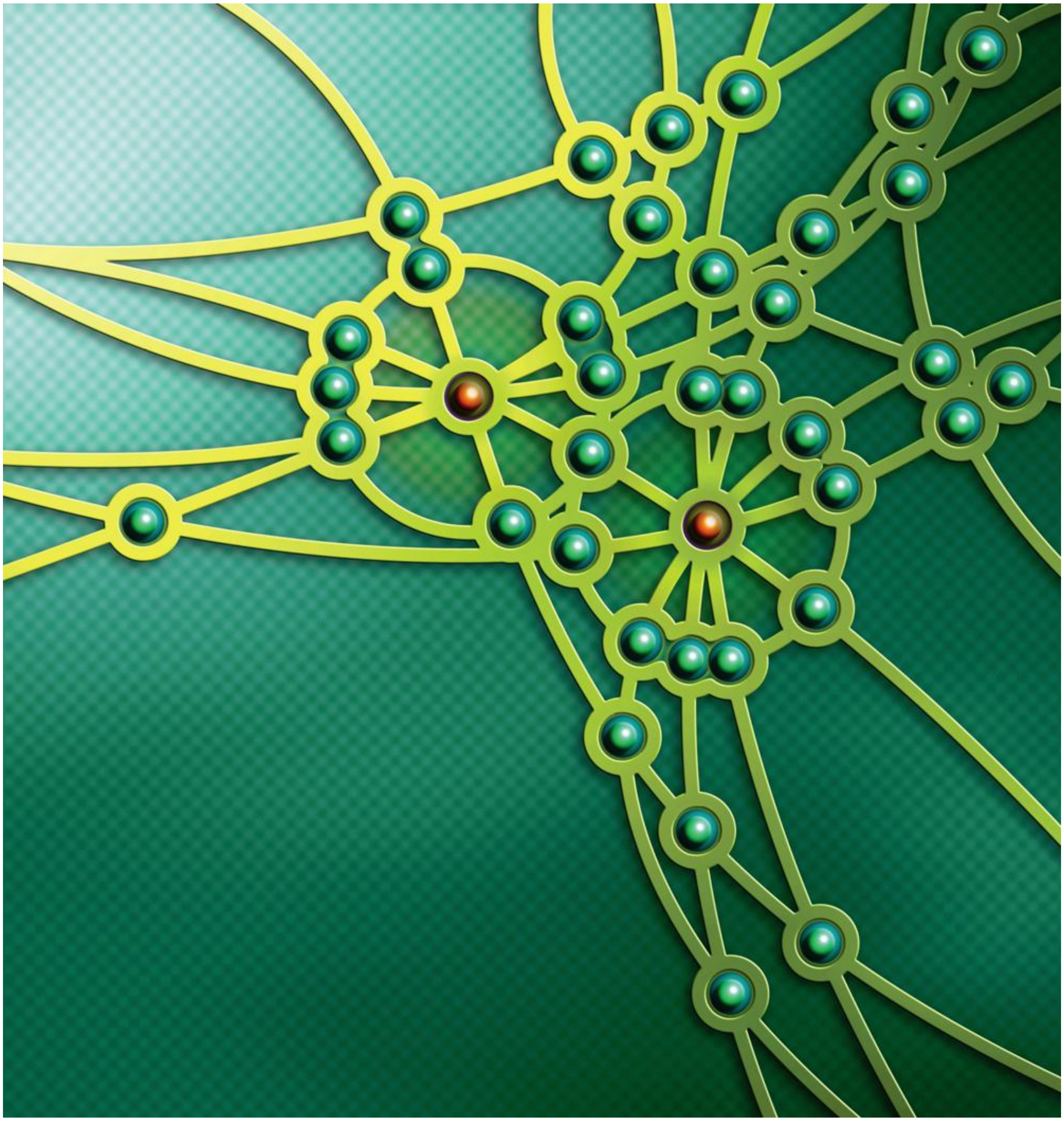

Nanoinformatics 2011

December 7-9

Arlington, VA

Nanoinformatics 2011

Hyatt Regency Crystal City
Arlington, VA
December 7-9, 2011

Nanoinformatics 2011 will bring together informatics experts, nanotechnology researchers, and other stakeholders and potential contributors to advance Nanoinformatics 2020 Roadmap goals. The workshop will set a clear path for Nanoinformatics participants through the presentation of projects and research, open discussions, and strategic planning sessions.

The conference will be held December 7-9, 2011 in Arlington, VA, at the Hyatt Regency Crystal City hotel. December 7-8 will feature nanoinformatics presentations on a variety of topics as well as focused talks on Quantitative Structure Activity Relationships and Minimum Required Characteristics. December 9th will be a working day where feedback and ideas on the Nanoinformatics 2020 Roadmap from meeting attendees will be especially welcome.

Nanoinformatics involves the development of effective mechanisms for collecting, sharing, visualizing, modeling and analyzing information relevant to the nanoscale science and engineering community. It also involves the utilization of information and communication technologies to help launch and support efficient communities of practice. Nanoinformatics is necessary for comparative characterization of nanomaterials, for design and use of nanodevices and nanosystems, for instrumentation development and manufacturing processes. Nanoinformatics also fosters efficient scientific discovery and learning through data mining and machine learning techniques.

Organizers

Jessica Adamick, National Nanomanufacturing Network
Nathan Baker, Pacific Northwest National Laboratory
Jean-Claude Bradley, Drexel University
Anne Chaka, National Institute of Standards & Technology
Yoram Cohen, University of California, Los Angeles
Martin Fritts, Nanotechnology Characterization Laboratory
Charles Geraci, National Institute for Occupational Safety and Health
Sharon C. Glotzer, University of Michigan
Stacey Harper, Oregon State University
Mark Hoover, National Institute for Occupational Safety and Health
Kristen Kulinowski, IDA-Science and Technology Policy Institute
Phil Lippell, Consultant, Nanoscience and Emerging Technologies
Michael McLennan, Purdue University
Jeff Morse, National Nanomanufacturing Network
Michele Ostraat, RTI International
Krishna Rajan, CoSMIC -- Iowa State University
Mark Tuominen, National Nanomanufacturing Network

This event was made possible by the National Science Foundation through grant number CMMI 1025020.

Supporting organizations include

Combinatorial Sciences and Materials Informatics Collaboratory
ICON GoodNanoGuide
nanoHUB.org
Nanoparticle Information Library
National Institute of Standards and Technology
National Nanomanufacturing Network
Nanotechnology Characterization Laboratory
Oregon Nanosciences and Microtechnologies Institute
The Safer Nanomaterials and Nanomanufacturing Initiative

Program

Wednesday, December 7

6:00 PM -	**Registration**	Regency Ballroom Foyer
7:00 - 7:45 PM	**Welcome Keynote: Infrastructure for a Connected World** *Christian Lehinger (HealthQuest Alliance)*	Regency Ballroom A
7:45 PM	**Reception and Poster/Exhibitor Session** Reception sponsored by ***NanoBusiness Commercialization Association***	Regency Ballroom Foyer

Thursday, December 8

8:00 - 8:30 AM	**Registration and Continental Breakfast**	Regency Ballroom Foyer
8:30 - 8:35 AM	**Welcome** *Mark Tuominen (National Nanomanufacturing Network)*	Regency Ballroom A
8:35 - 8:45 AM	**Opening Remarks** *Altaf Carim (White House Office of Science and Technology Policy)*	Regency Ballroom A
8:45 - 9:30 AM	**Keynote: Mythbusting Scientific Knowledge Transfer: nanoHUB usage Scenarios and Impact** *Gerhard Klimeck, (Purdue University, nanoHUB)*	Regency Ballroom A
9:30 - 10:20 AM	**Pilot Status Reports**	Regency Ballroom A
9:30 - 9:40 AM	**Consortium for Coordinating Nanomaterials Research** *Stacey Harper (Oregon State University)*	
9:40 - 9:50 AM	**Nano-SAR Education and Dissemination** *Nathan Baker (Pacific Northwest National Laboratory)*	
9:50 - 10:20 AM	**Knowledge Engineering for Nanoinformatics:** **Architecture** *Joe Glick (Expertool Software)* **Ontology** *Nathan Baker (Pacific Northwest National Laboratory)* **Quant Modeling** *Krishna Rajan (Iowa State University)*	
10:20 - 10:50 AM	**Break**	Regency Ballroom Foyer
	Q-SAR Theme *Theme chairs: Nathan Baker (Pacific Northwest National Laboratory), Yoram Cohen (UCLA), Krishna Rajan (Iowa State University)*	Regency Ballroom A
10:50 - 11:20 AM	**Featured Talk** *Yoram Cohen (University of California, Los Angeles)*	
11:20 - 11:45 AM	**QSAR Development for Toxic Chemical Sequestration** *Krishna Rajan (Iowa State University)*	
11:45 - 12:45 PM	**Lunch**	Regency Ballroom B

	Vincent Caprio (NanoBusiness Commercialization Association)	
	Q-SAR Theme (cont.)	Regency Ballroom A
12:45 - 1:10 PM	**Informatics and Standards for Nanomedicine Technology** *Nathan Baker (Pacific Northwest National Laboratory)*	
1:10 - 1:35 PM	**Quantitative Nanostructure-Activity Relationships (QNAR) Modeling: Applications to Rational Design of Nanomaterials with the Desired Bioactivity Profile** *Alexander Tropsha (UNC - Chapel Hill)*	
1:35 - 2:35 PM	**Government Panel**	Regency Ballroom A
2:35 - 3:00 PM	**Break**	Regency Ballroom Foyer
	MinChar Theme *Co-chairs: Stacey Harper (Oregon State University), Mark Hoover (NIOSH Nanotechnology Research Center), Phil Lippel (Nanoscience and Emerging Technologies Consultant)*	Regency Ballroom A
3:00 - 3:30 PM	**Featured Talk: Nanoinformatics Challenges for Occupational Exposure Limits, Medical Surveillance, Exposure Registries and Epidemiologic Research** *Paul Schulte (NIOSH Nanotechnology Research Center)*	
3:30 - 3:55 PM	**Development of Predicative Tools for Nanomaterials Risk Analysis** *Amy E. W. Bednar (US Army Engineer Research and Development Center)* *Jeffery A Steevens (US Army Engineer Research and Development Center)*	
3:55 - 4:20 PM	**Multi-Criteria Decision Analysis Tool to Support Selection of Nanomaterial Studies: Development Update** *Gretchen Bruce (Intertox)*	
4:20 - 5:00 PM	**Keynote: Data Intensive Computing for Science and Information Discovery** *Deborah Gracio (Pacific Northwest National Laboratory)*	Regency Ballroom A
5:00 - 5:05 PM	**Closing Remarks** *Vincent Caprio (NanoBusiness Commercialization Association)*	Regency Ballroom A
5:05 PM	**Reception and Poster/Exhibitor Session** Reception sponsored by ***NanoBusiness Commercialization Association***	Regency Ballroom Foyer

Friday, December 9

8:00 - 8:30 AM	**Continental Breakfast**	Regency Ballroom Foyer
8:30 - 8:40 AM	**Opening Remarks** *Sally Tinkle (National Nanotechnology Coordination Office)*	Regency Ballroom A
8:40 - 9:10 AM	**The Materials Genome Initiative: A Renaissance of American**	Regency Ballroom A

	Manufacturing *Cyrus Wadia (White House Office of Science and Technology Policy)*	
9:10 - 10:10 AM	LIGHTNING TALKS	Regency Ballroom A
9:10 - 9:20	1: **Nanoinformatics in Support of Defense Applications of Nanotechnology** *Christopher Detzel (NanoSafe, Inc.)*	
9:20 - 9:30	2: **An Integrated and Comprehensive Data Mining System for Studying Environmental Impact of Nanomaterials: NEIMiner** *Kaizhi Tang (Intelligent Automation, Inc.)*	
9:30 - 9:40	3: **A Predictive Model for Pulmonary Toxicity of Carbon Nanotubes – Implications for Nanomaterial Characterization Standards** *Jeremy Gernand (Carnegie Mellon University)*	
9:40 - 9:50	4: **Nanoinformatics: Current Challenges and Trends on Nanomedical Information Management** *Diana De La Iglesia (Universidad Politecnica de Madrid)*	
9:50 - 10:00	5: **Intellectual Property Aspects of the Nanoinformatics 2020 Roadmap** *Francisco Castro (McAndrews, Held & Malloy Ltd.)*	
10:00 - 10:10	6: **Using Informatics Tools to Survey the Nano Patent Landscape** *Phil Lippel (Nanoscience and Emerging Technologies Consultant)*	
10:10 - 10:30 AM	**Break**	Regency Ballroom Foyer
10:30 - 11:30 PM	**Roadmapping Strategy for 2012**	Regency Ballroom A
11:30 - 12:30 PM	**Nanoinformatics Governance**	Regency Ballroom A
12:30 - 1:15 PM	**Lunch**	Regency Ballroom B
1:15 - 1:45 PM	**General Networking and Information Technology Research and Development (NITRD) Program Overview** *George O. Strawn (Networking and Information Technology Research and Development Program)*	Regency Ballroom A
1:45 PM -	**Pilot Work Groups**	Regency Ballroom A/B

Abstracts

Lightning Talks

1. **Nanoinformatics in Support of Defense Applications of Nanotechnology**
Christopher Detzel (NanoSafe, Inc.)
Matthew Hull (NanoSafe, Inc.)

Nanoscale technologies offer the potential to transform military defense systems in numerous ways ranging from enhancement of weapons and munitions to the formulation of stronger lightweight composite armor. Realizing these materials in ways that are both practical and safe requires tools that enable understanding of the physicochemical and toxicological properties of numerous nanoparticle variants. NanoSafe, Inc. is currently supporting nanoinformatics approaches under development within the US Army and Air Force to improve understanding of nanomaterial properties as well as Environmental Safety and Health (ES&H) risks. This presentation will describe efforts underway at NanoSafe, Inc. in support of these military nanoinformatics projects and will discuss how recent progress can be applied beyond the military and defense communities.

2. **An Integrated and Comprehensive Data Mining System for Studying Environmental Impact of Nanomaterials: NEIMiner**
Kaizhi Tang (Intelligent Automation, Inc.)

As more engineered nanomaterials (eNM) are developed for military use, it is crucial to minimize any unintended environmental impacts (NEI) resulting from the application of eNM. To realize this vision, industry and policymakers must base risk management decisions on *sound* scientific information about the environmental fate of NM; their availability to receptor organisms, including related concepts such as uptake; and any resultant biological effects, e.g. toxicity. Intelligent Automation, Inc. (IAI) is developing a Model driven Data Mining System for studying Environmental Impact of Nanomaterials, NEIMiner, which consists of four components: nanomaterial environmental impact (NEI) modeling framework, data integration, data management and access, and model discovery and composition. The NEI modeling framework defines the scope of NEI modeling and the strategy of integrating NEI models to form a layered, comprehensive predictability similar to the Framework for Risk Analysis of Multi-Media Environmental Systems (FRAMES). The data integration layer brings together heterogeneous data sources related to NEI via automatic web services and web scraping technologies. The data management and access layer reuses and extends a popular Content Management System (CMS), Drupal, and consists of modules that model and enable interactions over a complex data structure for NEI related bibliography and characterization data. The model discovery and composition layer provides an analysis capability for NEI data. The NEI modeling framework serves the guiding force to design, develop, and implement the NEIMiner information system.

3. **A Predictive Model for Pulmonary Toxicity of Carbon Nanotubes – Implications for Nanomaterial Characterization Standards**
Jeremy Gernand (Carnegie Mellon University)
Elizabeth Casman (Carnegie Mellon University)

The ability to map nanoparticle properties to nanotoxicity would be a significant advancement in nanotoxicology. This goal has been thwarted by inconsistencies and omissions in nanoparticle characterization measurements reported in the nanotoxicology literature. Yet, even with this imperfect data base it is possible to identify nanoparticle characteristics with high information content using machine learning techniques. We identify such characteristics for pulmonary exposures to carbon nanotubes (CNTs) and make recommendations for future CNT measurement and reporting.

To develop predictive models of CNT pulmonary toxicity from CNT properties, we performed a meta-analysis of CNT *in vivo* pulmonary inflammation and toxicity studies. From the predictive models we ranked nanomaterial attributes and experimental parameters according to their influence on toxicity indicators. The analysis employed random forest models based on ensembles of regression trees, a machine learning technique useful for identifying high information value attributes in sparse, high-dimensional, and non-linear contexts. The information contents of attributes were quantitatively compared with each other for both uniqueness and the degree of correlation for several measures of toxicity. Together with model complexity criteria, these metrics were used to provide a quantitative commentary on proposed characterization standards for nanomaterial experiments, such as those of the MinChar Initiative.

To facilitate the mapping of CNT properties to toxicity, our results suggest that future CNT toxicity studies should at a minimum report high information value nanomaterial characteristics. Distributions of measurements of some parameters carry important information that is lost when the attributes are reported as means or modes. For CNTs, these include distributions of the unaggregated CNT fragment lengths and distributions of aggregate dimensions. When distributions of geometric parameters are reported, the fractions responsible for the toxicity can be identified by the random forest method and irrelevant fractions do not obscure the relationship. Several other characteristics were found to be important, including CNT diameter (a surrogate for multi or single walled structure) and impurity content. When measuring toxicity by total cell count in bronchoalveolar lavage (BAL) fluid, the influence of impurities on toxicity was typically less than a quarter the influence of the CNTs themselves. By contrast when measuring toxicity by total protein in BAL fluid, impurity content including oxidized carbon and metals (particularly cobalt and aluminum) did play a significant role in toxicity, followed by CNT diameter.

4. **Nanoinformatics: Current Challenges and Trends on Nanomedical Information Management**
Diana De La Iglesia (Universidad Politecnica de Madrid)
Miguel Garcia-Remesal (Universidad Politecnica de Madrid)
Jose Crespo (Universidad Politecnica de Madrid)
Miguel Muñoz (Universidad Politecnica de Madrid)
Alejandro Pazos (University of A Coruña)
Victor Maojo (Universidad Politecnica de Madrid)

Although its applications are still in their early stages, professionals working on nanomedicine already generate huge volumes of data resulting from the active research in the field. This information needs to be collected, filtered, managed, and, finally, organized and presented in a standardized way by using informatics methods and techniques —such as, among others, ontologies, semantic search, text mining, imaging and standards [1]. Here we present a summary of current research carried out by members of the Biomedical Informatics Group at the Universidad Politecnica de Madrid in nanoinformatics, along various directions.

1) Text Mining for Nanotoxicity
During the last years, the scientific community —as well as other specialists and the general public— has expressed concern towards toxicity issues related to nanoparticles [2]. A more rigorous assessment of the potential health impact of innovative nanoparticles, along with more stringent regulations, is necessary before introducing nanotechnology more broadly into everyday life. In this regard, we have been working on the development of different computational applications for automatically retrieving information about nanotoxicity. We have analyzed the scientific literature related to this issue, dealing with toxic effects of nanoparticles, which has been semantically annotated by applying text mining and machine learning methods [3].

One of our tools provides an automatic matching engine which extracts and links terms from scientific articles with the concepts from two ontologies: the Nanoparticle Ontology [4] and the Foundational Model of Anatomy [5]. The system retrieves information about those papers reporting which nanoparticles are more suitable for delivering a specific drug to a given anatomical location or identifying which nanoparticles have a toxic effect in a certain part of the body.

We have also developed a labeling system [6] which facilitates the automatic recognition of relations between nanoparticles and their toxic effects by applying machine learning techniques to the scientific literature. Our system parses the publications identifying and marking the text corresponding to the target entities –name of the nanoparticle, toxic effect, target or affected organ/tissue/cell and type of exposure— with a concrete color, each denoting a different category.

2) Nanoparticle Characterization: Ontology of nanoparticles shapes
The difficult characterization of the nanoparticles and their different combinations constitutes a major challenge for managing information related with the use of nanoparticles. Our group is currently working on an ambitious project for analyzing nanoparticles shapes and 3D structures that could be useful for their further characterization [7]. The system aims to analyze the morphological characteristics of the nanoparticles to subsequently perform a taxonomic classification based on the geometrical shapes of the nanoparticles and their components.

3) Nanoinformatics Resources
Finally, we are also working on creating inventories of various types of information, such as existing nanomedical data sources, computational resources related to nanomedicine or nanoparticles and nanodevices. These inventories are automatically populated, with the support of text mining techniques, by extracting the target information from scientific papers describing recent research on nanomedicine.

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[2] Maynard AD, Warheit DB, Philbert MA. The new toxicology of sophisticated materials: nanotoxicology and beyond. Toxicol Sci. 2011 Mar;120 Suppl 1:S109-29.
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[7] Maojo V, Crespo J, García-Remesal M, De la Iglesia D, Perez-Rey D, Kulikowski C (2011). Biomedical ontologies: toward scientific debate. Methods Inf Med. 2011 May 13;50(3):203-16.

5. **Intellectual Property Aspects of the Nanoinformatics 2020 Roadmap**
Francisco Castro (McAndrews, Held & Malloy Ltd.)

Practitioners from the legal community, and particularly intellectual property attorneys, need to take an active role in assisting the various efforts of informatics experts, nanotechnology researchers, and other stakeholders and potential contributors that are required to achieve the significant benefits emerging from the field of nanoinformatics. Consequently, the guidance provided by intellectual property practitioners can be used to effectively advance the efforts being proposed in the Nanoinformatics 2020 Roadmap. In this lightning talk, I will describe the manner in which several areas related to intellectual property, including patents, trademarks, copyrights, licensing and standards are more than likely to arise in each of the three main themes that have been identified as part of an envisioned system of nanoinformatics. By understanding the different forms of intellectual property and their respective functions, members of the nanoinformatics community can make better use of intellectual property as a strategic tool in achieving the significant benefits that are expected to emerge from this field.

In achieving a vision of nanoinformatics as a workflow for research, product innovation, manufacturing, and environmental, health, and safety (EHS) practices, the nanoinformatics community needs to address and coordinate the many issues related to regulations, compliance, standards, security and safety that are likely to arise in the process. While all these issues are important and require careful consideration, matters specifically related to intellectual property tend to appear in each of the three main themes.

For example, with respect to the data collection and curation theme, issues related to content and data rights, as well as privacy, security, integrity, evaluation, and standardization require proper guidance from experts in those areas, especially intellectual property experts. With respect to tools and methods for data innovation, analysis and simulation, a similar set of issues as those listed above are likely to need consideration. In addition, making various tools available and/or allowing their interaction with commercial software tools may also raise various issues related to intellectual property, including the type of licensing models most suitable for particular arrangements. Finally, the third theme that deals with data accessibility and information sharing explicitly identifies governance and regulation of data and intellectual property and standards development, as major concerns of sharing data with the nanotechnology community.

6. **Using Informatics Tools to Survey the Nano Patent Landscape**
Phil Lippel (Nanoscience and Emerging Technologies Consultant)

The United States Patent and Trademark Office maintains a cross reference art collection of nanotechnology patents known as USPTO Class 977. With over 7000 patents currently listed and full patent text freely (if not readily) available, this collection is a large but not overwhelming data set that provides an interesting sandbox for playing with nanoinformatics tools. The organization of the class, with 263 subclasses in a six-level hierarchy, differs somewhat from that of typical knowledge structures. Correlations between this structure and that of nano-ontologies, taxonomies, or vocabularies can be interesting for several reasons. The connections between patents identified by USPTO examiners in the classification process could point to a set of relationships not obvious from the perspective of the researchers developing nanotechnology knowledge structures. Comparison of patent data and publication data over time, assisted by mapping concepts and vocabularies between structures, could illuminate the progression of research advances through the innovation ecosystem. Since patents are never classified strictly as nanotechnology – 977 is a cross reference class, and all patents receive at least one primary class number – patent office data also offers interesting possibilities for tracking industrial and commercial sectors where nanotechnology is being applied.

Posters

1. **The National Cancer Institute (NCI) caBIG® Nanotechnology Working Group (NanoWG)**
Jessica Adamick (National Nanomanufacturing Network)
Nathan A. Baker (Pacific Northwest National Laboratory)
Joseph Fisher (Oregon State University)
Gilberto Fragoso (National Institutes of Health, National Cancer Institute)
Elaine T. Freund (3rd Millennium)
Martin Fritts (Nanotechnology Characterization Laboratory, National Institutes of Health)
Elizabeth Hahn-Dantona (National Institutes of Health, National Cancer Institute)
Stacey L. Harper (Oregon State University)
Mark D. Hoover (National Institute for Occupational Safety and Health)
Fred Klaessig (Pennsylvania Bio Nano Systems)
Juli D. Klemm (National Institutes of Health, National Cancer Institute)

David S. Paik (Stanford University)
Dennis G. Thomas (Pacific Northwest National Laboratory)

The National Cancer Institute (NCI) Cancer Biomedical Informatics Grid (caBIG®) project provides a collaborative information network for scientists and institutions. The infrastructure is open and broad, supports interoperability and access to data and information from basic through clinical research. The Nanotechnology Working Group (Nano WG) was established as part of caBIG in 2008 to support the specific informatics needs of its nanotechnology researchers. It is comprised of over 20 active participants with a broad range of expertise and background who communicate regularly with the goal of demonstrating the use of interoperable and open data information systems for the nano related sciences. The Nano WG has documented its objectives and timetable. This list is publicly maintained and periodically reviewed. Weekly web teleconferences promote direct communication and discussion. Content is shared freely through open web standards. A large community of collaborative participants interacts with the Nano WG and provides valuable input, feedback, and exchange.

The Nano WG activities focus on critical needs to support computational approaches such as modeling and prediction, including: (1) reliable curated data and a common understanding of nanomaterial characterization (2) advancing the interoperability of databases for aggregation of data and to support modeling and simulation (3) semantic search and retrieval of nanomaterial, protocol, and outcome data-sets and information to support prediction. Outcomes of the ontology and discovery tools include support for semantic search, nano bio-compatibility and design, and pharmacokinetic modeling. Major projects include the ongoing development of and support for both the NanoParticle Ontology (NPO) and the nano-TAB data exchange format. NPO represents the description, preparation, and characterization of nanomaterials in nanotechnology research. It is developed within the Basic Formal Ontology framework and is implemented in OWL (Ontology Web Language) and is accessed through the NCI. The nano-TAB exchange format is a specification developed to facilitate the import/export of data on nanomaterials and their use to and from nanotechnology informatics resources. The nano-TAB is a human and machine readable specification utilizing delimited files (where most data is initially captured), to leverage and extend concepts from the caBIG Life Sciences Domain Analysis Model (LS DAM), and to use the NanoParticle Ontology and other ontologies as sources for its terms. It leverages and extends the ISA-TAB standard because of its flexibility in supporting several different types of assays of interest including: *in silico, in vitro*, and *in vivo* assays as well as nanomaterial characterization attributes.

The Nano WG currently supports the design and development of new and existing nanomaterial bio-informatics information systems by supporting and developing the standards and schemas for its related data interoperability. Several examples of Nano WG support include: (1) the Nanomaterial-Biological Interactions (NBI) knowledgebase (2) the cancer nanotechnology laboratory portal (caNanoLab) (3) BioPortal (4) and PubNano. These resources support scientists, regulators, medical, and occupational professionals with their nanotechnology informatics needs.

caBIG® Nanotechnology Working Group (caBIG® Nano WG)
https://wiki.nci.nih.gov/display/ICR/Nanotechnology+Working+Group

2. **Nanoinformatics to Explore the Chemical Origin of Cytotoxicity of Oxide Nanoparticles**

Prasanna V. Balachandran (CoSMIC , Iowa State University)
Krishna Rajan (CoSMIC, Iowa State University)

Quantitative structure-activity relationships (QSARs) provide a well-established informatics tool to explore cytotoxicological effects of metal oxide nanoparticles. In this presentation, we expand the QSAR formulations to include fundamental materials characteristics at the crystal structure and electronic structure scale. We use that information to predict the potential cytotoxicity of new and unexplored metal oxide nanoparticles. Examples are provided where we have predicted for the first time the cytotoxicity of new metal oxide nanoparticles and suggested new dopants for reducing the cytotoxicity of some of the highly toxic metal oxide nanoparticles.

CoSMIC (Combinatorial Science & Informatics Collaboratory)
http://cosmic.mse.iastate.edu

3. **Comprehensive Environmental Assessment - Conceptual Model Developer**

Amy E. W. Bednar (Information Technology Laboratory, U.S. Army Engineer Research and Development Center)
David Boehm (Information Technology Laboratory, U.S. Army Engineer Research and Development Center)
David Johnson (Environmental Laboratory, U.S. Army Engineer Research and Development Center)
Alan Kennedy (Environmental Laboratory, U.S. Army Engineer Research and Development Center)
Aimee Poda (Environmental Laboratory, U.S. Army Engineer Research and Development Center)
Chris Griggs (Environmental Laboratory, U.S. Army Engineer Research and Development Center)
Chuck Weiss (Environmental Laboratory, U.S. Army Engineer Research and Development Center)
Jeff Steevens (Environmental Laboratory, U.S. Army Engineer Research and Development Center)
J. Mike Davis (U.S. Environmental Protection Agency)
Christina Powers (U.S. Environmental Protection Agency)
Dana Genya (U.S. Environmental Protection Agency)
Patricia Gillespie (U.S. Environmental Protection Agency)
Christine Hendren (Research Triangle Institute)
Katherine von Stackelberg (Harvard University)

With growing production and use of manufactured nanoparticles in DoD applications, the demand for capability to assess environmental risk of nanomaterials will increase. Additionally, regulatory requirements and DoD directives requiring consideration of hazards to soldiers, civilians, and environment will be implemented. An assessment with respect to ecosystem health requires current knowledge about nanomaterial properties, uses, environmental fate, and effects, to determine both predicted environmental concentrations and predicted no-effect concentrations.

This work presents a comprehensive environmental assessment approach (CEA) that is used to frame the problem to evaluate risks of nanotechnology through the entire life-cycle (e.g., feedstocks, manufacturing, distribution, storage, use, and disposal). The CEA process spans disciplines ranging from process engineering, physical chemistry, toxicology, and risk assessment.

The Comprehensive Environmental Assessment - Conceptual Model Developer (CEA-CMD) is a user-friendly software tool to support the development of a generic conceptual model of new materials for the CEA. CEA-CMD will facilitate the user's building the concept model of the life cycle and risk pathways for a material and/or chemical. The CEA-CMD separates the CEA into five divisions: life cycle stages, compartments, organisms, ecosystems and effects. Each division has multiple constituents and processes that can be added to the concept model. The user is required to answer a series of content-specific questions about each constituent and process. The model will output graphic and text descriptions outlining the specific constituents and processes of the material CEA. By using existing life cycle data, the CEA-CMD will identify common themes, data gaps, and health and safety issues that will help acquisition personnel, scientists, and risk assessors and managers make better decisions
prior to large-scale production, distribution, and use.

4. **Informatics Guided Atomistic Scale Imaging of Nanoparticle Degradation**
Scott Broderic (CoSMIC , Iowa State University)
Joaquin Peralta (CoSMIC , Iowa State University)
Krishna Rajan (CoSMIC , Iowa State University)

A new experimental approach for the study of the degradation of nanoparticles is introduced, via the technique of atom probe tomography (APT). APT is a data intensive imaging and spectroscopy technique that permits the imaging of hundreds of millions of atoms in three dimensions while simultaneously discriminating their elemental chemistry. We show how fundamental information on chemical bonding and structure at surfaces with nanoscale curvature can influence materials degradation. Informatics and data mining methods for experimental data, coupled to electronic structure calculations, are shown to form a powerful computational paradigm to extract the role of charge density distributions and diffusion mechanisms associated with the nanoparticle degradation. This work introduces a new paradigm in nanoinformatics, namely that of exploring "nano-surface science" via a data driven discovery approach.

CoSMIC (Combinatorial Science & Informatics Collaboratory)
http://cosmic.mse.iastate.edu

5. **Promoting Data Sharing To Expedite the Use of Nanotechnology in Cancer Research and Clinical Applications**
Sandra Chapman (Center for Strategic Scientific Initiatives, Office of Director, NCI/ NIH)
Dorothy Farrell (Center for Strategic Scientific Initiatives, Office of Director, NCI/ NIH)
George Hinkal (Center for Strategic Scientific Initiatives, Office of Director, NCI/ NIH)
Sara Hook (Center for Strategic Scientific Initiatives, Office of Director, NCI/ NIH)
Nicholas Panaro (NCI/SAIC)
Krzysztof Ptak (Center for Strategic Scientific Initiatives, Office of Director, NCI/ NIH)
Piotr Grodzinski (Center for Strategic Scientific Initiatives, Office of Director, NCI/ NIH)

The National Cancer Institute Office of Cancer Nanotechnology Research (OCNR) supports research in nanomaterials and devices for cancer detection, diagnosis and treatment. To promote clinical translation and commercialization of the nano-enabled technologies developed by its researchers, the OCNR also supports efforts to validate nanotechnologies and promote data-sharing across the research community. These efforts include the Nanotechnology Characterization Laboratory (NCL), the cancer Nanotechnology Laboratory (caNanoLab) portal and the NanoRegistry database.

NCL establishes standardized protocols and assays for the characterization of nanomaterials intended for use in cancer care. The full assay cascade includes physico-chemical characterization and *in vitro* and *in vivo* assays. To share the protocols developed and data gathered, NCL maintains caNanoLab. caNanoLab is a data sharing portal designed to facilitate information sharing in the biomedical nanotechnology research community. It provides support for the annotation of nanomaterials with characterizations resulting from physico-chemical and in vitro assays and the sharing of these characterizations and associated nanotechnology protocols in a secure fashion. The portal is expanding to include support for in vivo characterizations of nanoparticles and their functionalizing entities, analogous to those required for small molecules and other medical devices. These characterizations include rigorous testing to determine toxicity and PK/ADME properties and additional *in vivo* characterization of nanoparticles to address additional challenges stemming from the relationship of particle structural properties to biological activity. At present, caNanoLab allows researchers to submit and retrieve information on nanoparticles including the composition of the particle, the function of the particle (*e.g*. therapeutic, targeting, diagnostic imaging), the experimental characterization of the particle from physical *(e.g.* size, molecular weight) and in vitro (*e.g*. cytotoxicity, immunotoxicity) assays, the protocols for these characterizations, and related publications. caNanoLab provides access to publicly available data from characterizations performed at the NCL, information on over 800 nanoparticles, a list of 1100 peer-reviewed publications on cancer nanotechnology, and 41 protocols used to perform nanomaterial characterization assays.

Together with NIBIB and NIEHS, the OCNR is also engaged in developing a Nanomaterial Registry. The NanoRegistry supports the nanomaterial community by providing curated information about the physico-chemical characteristics as well as the environmental and biological interactions of well-characterized nanomaterials. The Registry builds a repository of curated nanomaterial information by extracting data from a broad collection of publicly available nanomaterial resources, from caNanoLab, among others. It also promotes the use of a well-defined Minimal Information About Nanomaterials (MIAN) framework and common nanomaterial standards.

6. **Nonlinear Dynamics Prediction with Application in Monte Carlo Simulation Speedup for Carbon Nanotube Synthesis**
Changqing Cheng (Oklahoma State University)

Prediction of the future states and performance is becoming crucial for improving monitoring and control of real-world complex systems, pertinently the synthesis of a variety of nanostructures. Significant developments have taken place in the application of nonlinear dynamic system theory to improve prediction. Despite these research efforts, effective prediction of the future states remains a challenge because these complex systems exhibit combined nonlinear and nonstationary dynamics, and the mathematical structure remains unknown if not indeterminable in most cases. The recent advances in nonparametric modeling approaches, such as Gaussian process regression model, can be used to simplify the modeling efforts. However, most GP models assume stationarity of the dynamics. This severely limits their predictability in many real-world systems. Our recurrence based local Gaussian process (LGP) model, which partitions the state space into near stationary segments, can overcome these limitations, and outperform most classical models in terms of prediction accuracy. The present investigation focuses on the synthesis of carbon nanotubes (CNTs) --- which are among the nanostructure materials with potential for rich industrial applications --- using chemical vapor deposition (CVD) process. While efforts have been made to address the optimization of the CVD process, the current CNT production and yield rates remain rather low to permit wider industrial application. Translating these nano-synthesis processes into viable manufacturing technologies is an imperative for the realization of the market potential, and the understanding of CNT growth mechanism is critical for this translation. Different approaches have been taken to study the CNT synthesis mechanism, such as experimental study and atomistic Molecular dynamics (MD)/Monte Carlo (MC) simulations. Experimental studies can generate CNTs with length between 500nm and 16cm. But they are expensive and the characterization is tedious and limited by the current in situ measurement precision technique. Atomistic simulation can explore the atomistic evolution during the synthesis process, and can explain the process not observed in experiments. But the computational overhead involved in MD/MC simulations has limited the atomistic simulation only to the initial stage of CNT synthesis process. We found that the LGP prediction model can be used to speed up the atomistic simulation. Our meso-scale MC simulation of vertical aligned CNT synthesis in CVD process shows that the CNT growth increment exhibits nonlinear and recurring near-stationary dynamics, and the majority (80-95%) of the computational overhead is due to the relaxation process implemented at every growth step. LGP model can be applied to predict the growth increment and the CNT structure is put to near-optimum position before MC moves in the simulation, and thus the relaxation time is largely reduced. The prediction based acceleration approach can reduce computation time by about an order of magnitude compared to conventional meso-scale MC models, leading to the growth of one of the longest CNTs reported from atomistic simulations. This accelerated simulation model can be applied to capture the CNT length variation during the synthesis, and can be used for control and monitoring purpose.

7. **A Predictive Model for Pulmonary Toxicity Of Carbon Nanotubes – Implications for Nanomaterial Characterization Standards**

Jeremy Gernand (Carnegie Mellon University)
Elizabeth Casman (Carnegie Mellon University)

The ability to map nanoparticle properties to nanotoxicity would be a significant advancement in nanotoxicology. This goal has been thwarted by inconsistencies and omissions in nanoparticle characterization measurements reported in the nanotoxicology literature. Yet, even with this imperfect data base it is possible to identify nanoparticle characteristics with high information content using machine learning techniques. We identify such characteristics for pulmonary exposures to carbon nanotubes (CNTs) and make recommendations for future CNT measurement and reporting.

To develop predictive models of CNT pulmonary toxicity from CNT properties, we performed a meta-analysis of CNT *in vivo* pulmonary inflammation and toxicity studies. From the predictive models we ranked nanomaterial attributes and experimental parameters according to their influence on toxicity indicators. The analysis employed random forest models based on ensembles of regression trees, a machine learning technique useful for identifying high information value attributes in sparse, high-dimensional, and non-linear contexts. The information contents of attributes were quantitatively compared with each other for both uniqueness and the degree of correlation for several measures of toxicity. Together with model complexity criteria, these metrics were used to provide a quantitative commentary on proposed characterization standards for nanomaterial experiments, such as those of the MinChar Initiative.

To facilitate the mapping of CNT properties to toxicity, our results suggest that future CNT toxicity studies should at a minimum report high information value nanomaterial characteristics. Distributions of measurements of some parameters carry important information that is lost when the attributes are reported as means or modes. For CNTs, these include distributions of the unaggregated CNT fragment lengths and distributions of aggregate dimensions. When distributions of geometric parameters are reported, the fractions responsible for the toxicity can be identified by the random forest method and irrelevant fractions do not obscure the relationship. Several other characteristics were found to be important, including CNT diameter (a surrogate for multi or single walled structure) and impurity content. When measuring toxicity by total cell count in bronchoalveolar lavage (BAL) fluid, the influence of impurities on toxicity was typically less than a quarter the influence of the CNTs themselves. By contrast when measuring toxicity by total protein in BAL fluid, impurity content including oxidized carbon and metals (particularly cobalt and aluminum) did play a significant role in toxicity, followed by CNT diameter.

8. **Collaboration, Data Management and Analysis Tools for Nanomaterial Characterization and Toxicity**

Taimur Hassan (University of California, Los Angeles)
Haven Liu (University of California, Los Angeles)
Rong Liu (University of California, Los Angeles)
Robert Rallo (University of California, Los Angeles)
Yoram Cohen (University of California, Los Angeles)

Assessment of the potential environmental impact of engineered nanomaterials (ENMs) requires fundamental physicochemical and toxicological characterization of nanoparticles in order to elucidate assess their potential environmental impact. In order to develop strategies for their safe design and use, adequate toxicity and physicochemical property databases of ENMs are required. In this regard, a crucial requirement is the development of an information technology platform for data and research collaboration. Accordingly, the Data Management Team at the Center for the Environmental Impact of Nanomaterials (CEIN) has developed a Data Management (CDM) platform that provides three important functions: (a) Data management, (b) Resource and communication management, and (c) hosting of web-based knowledge extraction tools. The Data management function includes an online data repository for CEIN generated data that makes use of a workflow for data submission that includes annotating data with related to the generated data, and a strict data files review and acceptance criteria. The above approach enables advanced searching capability and generation of tabulated summaries of experimental data and other related information. Resource and communication management is a center-wide resource for dissemination of nanomaterial related information, including online distance learning course sites, reports, forms, personal profiles and online storage. Web-hosted knowledge extraction tools (e.g., analysis of high throughput toxicity data, environmental distribution of nanoparticles) allow remote access to online data analysis tools. Tools for data retrieval, high throughput data analysis, as well as nanomaterial distribution modeling are currently deployed within CDM. Finally, in order to promote data sharing amongst researchers, the above functions are supplemented with outreach efforts that include: (a) periodic reporting and publicized site usage statistics to update researchers of compiled information and encourage timely uploads of new data, (b) online help manuals and multimedia demonstrations of system capability and use, and (c) keeping research groups abreast of new features and services via electronic newsletters and webinars.

9. **A Paradigm Advancing Toxicity Testing of Nanomaterials in the 21st Century and QSAR Models Development**

David Y. Lai (US Environmental Protection Agency)

In this proposed paradigm, the toxicological properties of a small number of well characterized reference materials of each class/subclass of nanoparticles are first characterized by short-term *in vivo* studies in rodents. *In vivo* and *in vitro* high-throughput genomics and/or proteomics studies are then performed to investigate the underlying molecular mechanisms/toxicity pathways and biomarkers of the toxic responses. Mechanism-based short-term i*n vitro* assays in appropriate cell lines are also conducted to aid in elucidation or interpretation of mechanisms, toxicity pathways and biomarkers data derived from the *in vivo* studies. Once these mechanistic data on reference materials are obtained, they can be used to benchmark and predict the effects and hazard potential of a particular nanoparticle belonging to the same class/subclass by comparing data of their *in vitro* high-throughput and mechanism-based short-term *in vitro* assays. Using this paradigm, hazard potential of a particular nanomaterial could be semi-qualitatively evaluated. Quantitative risk assessment can be conducted when dose-response modeling of perturbations of pathways function, toxicokinetics data and PBPK modelings for i*n vitro* and *in vivo* extrapolation are available. With well-designed experiments, testing nanomaterials of varying/selected physicochemical parameters may be able to identify the physicochemical parameters contributing to toxicity. The data so derived could be used for the development of computer model systems to predict the hazard potential of specific nanoparticles based on property-activity relationships.

Introduction

Currently, there are a number of issues on toxicity testing of nanomaterials by traditional *in vivo* and *in vitro* studies. Toxicogenomics and other technologies (*e.g*., proteomics) could contribute to the elucidation of molecular mechanisms of nanomaterials. For the emerging field of nanotoxicology, the use of high-throughput or low-throughput “predictive toxicity” appears to be the only possible solutions to effectively deal with the issues involved in hazard identification and safety assessment of diverse nanomaterials with varying physicochemical properties. However, at present, this approach alone is unlikely to succeed in evaluating the toxicity of the wide array of nanomaterials and requires validation from *in vivo* studies. This article proposes a paradigm for toxicity testing and elucidation of the molecular mechanisms of reference materials of specific nanomaterials classes/subclasses using short-term *in vivo* animal studies in conjunction with high-throughput screenings and mechanism-based short-term *in vitro* assays. The hazard potential of a particular nanomaterial can then be evaluated by conducting only *in vitro* high-throughput assays and mechanistic studies and comparing the data with those of the reference materials in the specific class/subclass. Using this paradigm, hazard potential of a particular nanomaterial could be semi-qualitatively evaluated. Quantitative risk assessment can be conducted when dose-response modeling of perturbations of pathways function, toxicokinetics data and PBPK modelings for i*n vitro* and *in vivo* extrapolation are available.

10. **Mining High Throughput Screening Data of Nanotoxicity**
Rong Liu (University of California, Los Angeles)
Saji George (University of California, Los Angeles)
Bryan France (University of California, Los Angeles)
Sijie Lin (University of California, Los Angeles)
Zhaoxia Ji (University of California, Los Angeles)
Taimur Hassan (University of California, Los Angeles)
Robert Damoiseaux (University of California, Los Angeles)
Tian Xia (University of California, Los Angeles)
Robert Rallo (University of California, Los Angeles)
Kenneth Bradley (University of California, Los Angeles)
Andre E. Nel (University of California, Los Angeles)
Yoram Cohen (University of California, Los Angeles)

Nano-sized materials are increasingly utilized in many industrial products and processes, with over numerous commercial products utilizing engineered nanomaterials (eNMs), primarily due to their unique nano-scale properties. Despite the many beneficial uses of nanomaterials, there is a growing public concern regarding the potential release of eNMs to the environment and the potential adverse impacts of exposures to eNMs. Although there are mounting studies on the toxicity of eNMs, understanding of the general principles governing eNMs toxicity potential and the long-term environmental health and safety associated with eNM containing products is in its infancy. In this regard, high throughput toxicity screening is critical for characterization of the potential hazard of eNMs, which is in turn indispensable information for subsequent risk assessment and development of environmental and health regulatory policies. In the present work, data mining demonstrated that it is an efficient and reliable approach for knowledge extraction from high throughput screening (HTS) data of nanoparticle toxicity. Particularly, with Self-Organizing Map (SOM) analysis, clusters (groups of similar nanoparticles) corresponding to sub-lethal pro-inflammatory responses associated with ROS generation, lethal genotoxic responses, and cytotoxicity were identified from a HTS data set of the activities of ten different signaling pathways of BEAS-2B cell line. Association rule mining led to discovery of relationships among various toxicity-related signaling pathway activities of RAW and BEAS-2B cell lines exposed to metal/metal oxide nanoparticles (at ~0.39-200 mg/L). The identified association rules revealed pathways that are co-regulated by the nanoparticles and are useful in the selection of proper endpoint development for nano-quantitative-structure-activity relations (nano-SARs). Based on a HTS toxicity data set of the BEAS-2B cell line, a classification nano-SAR for metal oxide nanoparticles was developed, which can be used to identify decision boundaries with respect to hazard ranking of nanoparticles. Another aspect of HTS data mining was the development of an automatic phenotype (e.g., hatched, unhatched and dead) recognition system in order to facilitate in-vivo HTS zebrafish toxicity screening of eNMs based on analysis of captured optical images. Finally, in the current research, rapid knowledge extraction was aided by an online HTS Data Analysis Tool (HDAT) developed with modules of HTS data visualization, outlier removal, normalization, summarization, and hit identification.

11. **COMBIOMED and Ibero-NBIC Networks, Promoting Nanoinformatics and Analysing the Synergies with Biomedical Informatics.**
G Lopez-Campos (Carlos III Health Institute)
V Lopez-Alonso (Carlos III Health Institute)
I Hermosilla (Carlos III Health Institute)
F Martín-Sánchez (Melbourne Medical School)
A Pazos (University of A Coruña)

A Freire (University of A Coruña)
JA Seoane (University of A Coruña)
J Dorado (University of A Coruña)
V Maojo (Universidad Politecnica de Madrid)

In recent years the developments and maturity achieved in the field of nanotechnology and other disciplines such as biotechnology, information technologies and cognitive technologies have been coming together in different fields and this confluence has coined the term of NBIC technologies. An important and common characteristic of these technologies is the necessity of dealing with a vast amount of information and the need of developing tools and methods for that purpose. In this context it is important the development of nanoinformatics and its confluence also with the other fields such as bioinformatics for the support of data storage and analysis of these confluent technologies. In this context the COMBIOMED and Ibero-American Networks represent an opportunity to include the development and follow up of the advances done in the nanoinformatics field and its biomedical applications into the broader biomedical informatics.

The Cooperative Thematic Research Network on Computational Biomedicine COMBIOMED was approved in the last call for Thematic Networks in Health Research within the Spanish National Plan for Scientific Research, Development and Technological Innovation and it is funded for the period 2008-2011. The COMBIOMED Network is currently addressing various aspects that range from basic to applied research in science for the development of methods and tools to solve problems in biomedical science in the context of personalized medicine including the development of the nanomedicine and the management and analysis of these new data types.

Ibero-NBIC network is funded by the CYTED (Ibero-American Program for Science and Development) for the period 2009-2012 has among its aims the nanoinformatics and its development and needs in the Ibero-American region. The network Ibero-NBIC has 11 nodes from 7 different countries (Spain, Portugal, Argentina, Brazil, Chile, Uruguay and Venezuela) with complementary expertise in the four areas of NBIC and it is coordinated by the Spanish Node of University of A Coruña. This project aims to gather a broad community of scientists from the Ibero-American region that know, develop and assess applications of Convergent Technologies in Healthcare from an integrative and multidisciplinary perspective. The network promotes synergies among countries, disciplines and methods, and it will pay special attention to the related nanoinformatics needs and developments. Training and mobility of researchers and knowledge management in the field are also issues to be addressed by this project.

12. **Informatics Guided Computation of Physical and Chemical Properties of Nanomaterials**
Claudia Loyola (CoSMIC , Iowa State University)
Krishna Rajan (CoSMIC , Iowa State University)

Understanding the fundamental mechanisms by which nanoparticles degrade is critical to aid in the understanding of their potential toxicity. The aim of this presentation is to describe how we use informatics to first identify key electronic and crystal structure and use that information to guide fundamental electronic structure of materials to explore their reactivity. Particular focus will be directed towards the use of density of states, band structure, charge density and electron localization functions, the last two properties are for studying bonding parameters in oxide nanoparticles.

CoSMIC (Combinatorial Science & Informatics Collaboratory)
http://cosmic.mse.iastate.edu

13. **A Computational Model for Integrating Nanomedical and Nanoinformatic Techniques to Build a Unified Centralized and Standardized System Applied to Nutrigenomics of Obesity and Cardiovascular Diseases**

F Madueño (Universitat Jaume I, Carlos III Health Institute)
Z Falomir (Universitat Jaume I, Carlos III Health Institute)
G Lopez (Carlos III Health Institute)
V Lopez (Carlos III Health Institute)
D Corella (Universitat de València, CIBER Physiolopatology of Obesity and Nutrition)
O Coltell (Universitat Jaume I, Carlos III Health Institute)

Introduction
Nanoinformatics is an emerging discipline that arises to organize and efficiently manage the amount of information exponentially generated in nanotechnology and nanomedicine research. This growing disciplines produce scattered and disorganized data that requires a complex interpretation process and it emphatically increases when applied to nanomedicine. The possible interactions of the new nanomaterials with alive beings imply an accurate definition of the involved risk assessment before its practical application because their interaction with the rest of particles can alter the system producing unknown effects, particularly in human beings.

Standards must be defined to deal efficiently with information, determining all the involved nanomaterials and the relationships among them. By applying these standards, a model explaining the relationships and interactions among the nanocomponents from the viewpoint of the global system can be generated. Currently, most of the developed ontologies and models have been centered in the field of cancer research. Moreover, as far as we are concerned, there are no similar studies or initiatives in literature related to cardiovascular genomic and obesity nutrigenomic research.

Objectives
The contribution of this work is the development of a computer system that integrates:
(i) nanomedical new conceptual models, (ii) an information architecture and (iii) computational mechanisms designed specifically for Nanoinformatics and Nanomedicine. A unified, centralized and standardized nanocomponent data model will be obtained and used to compare the characterization of features and properties of each nanocomponent and then it will be applied to the regulation of food intake and other metabolic processes involved in the prevalence of different phenotypes in obesity and cardiovascular diseases.

The requirements of such a computer system are: (1) defining uniquely the nanocomponents and their relationships; (2) defining an ontology for describing nanotechnology and applying it to Nanonutrigenomics; (3) creating a metasearch engine or metacrawler for automatically unifying information in different databases; (4) developing models for simulating interaction patterns with the safety, quality and health constraints in the administration to human patients; and (5) broadcasting results to all stakeholders.

Methods and results
This project is divided into the following work packages: (a) data collection and classification, (b) defining relationships among unique nanocomponents, c) creating a description logics (DL) based-ontology, (d) writing a metasearch engine or metacrawler, (e) development of an interaction model, and (f) dissemination of results.

Conclusions
Biomedical Informatics and Nanoinformatics are essential to support research in cardiovascular genomics and obesity nutrigenomics by managing, organizing, and securing nanotechnology processes otherwise

unworkable. As a result, a unified, centralized, tested and standardized data model will be generated to allow a more intelligent comparison of their characterization features of each nanocomponent. This is an step forward to the acceleration and development of nanotechnology and nanomedical research, and to the regulation of food intake and other metabolic processes involved in the prevalence of different phenotypes in obesity and cardiovascular diseases.

Acknowledgements
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14. **Nano-enhanced Remediation: Opportunities for Safety and Health Oversight at the State Level through Nanoinformatics**

Ephraim Massawe (Southern Louisana University)
Thomas Frazier (Southern Louisana University)
Chase Dupre (Southern Louisana University)

Nano-enhanced remediation is fast, cost-effective and a promising technique of conducting clean-up operations at thousands of hazardous waste sites in the country where persistent, bioaccumulative and toxic wastes are deposited. However, the lack of validated protocols and instrumentation needed to gather preliminary information on environmental, safety, and health impacts of various nanomaterials is a persistent problem. The promotion of nanomaterials, particularly for environmental remediation, calls for serious consideration in the collection, validation, storage and sharing of relevant information to support actions capable of limiting exposures to nanomaterials and preventing potential adverse health effects to workers and the general public. Nanoinformatics will likely play a greater role in providing a framework to support this endeavor.

This presentation is the analysis of responses from the state government agencies to a survey questionnaire focusing on nanoinformatics for nano-enhanced remediation. The questionnaire was derived from the conceptual nanoinformatics' framework previously developed to understand the role of nanoinformatics for safety and health oversight at the local level specifically during nano-enhanced remediation. It is hypothesized that the information collected and collated will support various regulatory initiatives designed to prevent occupational and non-occupational health risks from exposures to nanomaterials during environmental remediation operations. Nanoinformatics techniques presented here will also promote the development of predictive models and mechanisms to support regulatory and standards setting processes, and to provide the basis for safety and health oversight. Subsequently, nanoinformatics for nano-enhanced remediation will very likely expand the capability of the state agencies to respond to the challenges of managing exposures to nanomaterials during nano-remediation operations.

15. **Nanomaterial Registry**

Karmann Mills (RTI International)

The Nanomaterial Registry (NR) is a web-based tool for the nanomaterial community under development by RTI International, under the funding of the NIH. The NR will be a publically-available, curated database containing physico-chemical characteristics (PCC) and biological and environmental interaction data of well-characterized nanomaterials. The data curated into the NR will be the minimal information about nanomaterials (MIAN) needed to determine a biological or environmental behavior. This list of MIAN was developed with the agreement of stakeholder group representatives to give it broad community acceptance.

Nanotechnology is a fast growing and enabling technology with extremely diverse research and applications. As this growth occurs, so does the information produced from the broad range of stakeholder groups invested in nanomaterials. Because there is such vast growth across a wide variety of stakeholder groups, there are several ever growing needs within the nanotechnology community, including:

- Standards for testing
- Regulations for handling and processing
- Resources for data comparison
- Information on what data gaps exist
- Community agreement on the MIAN

To provide a tool that addresses the needs of the nanotechnology community, RTI is creating this web-based, curated data source. This resource is being built through collaborations with representatives from many stakeholder groups within the nanotechnology community, including: industry, regulatory, government, and academia.

The significant long-term impact expected from the NR on the nanotechnology community includes the aid in:

- Developing new models, assays, standards, and manufacturing methods
- Accelerating the translation of new nanomaterials for biomedical and environmental applications
- Promoting standards and support science-based regulatory decision-making

16. **Munging for Deeper Meaning in Nanotoxicologic Studies with Select Model-Driven Discovery, Cleaner Nano-Ontolytics, and Tightly-Targeted In Silico Text Queries**
LaVerne Poussaint(DeepMed Library)
Devashish Tyagi (DeepMed Library)

Background / Purpose:
NanoTox MDD is a nano-knowledge discovery interface. With improved tweaking and testing, it will address urgent and unmet needs within nanotoxicology and nanopathology subfields.

Main conclusion:
Model-driven discovery within the NanoToxicology sub-domain would better serve the knowledge needs of researchers. NanoBioInformatics is the leap forward in risk regulation, rather than presently prevalent reductionistic approaches.

The poster can be viewed at: http://f1000.com/posters/browse/summary/1089204

17. **Nanoinformatics: Lessons from Building Materials Data Systems**
John Rumble (R&R Data Services)

The last two decades of the last century saw a sharp increase in computerizing materials data. Activities included (1) digitizing existing data collections, (2), establishing data recording and integration standards, (3) designing portals, and (4) integrating data into computer-aided engineering systems. As the field of nanoinformatics grow, especially with respect to information about materials at the nanoscale, it is useful to look back at some of the lessons learned in building materials data systems. Because the majority on new data is now generated in digitally, we will discuss only the last three subjects, especially with respect to minimum required characteristics.

Several organizations engaged in developing standards to record or integrate materials data, including ASTM International and ISO. The standards covered materials description, reporting of test property data and the involved independent variables. Standards were developed for a wide variety of materials, leading to definition of seven classes of information for describing a material. Data recording standards identified key types of independent variables that needed to be recorded to make a test result usable. In both cases, information was divided into three types: the minimum data required for a test result to be meaningful; additional information often reported; and information less often reported.

One problem encountered in building these standards was the large number of test methods in common use. That fact that many material "properties" were really not intrinsic properties, but rather the results of a standardized protocol that correlated well with actual service conditions over time added further complications. Another issue were composite materials that did not exist as a material separate from the product they were built as.

During this time, several government agencies and professional societies worked together to develop "one-stop shopping" for materials data. A prototype system developed by NIST, DOE, and the Army led to a National Materials Property Data Network (NMPDN) operated in the private sector into the 1990s. One of the major challenges facing NMPDN was the diversity of materials and materials data types. As new materials classes and new types of properties were added, the cost of integrating a new data resource did not become incremental. This fact came about because different materials required different descriptions. An alloy is described much differently than a ceramic and both much differently from a polymer. The same was true for test data. With as many as 200+ independent variables involved in some property test results, simply handling the semantics of new variables was time consuming.

Because materials are the "stuff" from which physical products and systems are built, integration of materials data and data systems into computer-aided engineering systems was important. ISO 10303 – The Standard for the Exchange of Product Data (STEP) fully integrated materials data into its work. This required considering a material to be a "product" itself, and recasting its description into the language of product description.

In this poster presentation, I will provide examples of these three activities and describe lessons learned that are relevant to nanoinformatics today.

18. **What Is Minimum Characterization For Effective Informatics?**
Aleks Stefaniak (NIOSH Nanotechnology Research Center)

19. **An Integrated and Comprehensive Data Mining System for Studying Environmental Impact of Nanomaterials: NEIMiner**
Kaizhi Tang (Intelligent Automation, Inc.)
Wei Wang (Intelligent Automation, Inc.)
Thomas Wavering (Intelligent Automation, Inc.)
Roger Xu (Intelligent Automation, Inc.)
Stacey Harper (Oregon State University)

To reduce the risk of nanomaterials in military use, NM environmental impact analysis requires a comprehensive NEI modeling framework, centralized NEI database, powerful model discovering tool and integrated model composition strategy. An integrated information system for NEI utilizing data integration, CMS, data mining and data visualization based on a comprehensive NEI modeling framework will be a useful tool for NEI model discovery and assessment.

Keynote Biographies

Christian Lehinger (HealthQuest Alliance)

Christian Lehinger, MCSE, has been working in the field of health information management for over 15 years. Christian began his career in healthcare working with Inland NW Health Services. Here he was exposed to the hospital care technology infrastructure by discovering the disconnects that exist in health information dissemination between hospitals and private care. In 1999 Christian founded an organization thats purpose was to help medical clinics integrate technology into their practice to increase efficiency and profitability and to improve patient care. His experience both in the hospital and private care settings helped him to see how the lack of information interoperability has had dilatory effect on the health care system and this breakdown in communication is what is holding back the healthcare industry today, as well as many other industries that rely on information dissemination. In 2005 Christian formed what is now known as HealthQuest Alliance, an organization comprised of an information technology division supporting over 75 clients nationwide, a medical care services division that works with primary care medical clinics in three states, and a software development team with two products in commercial use today. Using the patent DDCNet Patent 7,810,145 that Christian invented in 2003, HealthQuest Alliance is working to bridge the gap in information interoperability by demonstrating how information management across all areas of healthcare is possible and will dramatically change the future of healthcare. Christian is Certified in Infrastructure by Microsoft.

Gerhard Klimeck (Purdue University, nanoHUB)

Gerhard Klimeck (http://nanohub.org/klimeck) is the Director of the Network for Computational Nanotechnology at Purdue University and a Professor of Electrical and Computer Engineering. He guides the technical developments and strategies of nanoHUB.org which served over 167,000 users worldwide with on-line simulation, tutorials, and seminars in the year 2010. He was the Technical Group Supervisor of the High Performance Computing Group and a Principal Scientist at the NASA Jet Propulsion Laboratory. Previously he was a member of technical staff at the Central Research Lab of Texas Instruments where he served as manager and principal architect of the Nanoelectronic Modeling (NEMO 1-D) program. At JPL and Purdue Gerhard developed the Nanoelectronic Modeling tool (NEMO 3-D) for multimillion atom simulations. The latest tools OMEN and NEMO5 developed in his research group scale almost perfectly to over 221,000 cores. Prof. Klimeck's research interest is in the modeling of nanoelectronic devices, parallel cluster computing, and genetic algorithms. Dr. Klimeck received his Ph.D. in 1994 on Quantum Transport from Purdue University and his German electrical engineering degree in 1990 from Ruhr-University Bochum. Dr. Klimeck's work is documented in over 160 peer-reviewed journals and 150 proceedings publications and over 160 invited and 330 contributed conference presentations. He is a fellow of the Institute of Physics, a senior member of IEEE and member of APS, HKN and TBP. His research group can be found at https://engineering.purdue.edu/gekcogrp/.

Deborah Gracio (Pacific Northwest National Laboratory)

Deborah Gracio joined Pacific Northwest National Laboratory in 1990 and is currently the Director for the Computational and Statistical Analytics Division. Since joining the laboratory, Gracio has led the research, development, and management of multiple cross-disciplinary, multi-laboratory projects focused in the basic sciences and national security sectors. Her work has included research and development of integrated computational environments for biodefense, computational biology, computational chemistry, and atmospheric modeling. Gracio was the director of the Data-Intensive Computing Initiative and research started in this program continue to address the acquisition challenges of high-throughput streaming data, workflow, provenance, and the development of an integrated architecture to support a distributed analysis environment. Since joining the Laboratory, Gracio has been involved in a variety of projects that have aided in developing a broad technical background in computer systems integration, software engineering, scientific computing, large-scale data management, and data acquisition.

Speaker and Theme Chair Biographies

Nathan A. Baker, Ph.D. is currently the Chief Scientist for Signature Sciences at Pacific Northwest National Laboratory. After his research training at UC San Diego, he joined the Department of Biochemistry and Molecular Biophysics at Washington University in St. Louis in 2002 and was promoted to Associate Professor with tenure in 2006. In June 2010, he moved to Pacific Northwest National Laboratory as Chief Scientist for Signature Science. Dr. Baker is currently Lead for the National Cancer Institute caBIG Nanotechnology Working Group, Chair for the ASTM E56.01 Subcommittee on Nanotechnology Informatics, and Editorial Board Member for the Biophysical Journal. His research is in the area of computational biophysics, nanotechnology, and informatics. He is actively involved in the development of new algorithms and software for computational biology and modeling in support of these research projects, including development of the APBS and PDB2PQR biomolecular electrostatics software packages (http://www.poissonboltzmann.org/) and the NanoParticle Ontology (http://www.nano-ontology.org/).

Dr. Amy E. W. Bednar is a Research Mathematician for the Information Technology Laboratory (ITL) at the U.S. Army Engineer Research and Development Center (ERDC), Vicksburg, MS. She performs numeric analyses and develops numeric models. Dr. Bednar earned a bachelor’s in mathematics with an emphasis in applied mathematics and English from Spring Hill College, Mobile, AL, in 2000. She earned a master’s and doctorate in mathematics with an emphasis in topology from the University of Mississippi in May 2002 and December 2003, respectively.

Dr. Bednar is currently leading the development of NanoExPERT (Nanomaterials Experiment-based Predictor of Environmental Risk and Toxicity). NanoExPERT is an internet-accessible predictive model by which an interested user may acquire information regarding the potential ecological risk posed by nanoparticles based on chemical, physical, or bioaccumulation data obtained through experimentation. The model utilizes a material property database that describes environmentally relevant attributes of nanomaterials for technology development. NanoExPERT uses available experimental data from groupings of nanoparticles that are chemically and physically similar to predict the fate of other nanoparticles. Nanoparticles that behave similarly will be grouped by hierarchical clustering based on their properties and toxicology information, and data available within each cluster will be leveraged to generate predictive output for nanoparticles for which full information is unavailable.

Dr. Bednar is also leading the development of CEA-CMD (Comprehensive Environmental Assessment - Conceptual Model Developer). CEA-CMD is a user-friendly software tool to support the development of a generic conceptual model of new materials for the CEA. CEA-CMD will facilitate the user's building the concept model of the life cycle and risk pathways for a material and/or chemical.

Gretchen Bruce, DABT, is a senior scientist with 20 years of professional experience as a toxicologist and risk assessor. Ms. Bruce's project and project management experience includes site characterization and regulatory based risk assessment, exposure assessment, litigation support services, public health evaluations, probabilistic exposure model development, and historical dose reconstruction. Ms. Bruce's primary expertise is in the conduct of toxicological evaluations. On a wide-range of litigation and human health risk evaluation projects, Ms. Bruce has conducted critiques of the toxicological data and literature and characterized likely effect levels and adverse health impacts. In addition, Ms. Bruce has provided toxic tort litigation support in cases where materials were released from industrial facilities and present in workplace environments and consumer products. These projects included assisting in the evaluation of animal and human data for use in establishing a reference dose for perchlorate; characterizing the state of knowledge regarding the toxicity of numerous compounds including metals, solvents, and other organics; assessing probable adverse health effects and toxicity thresholds for organophosphate compounds leaked into airplane cabin air from engine oils and hydraulic fluids; conducting historical reviews of the development of toxicity testing protocols for consumer products and the development of knowledge of lead and arsenic toxicity; and assessing risks of metals and dioxins released from manufacturing facilities.

As a risk assessor, Ms. Bruce has managed and conducted risk assessments for industrial and residential sites in accordance with federal CERCLA/RCRA, state, and local guidance for more than a dozen states. Project experience includes using mathematical models to assess fate and transport and establish site cleanup levels; negotiating with regulatory agencies; designing and conducting field sampling programs and laboratory QA/QC reviews; establishing safe worker-exposure levels to newly developed materials and chemical mixtures; completing a 40-year historical dose reconstruction of mercury released from the U.S. Department of Energy's Oak Ridge Reservation; conducting detailed evaluations of the validity of default assumptions for site-specific assessments; and designing multipathway probabilistic exposure models to characterize the uncertainty and variability in estimated doses.

Mr. Caprio is the Executive Director of the NanoBusiness Commercialization Association. In November 2008, Mr. Caprio co-founded The Water Innovations Alliance with Mark Modzelewski. Mr. Caprio is one of the foremost advocates for government funding of emerging technologies at both the State and Federal levels. Mr. Caprio has testified before the state legislatures of New York and Connecticut, and has participated in NanoBusiness' Washington, DC Roundtable for the past nine years. Mr. Caprio is the founder and event director of the 10th Annual NanoBusiness Conference being held in Boston, MA at the Seaport World Trade Center. During the past five years (2006-2011), Mr. Caprio was an invited speaker and guest lecturer on Nanotechnology at over 50 conferences. In 2010 Mr. Caprio has spoken at the NNI Strategic Planning Stakeholder Workshop and the Nanotechnology Partnership Forum at NIST.

Mr. Caprio is a 25-year publishing and tradeshow industry veteran with an impressive track record of launching events focusing on emerging technology markets. Mr. Caprio joined the NanoBusiness

Commercialization Association as the Founder and Event Director in 2002, to steer the launch of the highly successful NanoBusiness event series in 2008 & 2009. In 2003 & 2004, Mr. Caprio served as the Event Director in the launch of The Emerging Technologies Conference in association with MIT's Technology Review Magazine. Mr. Caprio has served as a consultant to the leading emerging technology research and advisory firm Lux Research, for its Lux Executive Summit in 2005 & 2006. In 2002, Mr. Caprio served as the Event Director and Program Director of the Forbes/IBM Executive Summit. Prior to joining the NanoBusiness Commercialization Association, Mr. Caprio was Event Director for Red Herring Conferences, producing the company's Venture Market conferences and Annual Summit reporting to Red Herring Magazine Founder and Publisher Tony Perkins. His industry peers have formally recognized Mr. Caprio on several occasions for his talents in both tradeshow management and sales. Mr. Caprio was named Sales Executive of the Year in 1994, while with Reed Exhibitions. Mr. Caprio, while employed with Reed Exhibitions, was honored with two Pathfinder Awards in 1995 for launching the New York Restaurant Show.

Mr. Caprio graduated from Villanova University in 1979 with a B.S in Accounting and completed a MBA from Northeastern in 1987. Mr. Caprio is a member of Villanova University's Financial Club and serves as an active member of Villanova's President Club. Mr. Caprio serves on the Board of Trustees for the Easton Community Center and the Easton Learning Foundation in Easton, CT. In the summer of 2008, Mr. Caprio was appointed to the Board of Directors for the Fabricators & Manufactures Association Communications, Inc. based in Rockford, IL.

Dr. Altaf Carim is currently the OSTP Assistant Director for Nanotechnology. He has overseen the development and operations of a number of major scientific user facilities supported by the Office of Basic Energy Sciences (BES) at the Department of Energy (DOE), including five Nanoscale Science Research Centers and three Electron Beam Microcharacterization Centers. He represented DOE on the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council â€“ the interagency body responsible for the NNI â€“ from 2002 through 2010, and co-chaired that body from 2006 to 2009. He currently leads the BES team that manages the Energy Frontier Research Centers, major research collaborations started in August 2009 that focus on the long term basic research needed to overcome roadblocks to revolutionary energy technologies.

Dr. Carim entered Federal service in the Office of Basic Energy Sciences at DOE in September 2001. Prior to joining the Scientific User Facilities Division in October 2005, he was a program manager in the Division of Materials Sciences and Engineering with primary responsibility for activities in the structure and composition of materials. Before joining DOE, Dr. Carim was on the faculty at The Pennsylvania State University (in the Department of Materials Science and Engineering and as Chair of the Electronic and Photonic Materials program. He was a faculty member at the University of New Mexico and had prior research posts and activities at the Philips Natuurkundig Laboratorium in The Netherlands, Philips Research Laboratories Sunnyvale, Bell Laboratories, and the Xerox Palo Alto Research Center. He also was a visiting investigator at the Carnegie Institution of Washington during a year-long sabbatical.

Dr. Carim's primary scientific expertise is in microstructural and microchemical characterization of materials, with research contributions in a variety of areas, including semiconductor interfaces, superconducting and ferroelectric oxide thin films and ceramics, crystal structure determination, crystalline defects, joining of ceramics and composites, development of anisotropic microstructures, electron holography, and morphology of nanoparticles and nanowires. He has authored or coauthored over 85 research publications in these areas and has given over 100 conference, seminar, and other presentations. He has been active in numerous professional societies, organized a number of technical meetings and symposia, and held editorial roles with several journals. His awards and honors include recognition as an Office of Naval Research Young

Investigator, receipt of an AIST Foreign Researcher Invitation to lecture in Japan, and participation in the project teams recognized with several of the Secretary of Energy's Project Management Excellence Awards.

Dr. Yoram Cohen received his B.A.Sc., M.A.Sc., in 1975 and 1977, respectively, both in Chemical Engineering, from the University of Toronto, and his Ph.D. from the University of Delaware in 1981. He has been on the Faculty of Chemical and Biomolecular Engineering at the University of California, Los Angeles (UCLA) since 1981. He is also an Affiliate Faculty at the UCLA Institute of the Environment and an Adjunct Professor at Ben-Gurion University. He was a Visiting Professor at the Technion (1987-1988), at Universitat Rovira i Virgili (1944) and a Distinguished Visiting Professor at Victoria University (2006). He is a founder and Director of the Water Technology Research Center and the Center for Environmental Risk Reduction, and a member of the UCLA/National Science Foundation (NSF) Center for the Environmental Implications of Nanotechnology (CEIN). Dr. Cohen is a UCLA Luskin Scholar and a recipient of the 2008 Ann C. Rosenfield Community Partnership Prize in recognition of his environmental research. He received the 2003 Lawrence K. Cecil award in Environmental Chemical Engineering from the American Institute of Chemical Engineers (AIChE), the AIChE Separations Division Outstanding Paper Award (1997 and 2009), and was elected Fellow of the AIChE in 2009. In 2008 he received a County of Los Angeles Commendation (2008), a State of California Senate Certificate of Recognition, and a Certificate of Special Congressional Recognition (US) for contributing to legislation to protect public health and dedicated service to the Los Angeles community. Dr. Cohen served as Chair of the AIChE Environmental Division (2002) and of the Separation Division (2008). He published over 180 research papers and book chapters, presented over 300 papers in scientific conferences and gave over 130 invited talks on environmental impact assessment, contaminant fate and transport, surface nano-structuring, water treatment and desalination, and membrane science and technology. He is also the Editor of three environmental volumes. Dr. Cohen developed patented technologies in water desalination technology, surface nano-structuring, membrane synthesis, and chemical sensors, as well as models and software for environmental multimedia assessment. His present research on the environmental implications of nanotechnology focuses on the development of models and tools for assessing the toxicity of nanomaterials based on high throughput screening, quantitative-structure relations for toxicity and physicochemical properties of nanomaterials, environmental distribution of nanomaterials, and environmental impact assessment. He is also engaged in research on water technology including the development of approaches for distributed smart water systems, optimization, monitoring and control of water treatment systems, water desalination, and membrane development. He has served on numerous Government Advisory Committees (including the USEPA Science Advisory Board and the NRC Board on Environmental studies and Toxicology), recently served on the Blue Ribbon Committee of the Metropolitan Water District of Southern California, and is an active participant in the Nanoinformatics initiative.. Dr. Cohen organized over thirty scientific conferences including the 2008 International Congress on Membranes and membrane processes (ICOM), the 2009 and 2010 West Coast Water Technology Transfer workshops, and he was the Meeting Program Chair of the 2010 Annual AIChE Meeting. He is a member of a number of professional societies including the, AIChE, ACS, NAMS, IDA, AWWA and AMTA.

Joe Glick is the founder of Expertool Software, LLC, and the chief architect of the Expertool universal knowledge modeling platform and methodology. He began architecting knowledge-based solutions for medicine and business in 1983. His current company, Expertool Software, was launched in 1995 and specializes in rationalizing interdisciplinary knowledge silos and capturing human expertise in a computable form. The technology and methodology was evolved in the course of delivering complex solutions for some of the world’s largest organizations. Joe’s flagship project at Pfizer won the Upjohn Innovation Award (Dec. 2007) for the integration and rationalization of Policy, Regulatory, Technology, Legal, Process and Control knowledge bases, creating an engine for holistic change analysis and response optimization.

Joe's current research focus is the use of cognitive architectures as models for the development of computational architectures to represent knowledge about dynamic and adaptive systems. The initial area of application is systemic risk modeling for Dodd-Frank compliance.

Stacey Harper, Ph.D., is a Signature Research Faculty Fellow of the Oregon Nanoscience and Microtechnologies Institute and an Assistant Professor in the Department of Environmental & Molecular Toxicology and the School of Chemical, Biological & Environmental Engineering at Oregon State University (OSU). She earned her bachelor's degree in natural sciences and mathematics from Mesa State College, CO and her master's and doctoral degrees in biological sciences from University of Nevada Las Vegas, NV. She then served two years as a post-doctoral research fellow with the Exposure and Dose Research Branch of the EPA. In her research at OSU, she employs in vivo approaches to evaluate the biological activity and toxic potential of novel nanomaterials, and has established a collaborative, multidisciplinary research program to develop a knowledgebase of Nanomaterial-Biological Interactions (NBI). She works closely with industry, academic and government partners to ensure that environmental and human health considerations are addressed together with the development of new nanomaterials. Dr. Harper has been a working member of the ICR Nanotechnology Working Group since 2009. She also serves as the co-chair of ASTM International E56 Committee on Nanotechnologies and a representative of the ANSI-Accredited U.S. Technical Advisory Group for ISO/TC 229 which functions to formulate positions and proposals on behalf of the U.S. with response to ISO standardization activities on environmental health and safety of nanotechnologies.

Dr. Mark D. Hoover is a senior research scientist in the Division of Respiratory Disease Studies at the CDC's National Institute for Occupational Safety and Health, in Morgantown, West Virginia. Mark is a critical area leader in the NIOSH Nanotechnology Research Center and also serves as coordinator of the NIOSH Exposure Assessment Cross-sector Research Program. NIOSH is the leading federal agency conducting research and providing guidance on the occupational safety and health implications and applications of nanotechnology. Mark earned a BS degree in mathematics and English in 1970 from Carnegie Mellon University and MS and PhD degrees in engineering in 1975 and 1980 from the University of New Mexico. He is board certified in the comprehensive practice of health physics and in the comprehensive practice of industrial hygiene. Mark has developed improved approaches, techniques, and instrumentation for aerosol characterization, generation, and control; served as chairman or contributor to the development of many national and international standards; is a past chairman of the AIHA Nanotechnology Working Group; and is author or co-author of more than 180 open literature publications. He recently completed co-editing and writing a new CRC Press handbook on Radioactive Air Sampling Methods. Special emphasis areas for Mark's work in nanotechnology include a graded approach to exposure assessment and characterization of nanoparticles in the workplace, development of a prototype Nanoparticle Information Library, and promotion of opportunities to apply performance-based occupational exposure limits or control banding approaches to nanotechnology. Detailed information about the NIOSH nanotechnology health and safety research program is available at www.cdc.gov/niosh/topics/nanotech/.

Philip Lippel is an expert consultant on innovative applications of nanoscience and emerging technologies. He has worked at the national and international level on a variety of technical, policy, and science communication issues in fields including nanotechnology R&D, science education and the technical workforce, informatics, and telecommunications. Currently he is particularly interested in the emergence of nanotechnology-based solutions to problems in the energy, water, and medical fields.

Dr. Lippel served government as a senior policy analyst at the National Nanotechnology Coordination Office and as an AAAS Science and Technology Policy Fellow at the National Science Foundation; industry as a Member of Technical Staff at Agilent Technologies and as founder of L Cubed Consulting; and academia as a faculty member in the Physics Department of the University of Texas at Arlington. He was appointed as a U.S. delegate to the Working Party on Nanotechnology at the Organisation for Economic Co-operation and Development, and as a U.S. expert to the ISO/IEC Joint Technical Committee on Information and Communication Technologies.

Prof. Alexander Tropsha, K.H. Lee Distinguished Professor and Associate Dean for Research, the UNC Eshelman School of Pharmacy, UNC-Chapel Hill, received his PhD in Chemical Enzymology in 1986 from Moscow State University, Russia. He immigrated to the United States in 1989 and has been affiliated with UNC-Chapel Hill since then rising over the years from postdoc to Assistant, Associate, Full, and Endowed Professor. His research interests are in the areas of Computer-Assisted Drug Design, Computational Toxicology, Cheminformatics, and Structural Bioinformatics. His has authored or co-authored more than 140 peer-reviewed research papers, reviews and book chapters and co-edited two monographs. His research is supported by multiple grants from the NIH, NSF, EPA, and private companies. He is a member of editorial boards of several scientific journals and an elected member of the Board and vice-chair of the international Cheminformatics and QSAR Society.

Professor Krishna Rajan is the Wilkinson Professor of Interdisciplinary Engineering and Director of the Institute for Combinatorial Discovery at Iowa State University. He is holds appointments in the Department of Materials Science & Engineering and the Bioinformatics and Computational Biology Program. He received his BASc in Metallurgy and Materials Science from the University of Toronto and the ScD in Materials Science with a minor in Science & Technology policy from the Massachusetts Institute of Technology in 1978. He was a postdoctoral fellow at MIT and Cambridge University and then joined the National Research Council of Canada as a research staff scientist in the 1980s; after which he joined the faculty at Rensselaer Polytechnic Institute before coming to Iowa State University in 2005.

Dr. Rajan is recognized as one of the world`s leading authorities on the development and use of informatics, statistical learning and combinatorial discovery methods for the development, design and characterization of materials. His research extends into coupling new developments in computer and mathematical sciences into array of multiscale materials modeling problems and atomistic scale characterization and imaging of materials . He has also established the first academic program in materials informatics and combinatorial materials science in the United States as director of the Combinatorial Sciences and Materials Informatics Collaboratory.

Paul A. Schulte, Ph.D., is the Director of the Education and Information Division, and Manager of the Nanotechnology Research Center and the Prevention through Design programs, National Institute for Occupational Safety and Health, Centers for Disease Control and Prevention. Dr. Schulte has extensive experience in conducting research and developing guidance on occupational cancer, nanomaterials, risk communication, and genetics. He is the co-editor of the textbook entitled, “Molecular Epidemiology: Principles and Practices.” He has served as guest editor of the Journal of Occupational Medicine and the American Journal of Industrial Medicine and was on the initial editorial board of Cancer Epidemiology, Biomarkers and Prevention. He currently is on the editorial board of the Scandinavian Journal of Work and Environmental Health, and the International Advisory Board of the Annals of Occupational Hygiene.

Dr. Jeffery A. Steevens is the Senior Scientist in Biotechnology for the US Army within the Environmental Laboratory at the US Army Engineer Research and Development Center in Vicksburg, MS. He obtained his bachelor’s degree in biochemistry from the University of Missouri at Columbia in 1994 and his doctorate degree in pharmacology and toxicology from the University of Mississippi in 1999. As the ERDC’s lead scientist in biotechnology he is responsible for leading the basic and applied research that focuses on innovation in science and engineering to support the peaceful and wartime mission of the soldier. In addition to this research, he also leads environmental research for the U.S. Army Corps of Engineers. His research activities include risk assessment and management of contaminated sediments, bioavailability and biological effects of military-relevant materials (e.g., explosives, nanomaterials, metals). One of his current responsibilities is leading a multi-disciplinary ERDC research cluster focusing on the fate, transport, and toxicology of military nanomaterials and nano-enabled technologies. In addition to his research on nanomaterials, he is also a technical advisor to the World Bank on international projects, EPA Superfund Program, and provides expertise on many contaminated sediments projects throughout the U.S. His recent research activities have included leading a technical response to the recent Deepwater Horizon oil spill, response to the TVA fly ash spill in Tennessee, red mud spill in Hungary, and several Superfund sites.

Dr. George O. Strawn is the Director of the National Coordination Office (NCO) for the Federal government's multiagency Networking and Information Technology Research and Development (NITRD) Program. He also serves as the Co-Chair of the NITRD Subcommittee of the National Science and Technology Council. The NCO reports to the Office of Science and Technology Policy (OSTP) within the Executive Office of the President.

Dr. Strawn is on assignment to the NCO from the National Science Foundation (NSF), where he most recently served as Chief Information Officer (CIO). As the CIO for NSF, he guided the agency in the development and design of innovative information technology, working to enable the NSF staff and the international community of scientists, engineers, and educators to improve business practices and pursue new methods of scientific communication, collaboration, and decision-making.

Prior to his appointment as NSF CIO, Dr. Strawn served as the executive officer of the NSF Directorate for Computer and Information Science and Engineering (CISE) and as Acting Assistant Director for CISE. Previously, Dr. Strawn had served as the Director of the CISE Division of Advanced Networking Infrastructure and Research, where he led NSF's efforts in the Presidential Next Generation Internet Initiative. During his years at NSF, Dr. Strawn was an active participant in activities of the interagency IT R&D program that is now called NITRD.

Prior to coming to NSF, Dr. Strawn was a Computer Science faculty member at Iowa State University (ISU) for a number of years. He also served there as Director of the ISU Computation Center and Chair of the ISU Computer Science Department. Under his leadership, ISU became a charter member of MIDNET, a regional NSFNET network; he led the creation of a thousand-workstation academic system based on an extension of the MIT Athena system; and the ISU Computer Science department was accredited by the then-new Computer Science Accreditation Board.

Dr. Strawn received his Ph.D. in Mathematics from Iowa State University and his BA Magna Cum Laude in Mathematics and Physics from Cornell College.

Dr. Sally Tinkle is the Deputy Director of the National Nanotechnology Coordination Office of the National Science and Technology Council. Her responsibilities include facilitation and coordination of the National Nanotechnology Initiative, especially the environment, health, and safety activities. Previously, as Senior Science Advisor in the Office of the Director, National Institute of Environmental Health Sciences (NIEHS), National Institutes of Health (NIH), Dr. Tinkle developed the NIEHS nanotoxicology extramural research portfolio and the NIEHS NanoHealth and Safety Enterprise, a framework for public-private partnerships. She has been an active member of the trans-NIH Nanotechnology Task Force and is senior author of the health implications section of the NIH Nanotechnology Report to the NIH Director. At the federal level, Dr. Tinkle co-chaired the Nanoscale Science, Engineering and Technology (NSET) subcommittee of the National Science and Technology Council (2009 – 2010) and is the NSET Nanotechnology Environment and Health Implications working group (NEHI) Task Group Leader for human health and nanomaterials. She is a senior author on the human health sections of the three NEHI environment health and safety (EHS) documents that form the federal approach to EHS research. She is frequently an invited speaker at nanotechnology meetings, both nationally and internationally.

Dr. Tinkle received her PhD from the Department of Physiology at the University of Colorado School of Medicine in Denver, CO and was a postdoctoral fellow at the National Jewish Center for Immunology and Respiratory Medicine, Department of Occupational and Environmental Health Science. Prior to joining NIH, she was the leader of a pulmonary and dermal toxicology laboratory at the National Institute of Occupational Safety and Health in Morgantown, WV.

Mark Tuominen is a Professor of Physics and Director of the Center for Hierarchical Manufacturing and MassNanoTech at the University of Massachusetts Amherst. His research interests include experimental condensed matter physics. Research in the fabrication and physics of nanoscale devices and materials. This includes two primary research areas: nanostructures from self-assembling block copolymer templates and nanoscale device physics. The first area addresses the general scientific challenge of fabricating nanoscale structures by a convenient method and providing appropriate electrical interfacing to these structures. To address this challenge, diblock copolymer films are used as a convenient self-assembling template for the fabrication of arrays of nanoscale elements. This results in a new fabrication method for producing integrated devices using block copolymer templates in combination with other lithographic methods. Research includes work on terabit-density single-domain magnetic arrays, magnetotransport devices, field-emission arrays, electrochemical sensor arrays, and thermoelectric cooling elements. The second research area explores issues involved in single charge transport. This includes single-electron investigations of mesoscopic superconductors and, more recently, experimental and theoretical studies on charge shuttle devices, which involves quantum charge transport coupled with mechanical vibration.

Dr. Cyrus Wadia is the Assistant Director for Clean Energy & Materials R&D with the White House Office of Science and Technology Policy where he is advising the Executive Office of the President on Federal policy that accelerates innovation and deployment of advanced material systems for energy, national security, and human welfare. Cyrus is on leave from Lawrence Berkeley National Lab (LBNL) and the Haas School of Business where he holds a dual appointment as: Faculty & Co-Director of Clean Tech to Market and Research Scientist. His research in both exhaustible resource economics and the aqueous chemistry of nanoparticles is motivated by the pursuit of new low cost energy technologies using earth abundant materials. Cyrus was recently honored for his groundbreaking work with earth-abundant nanoparticle solar cells as a recipient of the MIT Technology Review Young Innovator award.

Prior to his work at LBNL, Cyrus spent over 7 years in Silicon Valley launching new technology to market. First as an engagement manager with R.B. Webber & Co where he worked with over 15 different venture backed startups; and next as a Senior Product Manager with AvantGo, where he completed several successful new product introductions. More recently, Cyrus founded a boutique Internet services startup specializing in complex data analysis for which he now serves as Chairman of the Board. Cyrus earned his PhD in Energy & Resources from U.C. Berkeley and holds both an M.S. and S.B. in Chemical Engineering from MIT.

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