XRD, UV-Vis and photoluminescence spectral analyses. Chemical and physical properties of crosslinked hydrogel and the nanocomposite hydrogel materials have been characterized using FTIR, ¹H NMR and ¹³C NMR spectral analyses. The gelling nature and thermoresponsive swelling nature of both cl β -CD/pVCL hydrogel and cl β -CD/pVCL/CQDs composite hydrogel have been confirmed by temperature dependent rheological and swelling characteristics respectively. Developed cl β -CD/pVCL/CQDs composite hydrogel has LCST at 33 °C which has been confirmed by measurement of % transmittance with respect to gradual increase (1 °C increase) in temperature. The biocompatible nature of the developed composite hydrogel has been confirmed by MTT assay and live dead assay using MG 63 cells. The *in-vitro* release of model drug gentamicin sulfate from composite hydrogel showed that the fabricated composite hydrogel releases the transdermal drug in a sustained way.

2:15 PM BI01.09.03

Direct Conversion of Shrimp Shells to the Antibacterial Chitin/Zn Composite with Deep Eutectic Solvent Aqueous Solution [Xingmei Lu](#)^{1,2}, Mi Feng^{1,2}, Jie Zhang¹ and Suojiang Zhang^{1,2}; ¹Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China; ²University of Chinese Academy of Sciences, Beijing, China.

With the development of marine fishery, the amount of waste shrimp shells has been grown tremendously leading to serious environment pollution and resource waste. Converting the waste shrimp shells to the value-added products is a meaningful way to solve the problems. Among the products, the chitin-based material has been attracted wide attention due to its biodegradability, non-toxicity, and physiological inertness [1]. However, the traditional method of preparing chitin-based material from shrimp shells needs acid and alkali repeated treatment and additional modification step [2]. It is meaningful to develop a green and simple strategy of chitin-based material synthesis from shrimp shells.

Herein, we report a green and simple method to prepare chitin/Zn composite using deep eutectic solvent (DES) aqueous solution. The used DES aqueous solution involved three functions, namely decalcification, deproteinization and Zn-loading. Under the optimal conditions, the chitin/Zn composite material with 34.6 wt% zinc, 0.2 wt% calcium carbonate and 2.5 wt% protein was obtained, which presented antibacterial effect against Gram-negative bacteria *Escherichia Coli* and Gram-positive bacteria *Bacillus subtilis* at certain bacterial concentration. The reason for calcium removal and zinc loading may be ion exchange and investigated by experiments with metal salt aqueous solution. Protein removal was ascribed to aggregation proved by particle size analysis and morphology observation.

Acknowledgments

This work was supported financially by National Natural Scientific Fund of China (No.21476234, No.21506231).

Reference

- [1] P. T. Wansapura, R. S. Dassanayake, A. Hamood, P. Tran, H. Moussa and N. Abidi, *Journal of Applied Polymer Science*, 2017, 134, 44904 (1-10).
- [2] P. T. S. Kumar, V.-K. Lakshmanan, R. Biswas, S. V. Nair and R. Jayakumar, *Journal of Biomedical Nanotechnology*, 2012, 8, 891-900.

2:30 PM BREAK

3:30 PM BI01.09.04

Sustainable Synthesis of Monodisperse Starch-Based Magnetic Polymer Beads Through Molecular Rearrangement of Glucans from Natural Starch Ke Luo, Ki-Baek Jeong, Sang Mook You and Young-Rok Kim; Kyung Hee University, Yongin, Korea (the Republic of).

Magnetic polymer beads (MPBs) have attracted extensive attention due to their excellent properties of instant action and contactless control driven by the external magnetic field. With combination of inherent features of magnetic particles and polymer, MPBs are used for various biological applications, such as immunomagnetic separation, which is a powerful and widely used technique in bioassay through the selective concentration and isolation of the biological and chemical target molecules from some complex and heterogeneous matrices. However, the conventional methods for synthesis of MPBs are still facing substantial challenges, such as potential toxicity, complicated process, and high energy consumption, which limit their applications and large-scale production. Short-chain glucan (SCG), a linear homopolymer of glucose linked with α -(1,4) glycosidic bonds, could be a promising polymer for synthesis of MPBs due not only to its abundance, renewable nature, low cost, and biodegradability, but also to its intrinsic properties of crystallization and self-association in aqueous solutions without need of energy consumption. Herein, we report a fairly simple and environmental friendly approach for the fabrication of starch-based magnetic polymer beads (SMPBs) with uniform shape and size through rearrangement of SCG produced by enzymatic debranching of waxy maize starch. The paramagnetic materials, dextran-coated iron oxide nanoparticles (Dex@IONPs), were readily incorporated into the starch microstructure and rendered a superparamagnetic property to the SMPBs. The morphology and size of resulting SMPBs turned out to be modulated by Dex@IONPs in concentration dependent manner, of which Dex@IONPs was assumed to be acting as a seed inducing the epitaxial crystallization of SCG and further transforming it into homogeneous microparticles. The surface of SMPBs was readily functionalized with antibody through one step reaction using a linker protein. The immuno-SMPBs showed great capture efficiency and specificity (>90%) to target bacteria. Furthermore, the captured bacteria along with antibody and linker protein were effectively eluted from the surface of SMPBs by free maltose, indicating the excellent recyclability of SMPBs, making this new material suitable for various chromatographic applications. The biocompatible nature of this materials would also be advantageous for its potential applications in diagnostics and delivery of drugs or physiologically active compounds to a target sites.

3:45 PM BI01.09.05

Green Synthesis of Amine-Functionalized Starch Magnetic Beads and Its Application as Recyclable and Rapid Efficient Removal of Bacterial Pathogens in Drinking Water Sang Mook You, Young-Rok Kim and Ke Luo; Kyunghee University, Yongin, Korea (the Republic of).

Microbial contamination of drinking water is still a cause of major outbreaks of diarrheal diseases and deaths, particularly in developing countries. Polymeric magnetic particles (PMPs) are promising materials for removal of bacterial pathogens from drinking water because of their intrinsic permanent magnetic properties. Nevertheless, current methods for their synthesis generally require complicated procedures and large energy consumption, which unfavorably hinder their practical implementation of bacterial removal from drinking water. In addition, functionalization of PMPs using recognition elements, such as antibodies, aptamers, and phages, is not suitable for this purpose, since most of contaminated drinking water environments are polymicrobial. In this study, we report a fairly simple and low-cost approach for the fabrication of starch magnetic microparticles (SMMPs) through spontaneous rearrangement of short-chain glucan (SCG) produced by enzymatic debranching of waxy maize starch. The surface of SMMPs was readily functionalized with poly-L-lysine through hydrogen-bonding interaction. The poly-L-lysine-coated SMMPs (PLL@SMMPs) showed great capture efficiency (>90%) for bacteria in water regardless of gram-positive and gram-negative under slightly acidic conditions (pH 5-6). Furthermore, we found that the surface charge of Gram-negative bacteria varied depending upon the length of lipopolysaccharide (LPS) O-side chains since the phosphate groups are mostly located in the inner core of LPS. Upon the presence of LPS, PLL@SMMPs showed greater capture efficiency for Gram-positive bacteria compared to that of Gram-negative bacteria at the same pH-level. More importantly, the captured bacteria were effectively eluted from the surface of PLL@SMMPs by aqueous ammonia solution along with recycling use, making them promising candidates for practical implementation not only for rapid capturing and removal of bacterial pathogens from drinking water but also for the sample preparation giving aid to bacterial detection and identification.

4:00 PM BI01.09.06

Spectroanalytical and Microstructural Investigation for Arsenic Removal from Water Media by Modified Ceramic Filter Membranes (Mo-CFM) for Household Water Treatment Application Amrita Kaurwar¹, Manoj K. Tiwari², Ajay Khooha², Ajit Kumar Singh², Abhineet Nighojkar³ and Anand K. Plappally¹; ¹Indian Institute of Technology Jodhpur, Jodhpur, India; ²Raja Ramanna Centre for Advance Technology, Indore, India; ³Shri Govindram Seksaria Institute of Technology and Science, Indore, India.

This study aims to evaluate the effect of modified ceramic filter composition in removing As (V) ions from water media. The filter composition was modified through the addition of low-cost iron-rich waste powder into the local clay-saw dust mixed ceramic matrix. The modified ceramic filters (Mo-CFM) membranes were manufactured with dimensions of 10 cm by 10 cm and 1.5 cm thickness. The membrane fabrication involved mixing of local clay

with an equal volume fraction of sawdust and 5% volume fraction of iron-rich waste. The raw materials and modified ceramic membranes were characterized using Energy dispersive X-ray fluorescence (EDXRF) and scanning electron microscopy. The arsenic solution was prepared in the laboratory and filtered through the modified ceramic units. The effect of prominent parameters like – pH, initial pressure head and arsenic concentration on their arsenic removal efficiency by Mo-CFM was examined. The concentration of arsenic before and after filtration process was assessed using Atomic absorption spectroscopy. The spectroanalytical results displayed high removal efficiency up to 99% for the As (V) ions. The ED-XRF and SEM images of ceramic membranes after the filtration process showed the presence of arsenic adsorption on the porous surface of the modified ceramic membrane (Mo-CFM).

4:15 PM BI01.09.07

Detection of Cd Ions Using an Ion-Selective Field Effect Transistor with a Chalcogen-Doped Gate Oxide for Water Quality Monitoring Priya Vinayak¹, Sushma Yadav², Ajeet Singh¹, Soumen Saha¹, Henam Sylvia Devi¹, Sameer Sapra¹, Madhusudan Singh¹ and Bhaskar Mitra¹; ¹Indian Institute of Technology Delhi, New Delhi, India; ²Institut für Physikalische Chemie und Elektrochemie, Leibniz University, Hannover, Germany.

The American Cancer Society lists cadmium and its compounds as group 1 carcinogens in humans as exposure to these species through food, water, and the air is known to increase the lifetime risk of cancer. In this work, we report a field-effect transistor (FET) based electrolyte insulator semiconductor (EIS) sensor with a CdSe doped silica gel used as the sensing membrane. The EIS structure has a metallic layer as the back contact and the sensing membrane as the top layer with a pseudo-reference platinum electrode as top contact. The electrolyte consists of spiked cadmium acetate solutions and 0.1M KNO₃. The back contact (150 nm Al) was first deposited, with a Cr/Au(10nm/50nm) capping layer using thermal evaporation at 4.2 x 10⁻⁶ Torr, followed by a rapid thermal annealing step at 450°C. Silica gel synthesis was carried out using hydrolysis and condensation of tetraethylorthosilicate in ethanol, distilled water, and HCl. Thin film X-ray diffraction (XRD) measurements on spin-coated silica gel revealed amorphous silica sol-gel formation. CdSe nanoparticles (~3.4nm) with photoluminescence (PL) and absorbance peaks at 570nm and 562nm, respectively, were mixed with the silica sol to form a stable ink. This ink was spin-coated over a silicon wafer with 100 nm of thermal oxide. Capacitance-voltage (CV) measurements were carried out using an AC voltage of 50mV superposed on a DC voltage ramp in the range -1.5V to +1.5V at the 100 kHz. The CV curve was detected in current mode with the Stanford Research SR830 lock-in amplifier (gain = 1M Ohm). Threshold voltage shifts (ΔV_T) were extracted from the CV curve was monitored as a function of varying Cd concentration (1M to 10⁻⁷M) in solution. The relationship between the shift and the concentration is linear down to the detection limit of 1 ppm in this initial study, which establishes this baseline FET-based platform for real-time detection of Cd ions in the environment in a low-cost and sustainable manner.

4:30 PM FINAL SYMPOSIUM CONCLUSIONS AND PERSPECTIVES