# NANOINFORMATICS 2010 Poster Session Abstracts

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### 1. The Center for Environmental Implications of Nanotechnology (UC-CEIN)

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The goal of the University of California Center for Environmental Implications of Nanotechnology (UC CEIN) is to develop a paradigm for predictive toxicology and risk ranking premised on nanomaterial property-activity relationships, fate and transport analysis, exposure implications, as well as biological injury at molecular, cellular, organismal, and ecosystems levels. The integrated and multidisciplinary research effort, assisted by various modeling efforts, will help to establish functional decision tools regarding the design and safe implementation of nanotechnology. UC CEIN has successfully integrated the expertise of engineers, chemists, colloid and material scientists, ecologists, marine biologists, cell biologists, bacteriologists, toxicologists, computer scientists, and social scientists to create the scientific platform to identify possible hazards and guide the safe design of nanomaterials (NMs). Noteworthy accomplishments of the UC CEIN include (i) the development of a combinatorial library of nanomaterials (metal oxides, SWCNT, metals, clays) that includes 60 variants of nanoparticles in various stages of characterization and introduction into environmental relevant systems; (iii) modeling of nanoparticle aggregation; (iv) development of an architecture for nanoparticle data management, analysis and modeling; and (v) studies on nanotechnology risk perception.

### 2. Interactive Taxonomy for Content Exploration and Discovery

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Interactive taxonomic functionality enables visitors to explore relationships between concepts and access content within the nanomanufacturing domain.

InterNano is an information portal and subject repository for nanomanufacturing hosted by the National Nanomanufacturing Network at the University of Massachusetts Amherst, which combines a dynamic open source content management system (Joomla!) for managing original content with the reliable EPrints repository software system for managing archived publications, educational material, and workshop presentations. Because nanomanufacturing is a small, interdisciplinary subdomain of nanotechnology, an important component of the project is a specialized taxonomy for domain definition and information discovery.

The InterNano Taxonomy is a unique, custom-built terminology to describe the nanomanufacturing



enterprise—from areas of application to nanomanufacturing processes—with three levels of granularity. The Taxonomy is fully integrated into the InterNano system, linking all tagged content both in Joomla! and in EPrints. By browsing the taxonomy either through a hierarchical list or through a tag cloud, visitors can review and access all of the tagged content within the InterNano portal and repository.

InterNano has expanded its taxonomic functionality to enable a more interactive user experience. Spring graphs display Taxonomy terms with respect to their relationship to other taxonomy terms via content tagging and reflect terms' relative usage statistics. The spring graphs are generated with open source libraries for Python: matplotlib and NetworkX. This capability allows users to explore the different concepts within the nanomanufacturing domain as well as review and access tagged content throughout the integrated InterNano system.

### 3. INFONANOSAFE: A Web Resource for Knowledge Integration in the Field of Nanosafety

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The Medical NanoBioInformatics Department of the Institute of Health Carlos III, as part of its contribution to the NanoSost Project [1], has designed and implemented a web portal, INFONANOSAFE, that aims to collect incoming knowledge about nanotechnology safety issues and to offer it through



Internet, so becoming a reference resource in these matters for the spanish speaking community.

INFONANOSAFE website is based on Drupal CMS [2] and implements some of the cutting edge web design trends and techniques as faceted browsing, taxonomy tagging, URL rewrite, XML sitemaps and Search Engine Optimization, among others, to improve user navigation experience and search features, reducing the time to retrieve relevant data.

INFONANOSAFE categorizes the information into three axis:

• News related with the area of nanosafety and the

process of characterization of nanomaterials;

- Guides designed to provide information on how to handle nanoparticles and nanomaterials, as well as their manufacturing and destruction, in order to facilitate the work of researchers and engineers;
- Catalogue of best-practices, that refers to successful experiences that can be shared in a concrete context or industrial domain.

Four lexicons, that we call facets, have been defined to be associated with documents enabling the use of advanced techniques for content retrieving and a simple and quick access to the stored documents.

a) Nanomaterial: This facet maps the family of nanoelements or nanocompounds referred by the documents. It is based on Tomalia's framework reference for classifying nanomatter [3], that could catch sight of a future nanoperiodic system and therefore predict functional properties including toxicology aspects.

- b) Potential risk: Based on European directive 67/548/EEC, this facet describes potential hazards caused by nanomaterial handling (corrosive, explosive, inflammable, toxic, irritant, etc...). In order to use a more suitable classification within the field of nanoscience, it is going to be replaced by GHS—Globally Harmonized System of Classification and Labeling of Chemicals.
- c) Risk management: It refers to the two most important issues that address nanosecurity—risk assessment to identify potential threats (threatened groups, measurement equipment, exposure threshold, measurement procedures, and health observation) and risk management to learn how to manage risks and to avoid its harmful consequences (engineering control, personal protection equipment, training, communication and information, organization, collective protection).
- d) Economic sector: To highlight the main economic sector for which the information is relevant.

To achieve a secure development of nanotechnology it is necessary to take action in order to identify potential threats, learn to manage them, and avoid potentially harmful consequences. INFONANOSAFE will offer the user a broad spectrum of high-quality, evidence-based nanotechnology safety information accessible to the public, industry, health providers, and policy-makers.

References
[1] Balas, F et al., Nanosost: towards a sustainable, responsible and safe nanotechnology.
NanoSpain2009 Zaragoza-Spain.
[2] http://drupal.org/
[3] Tomalia, Donald A. In quest of a systematic framework for unifying and defining nanoscience. Journal of Nanoparticle Research, (2009) 11 (6):1251-1310.

### 4. Insitu Growth of Multiwalled Carbon Nanotube on Alumina Matrix as Reinforcing Agent by

### **Ethylene CCVD Method Using Fe as Catalyst**

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We report the *in situ* growth of multiwall carbon nanotubes (MWCNT) by catalytic chemical vapor deposition (CCVD) using Fe nanoparticles as catalyst. Due to special characteristics of CNTs, such as high Young modulus, (~ T Pascal), good thermal and electrical conductivities, et cetera, these materials are known as the most suitable candidates for reinforcing metals, polymers, and ceramics composites. In this work, MWCNTs are used to reinforce Alumina matrix. We employed CCVD method to grow *in situ* MWCNT on bi powder Fe/Alumina mixed in Ball milling for two hours with different percentages. Ethylene was used as the feed gas and Argon as the carrier gas. Scanning electron microscope (SEM) and tunneling electron microscope (TEM) as well as X-ray Diffraction (XRD) and Raman spectrometer were used to characterize the synthesized nanocomposite. Results show that with an increasing percentage of Fe in the mixed powder Fe/Al, the amount of CNT in the composites increases, and the distribution of CNT in the composites improve. We also find that increasing percentage of Fe leaves more impurity particles in the composite which needs to applying various purification procedures on the synthesized composite.

**5. INSCX™ Exchange: Delivering a Commercial Framework for Nanomaterials** Charles McGovern INSCX Exchange, United Kingdom INSCX is a patent-pending commodity exchange trading platform devoted to the trading of a wide range of nanomaterials to be launched in Europe and the United States during 2010 with global rollout to include Asia earmarked 2011. The Integrated Nano-Science and Commodity Exchange (INSCX exchange) will structure trade in accredited, compliant, and validated nanomaterials, ranging from basic raw materials such as carbons and metal oxides and advanced materials/composites to high-end, processed goods such as photonics and programmable matter.

INSCX is based in the United Kingdom and will have satellite operations in the United States and Asia. The aim of the exchange, which is supported by various companies, organizations from government in the United Kingdom, academia, the world of commodity trading and various fields of nanotechnology, is to be the focal point of the emerging world trade in nanomaterials providing tools to structure the organic growth of supply capacity in nanomaterials. The exchange process will act as a driver affording buy-side interest in the diverse suite of materials assurance on quality, transparency, and pricing in addition to permitting use of material hedging, a risk management tool offering certainty, enabling organisations to lock-in future price exposure in nanomaterials and therefore remain disposed to more confidently focus investment on research, development and other capital expenditure.

Hedging is a means to overcome price volatility where excessive volatility proves unmanageable for many parts of the supply chain. The problem posed by excessive price volatility causes immense problems in emerging materials markets especially where no effective hedging technique exists. For example, across many sectors such as the polymers industry, producers attempting to pass on rising prices to converters are meeting resistance as converters are typically under pressure from consumers to maintain previously agreed prices. This means converters are increasingly 'squeezed' in the middle, and supply chains, rather than the suppliers, are competing. Similar difficulties are already becoming manifest in the context of nanomaterials likely to compound in the absence of an effective means to plan the allocation of nanomaterials from source to end product. The structured allocation of these commodities remains the central purpose of INSCX exchange.

The opening of the exchange means that, for the first time, nanomaterials will be traded in the same way as basic commodities, adopting many of the practices and conventions long associated with formalized physical commodity trading, where the use of hedging techniques, price discovery, supplier trade financing, quality assurance, and adherence to official regulations are standard features. INSCX exchange means nanomaterials can now harness these commercial essentials with purchasers assured of quality and competitive prices, while suppliers will be provided a direct route to market, essential trade supports, and flexibilities designed to engender organic growth from within. In equal measure official regulation agencies can be confident that a formalized adherence to trade standards in the manufacture, use, application, and exchange of nanomaterials exists by way of the INSCX exchange process to support continued effort to safeguard societal interest.

### 6. The Knowledgebase of Nanomaterial Biological Interactions

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A risk characterization framework to classify nanomaterials based on their physical or chemical properties as well as their biological impacts is necessary to reduce the uncertainty around potential nanomaterial hazards. Structure-property relationships that can be used to predict nanomaterial

impacts in lieu of empirical data can provide significant support for the nanotech industry in developing safer nanomaterials. Knowledge on the governing principles of nanomaterial-biological interactions can more effectively be utilized once computational tools are available for data integration and consensus analysis. The Nanomaterial-Biological Interactions (NBI) knowledgebase was developed to consolidate and integrate disparate data on nanomaterial effects in model systems and provide unbiased informatics approaches to identify the relative importance of characterization parameters on biological effects. The NBI serves as an open-source data repository for nanomaterial characterization, synthesis, and biological interactions, and houses a reference dataset from embryonic zebrafish evaluations on over 200 distinct nanomaterials. Various data mining and computational tools are used to organize the existing body of data in a systematic and logical way. The goal is to identify nanomaterial structure-property relationships that can be used to determine which material features can be altered to gain functionality in a predictable manner.

#### 7. NanoGold-Bio Interaction: A Big Concern in Nanomedicine Era

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Nanotechnology is known as a set of promises to reengineer the man-made world, molecule by molecule, successfully sparking a wave of innovation in every field from mechanics to medicine. From thousands of variations of nanomaterials, gold nanoparticles (AuNPs) seem to be a promising choice as they show excellent bio-compatibility and are one of trace elements that regulate the cells coenzymes. However, as the advancement of AuNPs in the medical field increases, people come to question the safety of AuNPs. Many studies were conducted, both *in vitro* and *in vivo*, to evaluate these biological effects on human cells. Many have proved that AuNPs can induce cell damage, gene damage, but some have proven that AuNPs are not toxic and have anti-oxidative properties as well. Here, in this study, interesting data of AuNPs, compared with non-metal nanoparticles, their influence to cellular morphology, and protein interaction and level of gene expression are presented. *In vitro* alteration of cellular functions induced by nanoparticles are also presented.

### 8. Mosfet Analysis at Nanoscale Using Nano Simulator Version-I

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### 9. Developing a Collaborative Environment Supporting the Application of Nanotechnology in Biomedicine

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The application of nanotechnology in cancer promises advancements in early detection, targeted therapeutics, and cancer prevention and control. The use of nanotechnology in biomedicine involves

the engineering of nanomaterials to act as therapeutic carriers, targeting agents, and diagnostic imaging devices. To assist in expediting and validating the use of nanomaterials in biomedicine, the NCI Center for Biomedical Informatics and Information Technology (CBIIT), in collaboration with the NCI Nanotechnology Characterization Laboratory (NCL) and other Cancer Centers of Nanotechnology Excellence (CCNEs), has developed a data sharing portal called caNanoLab (<u>http://cananolab.nci.nih.gov/caNanoLab/</u>). caNanoLab provides access to experimental and literature-curated data from the NCL and other CCNEs and facilitates data sharing via the use of caBIG<sup>®</sup> technologies enabling semantic interoperability.

caNanoLab provides a model for representing the composition of nanomaterial types (dendrimer, carbon nanotube) and associated functionalizing entities (e.g. small molecules, antibodies). caNanoLab supports the annotation of nanomaterials with characterizations resulting from physico-chemical (size, molecular weight) and in vitro (cytotoxicity, immunotoxicity) assays and the sharing of these characterizations and associated protocols in a secure fashion. The caNanoLab project is expanding to include support for *in vivo* characterizations (pharmacokinetics, toxicology) of nanomaterials. To represent nanomaterials and associated characterizations, caNanoLab leverages concepts from the NCI's Enterprise Vocabulary Services (EVS) and the Nanomaterial Ontology (NPO) designed by Washington University. The caNanoLab project is collaborating with members of the biomedical nanotechnology community through the caBIG<sup>®</sup> Nano WG in the development of nano-TAB, a standard supporting data import/export between disparate nanotechnology systems.

## 10. nano-TAB: A Standard File Format for Data Submission and Exchange on Nanomaterials and Characterizations

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The field of nanomedicine faces many challenges in the development of standards to support meaningful data submission and information exchange. Numerous physico-chemical, *in vitro*, and *in vivo* assays must be addressed, with measurements currently dependent on non-standardized protocols and diverse technology types. Representing Structure-Activity-Relationships (SARs) in nanomedicine, in particular, is critical to understanding the effects of nanomaterial structure on biological activity. Unfortunately, information describing the nanomaterial including functionalizing entities and 3D structure is often represented in an undisciplined fashion. This lack of standardization has been a significant deterrent to meaningful data sharing across the nanotechnology community; few publications contain sufficient information to enable adequate interpretation of results and successful achievement of experimental reproducibility.

The nano-TAB effort aims to address data sharing challenges in nanotechnology by providing a standard means for identifying nanomaterials and characterizations in a tab-delimited format. nano-TAB is based on existing standards developed by the European Bioinformatics Institute (EBI) and the Investigation/Study/Assay (ISA-TAB) file format, which represents a variety of assays and technology types. The nano-TAB specification leverages ISA-TAB files describing investigations, study-samples, and assays and provides extensions to support nanomaterial structural information and assay measurements

from the Washington University NanoParticle Ontology (NPO). The nano-TAB standard specification will enable the submission and exchange of nanomaterials to/from nanotechnology resources like the NCI's caNanoLab nanotechnology portal and the Oregon State Nanomaterial-Biological Interactions (NBI) knowledgebase; empower organizations to adopt standards for representing data in nanotechnology publications; and provide researchers with guidelines for representing nanomaterials and characterizations to achieve cross-material comparison.

The nano-TAB effort is a collaboration between a variety of organizations including the NCI, Washington University, Oregon State, ONAMI, NIOSH, Stanford University, and ISA-TAB. nano-TAB is registered as an ASTM Work Item, which facilitates a broad community outreach and input to the development of nano-TAB and other standards needed to support nanomedicine.

# **11. Web-Interfaced Nanotechnology Environment, Safety, and Occupational Health Guidance System–WINGS**

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In order to streamline access to strategies and tools for quantifying and managing emerging environment, safety, and occupational health (ESOH) risks related to nanomaterials, Luna Innovations Incorporated developed a web portal capable of providing up-to-date ESOH information in the rapidly growing field of nanomaterials. This Web-Interfaced Nanotechnology Environment, Safety, and Occupational Health Guidance System—WINGS—will be instrumental in guiding the end user through cradle-to-grave considerations for handling of nanomaterial sources. The site provides comprehensive guidance modules related to regulations and industry best practices, while also serving as a repository for related literature as well as localized medical surveillance documents. Additional tools and modules allow the user to assess risk and implement necessary control methods prior to bringing the material on site, thus allowing for educated decision making with respect to nanomaterial handling, storage, and disposal considerations in advance.

The centralization of ESOH resources through WINGS will allow Air Force personnel and OEMs to save valuable man hours by eliminating tedious searching through various sites and databases for the relevant information or regulations related to the nanomaterial of interest. Additionally, tools such as the Multi Criteria Decision Analysis (MCDA) tool will allow for rapid risk assessment through the life cycle of the nanomaterial of interest via a concise on-line questionnaire and simple scoring system. The site provides a framework that can easily be expanded to include additional data base sets, nanomaterial exposure tracking, medical surveillance tools, and information exchange forums. Additionally, the site framework is suitable for rapid modification to suit other business interests or braches of the government.

### 12. Nanoinformatics: Informatics for Nanomaterials Discovery and Design

C. S. Kong, S. R. Broderick, and K. Rajan Department of Materials Science and Engineering & Institute for Combinatorial Discovery, Iowa State University

Today nanomaterials, which encompass all levels of studies and applications of materials properties revealed in unique ways under the nano-length scale, are used in numerous fields. Prompted by the

highly diverse and ceaseless needs for novel functionalities of materials, the intensive efforts to extend our materials domain towards this new scale have long been continued by means of both experimental and computational approaches. At present, the nanomaterials research is guided by materials knowledge/databases accumulated over the past several decades. Along with the accelerated acquisition speed of materials data, informatics has been recognized as a powerful tool of materials research for extracting useful and comprehensive knowledge on the materials behavior from the data obtained.

In this poster presentation we discuss the application of informatics for both the design of novel functional materials, as well as for atomic-length scale characterization and analysis. In this poster presentation, we describe the application of nanoinformatics for three different fields. Applications include nanoinformatics to the analysis of nanoscale chemical imaging and characterization through atom probe tomography, design of new nanoscale biomaterials for drug delivery and finally nano-crystallography combined with informatics for the development of new inorganic scintillator materials.

### 13. Informatics in Relation to Nanomaterials and Worker Health

Mark D. Hoover

National Institute for Occupational Safety and Health (NIOSH)

Informatics is the science and practice of collecting, validating, sharing, visualizing, analyzing, modeling, and applying information. Modern informatics tools can be used to organize, guide, and interpret occupational safety and health research for nanotechnology specifically, and for worker protection in general. An expansion of informatics efforts is needed within the research and public health communities to ensure that risks are minimized and benefits are realized. As we attempt to move to an agreed set of minimal parameters and techniques for nanomaterial characterization, data from the use of current material characterization techniques can be organized in a manner that supports the construction of a logical taxonomy and enables the organization of materials into biologically meaningful categories. In particular, use of a categorical approach (such as grouping metal oxides or carbon-based materials according to mechanisms of toxicity versus a one-particle-at-a-time approach) will accelerate NIOSH's efforts in its key research areas of Hazard Determination (design, conduct, and interpretation of toxicology studies); Risk Assessment (dose-response evaluation of biologic effects); Exposure Assessment (metrics, methods, and the supporting research); Risk Characterization; Controls and Risk Management Methods; and Medical Screening/Surveillance and Epidemiology (including identification and tracking of nanomaterial workers who could be enrolled in exposures registries or included in epidemiological studies).

One example of an ongoing nanoinformatics initiative with which NIOSH is partnering in the National Cancer Institute's caNanoLab web-based portal (http://cananolab.nci.nih.gov/caNanoLab/), which allows researchers to share information on nanoparticles (including size, composition and other physico-chemical parameters) and information on the supporting protocols and results of in vitro and in vivo biological assays. Information from nanotechnology health and safety studies at NIOSH is available at http://www.cdc.gov/niosh/topics/nanotech/. Tools for prioritizing and controlling health risks to dangerous substances can be found at http://www.stoffenmanager.nl. The NANEX project (http://nanex-project.eu) has developed a catalogue of generic and specific (occupational, consumer, and environmental release) exposure scenarios for manufactured nanomaterials taking account of the entire lifecycle of these materials. The patient-centered, computer-based health records initiative (www.hhs.gov/healthit/ahic/healthrecords/) might support improved tracking of nanotechnology

workers and improved worker health in general. Challenges for the community are to understand and improve the linkage among existing informatics initiatives; establish standards to support terminology, characterization and testing protocols, data acquisition and validation, and contents of worker health records; develop "data mining" approaches to cull the massive amounts of data from biological studies into knowledge about key parameters for occupational safety and health; and provide incentives for the community to contribute to robust platforms for nanotechnology health and safety informatics.

### 14. ART: Advanced REACH Tool

Chemical Safety Assessment under the European Commission's Registration, Evaluation, Authorization and Regulation of Chemicals (REACH) program can be complex and time consuming. Assessing risk requires a clear knowledge of exposure to chemicals. While Tier I models estimating exposure are available, should they be unable to show safe use, then refinement with more data or better assumptions is the only way forward. A large collaborative project is therefore initiated by TNO, bringing together leading scientist across Europe from major research organization in the field of occupational health (TNO, IOM, HSL, IRAS, BAUA and NRCWE) aiming to develop an Advanced REACH Tool (http://www.advancedreachtool.com). The ART provides a cost-effective higher tier exposure assessment approach without diminishing the protection of workers in Europe.

The ART incorporates a mechanistic model of inhalation exposure and a database of empirical exposure information from a wide variety of exposure scenarios and substances. Information from the model and the exposure database is combined using sophisticated statistical techniques to produce more refined estimates of exposure and related uncertainty. Assessors may also include their own data to update and refine estimates. The mechanistic model is calibrated using a range of data sources so that even if there are no relevant data available the ART provides useful exposure estimates.

The development of the ART started in January 2008 and received broad support from member states, industry, and ECHA and is considered as a robust and necessary way forward in exposure assessment. Several industry- and sector-specific features have been built into the ART resulting in a version 1.0 that combines the mechanistic model with a facility for statistical updates with the user's own data. This version 1.0 was released in March 2010 and is freely available at www.advancedreachtool.com. Examples convincingly show that updating the mechanistic model estimates with available exposure data results in a substantial reduction in model uncertainty.

### **15. A Service-Oriented, Federated Approach for Nanoinformatics** *Matt Sedlak RJLee Group, Inc.*

A federated architecture is an implementation of a Service-Oriented Architecture (SOA) centered on web services amongst an organization of systems or partners in a trust relationship called a Federation. It facilitates the secure communication of information assets amongst human and system members of a federation, where the terms of the information assurance and security are agreed upon when a system joins the Federation.

A contemporary federated solution supports distributed computing over the internet eliminating traditional point-to-point interfaces leveraging Web 2.0 (social networking) and Web 3.0 (semantic discovery) technologies with extensions for cloud and high performance computing (HPC) to support

computing processing needs. Once a system defined as a "data provider" is established as part of the Federation, data is then exposed and made available to federated members. Once a system or human is defined as a "data consumer" and established as part of the Federation, data can then be accessible or discovered for consumption and sharing.

The Department of Defense (DoD) is actively implementing similar federated solutions. RJ Lee Group's expertise within informatics and scientific solutions developed an innovative Web-Service Integration Framework Tool using open standards for the DoD as a federated baseline framework called swift. The swift toolset includes Web 2.0 Exposure services, Mashup services, Widget services, Federated Security services, and Web 3.0 Discovery services.

The Exposure services quickly enable an organization to expose data from relational databases as informational assets in the form of standard XML Web Services. The Mashup services provide system and user controlled data integration and visualization of the XML Web Services combining the data sources, data translation, and data consumption into an easy to use structure. The Mashup services are also uniquely designed for HPC of 3rd party algorithms against large data sets that are commonly found within Scientific, Engineering, and Research communities. The Widget services consume the XML Web Services for Remote Portlets (WSRP) standards. The Discovery services provide a "Google-like" natural language semantic search on exposed data sources that allow users to easily and quickly discover valuable information assets that are part of the Federation. The Federated Security services provide cross-domain application level security assurance for the swift services (exposure, discovery, mashup, widgets) by establishing a contract or trust relationship with the disparate information systems within the Federation. The security is customizable to satisfy requirements for the enterprise and is independently built on-top of an organizations existing network level security.

The Service-Oriented, federated approaches developed for the DoD can also be adopted and applied to nanoinformatics supporting the nanotechnology domain. Utilizing these approaches and technologies correctly can provide an unprecedented capability to the scientific, engineering, research ,and academic communities enabling the accessibility and sharing of nano data without geographic boundaries for the advancement of nanotechnology worldwide.

### 16. NANOSAFEWARE™: Compliance Management Software for Industries Supported by Emerging Nanotechnologies Matt Hull

NanoSafe, Inc.

Much speculation remains as to whether and to what extent nanotechnology driven industries will be regulated. What is clear, however, is that as best practices and guidance strategies continue to emerge with remarkable frequency, management of key nanotechnology health and safety risks in the laboratory and workplace is becoming increasingly complex and difficult to verify. This poster presentation will describe NANOSAFEWARE<sup>™</sup>, which is an electronic compliance monitoring tool suited specifically for industries supported by emerging nanotechnologies. The program, which has been adapted from heavily regulated industries where compliance with state and federal regulatory standards is a frequent challenge, simplifies and streamlines document management, workflows, process control, workforce training, auditing, and enforcement, and keeps users updated on state-of-the-industry compliance requirements—regardless of whether such requirements are motivated by government

regulations or organization specific standards of performance and safety. With representatives from both the legal and insurance communities urging organizations to minimize future liabilities by adopting proactive risk management strategies, tools like NANOSAFEWARE<sup>™</sup> should play an increasingly important role in the organization, implementation, and verification of such strategies.

### 17. Pilot of the Communication and Education Message and Audience Planning Tool for the Nanoinformatics 2020 Roadmap and Plan: Illustration of Findings Related to Public Perception

Stephanie Mathews, MPH, CHES, Department of Epidemiology and Biostatistics, University of Georgia

The Nanoinformatics 2010 Workshop is designed as a community-wide, public forum to survey the current nanoinformatics landscape, to stimulate collaborative activities and pilot projects, and to craft a broad-reaching Nanoinformatics 2020 Roadmap and Plan for the development and implementation of informatics in the nanotechnology domain. The draft roadmap that will be discussed at the workshop includes a table illustrating the concept of "A Communication and Education Message and Audience Planning Tool for the Nanoinformatics 2020 Roadmap and Plan". The table recognizes a diversity of stakeholders and community roles that can make informatics contributions and have informatics needs, including workers, health and safety practitioners, management, policy makers and regulators, equipment and system vendors, consumers, the legal community, researchers, educators, the media, and society in general. The table further recognizes the common and potentially unique needs of each stakeholder and partner to (1) Emphasize literacy and develop critical thinking; (2) Develop and use real-life data examples; (3) Stress conceptual understanding rather than mere application of procedures; (4) Foster continuous improvement and active discussions; (5) Use technology for developing conceptual understanding and for analyzing and sharing information (e.g., modeling and simulation, databases, etc.); and (6) Use assessments to improve and evaluate the efficacy and impact of these activities.

Success of the Nanoinformatics 2020 Roadmap and Plan will require detailed considerations of how the vision of a communication and education message and audience planning tool can be specifically and effectively refined and applied across the many disciplines and many aspects (both scientific and societal) of nanotechnology research, development, and application. In this pilot illustration an example table was prepared to stimulate discussion of possible Pilot Project ideas for application of the Communication and Education Message and Audience Planning Tool proposed in the Nanoinformatics 2020 Roadmap and Plan. Current entries represent portions of a first layer of evidence-based communication considerations for the perception of nanotechnology. Subsequent dimensions of the matrix could include parallel information related to other areas of interest such as health and safety, technical feasibility, economics, and population disparities. (The invaluable contributions of Dr. Mark D. Hoover of the National Institute for Occupational Safety and Health to this work are gratefully acknowledged.)