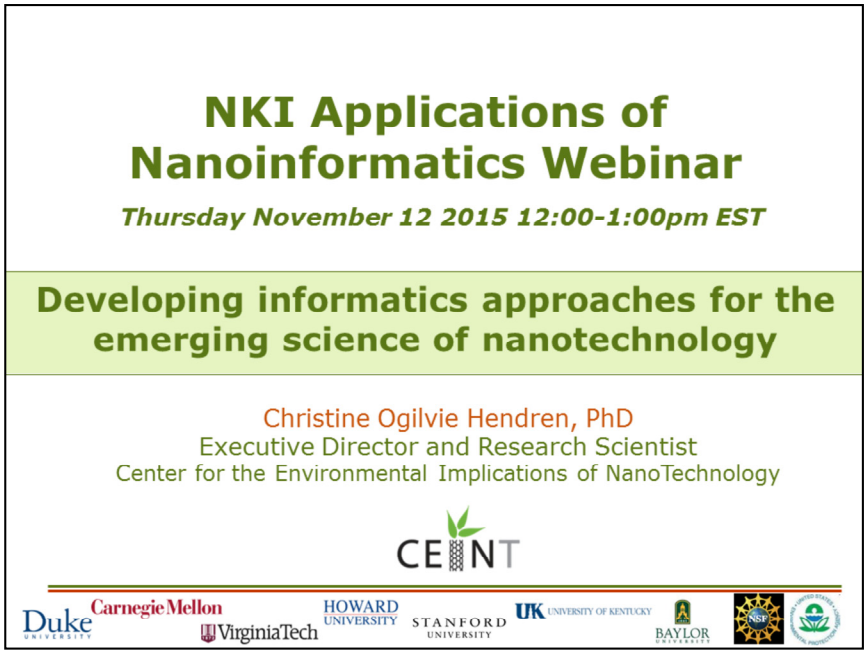
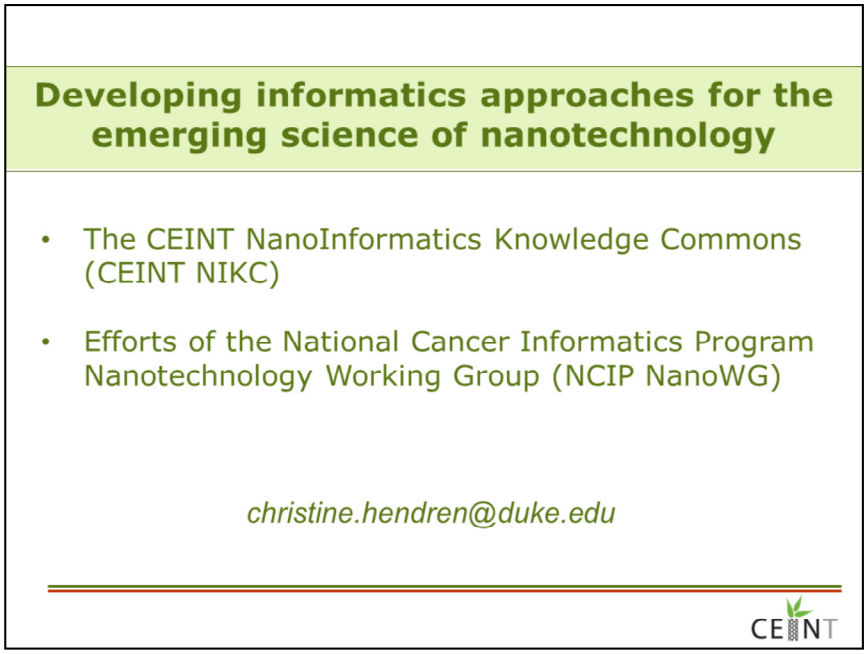
>> Stephen Lehrman: Greetings. It is my pleasure to welcome you to today's webinar titled "Applications of Nanoinformatics." My name is Stephen Lehrman, and I am with the National Nanotechnology Coordination Office. I will be today's moderator. We have a great panel of speakers today, and I invite you to read their bios online. By way of a brief introduction, Dr. Christine Ogilvie Hendren is Executive Director of the National Science Foundation and the U.S. Environmental Protection Agency sponsored Center for the Environmental Implications of Nanotechnology, headquartered at Duke University. She is also co-chair of the National Cancer Institute's National Cancer Informatics Program Nanotechnology Working Group. Dr. Bruce Lippy is the Director of Safety Research at CPWR, the Center for Construction Research and Training. He currently serves on the American Industrial Hygiene Association's Nanotechnology Working Group, and represents the group as the member of the ISO Technical Committee 229 on nanotechnology.

The National Nanotechnology Initiative, also known as the NNI, is a partnership of 20 Federal agencies and departments with activities in nanotechnology research and development, policy, and regulation. More information on the NNI, including reports, nanotechnology news, upcoming events, and solicitations can be found at the nano.gov website. These agencies have established five Nanotechnology Signature Initiatives in order to enhance interagency coordination and collaboration. The Signature Initiatives leverage resources and capabilities of the NNI agencies to maximize progress and provide a forum to maximize communications. The Signature Initiatives are not intended to be a purely Federal activity, but to catalyze communities of interest that extend into academia and industry.

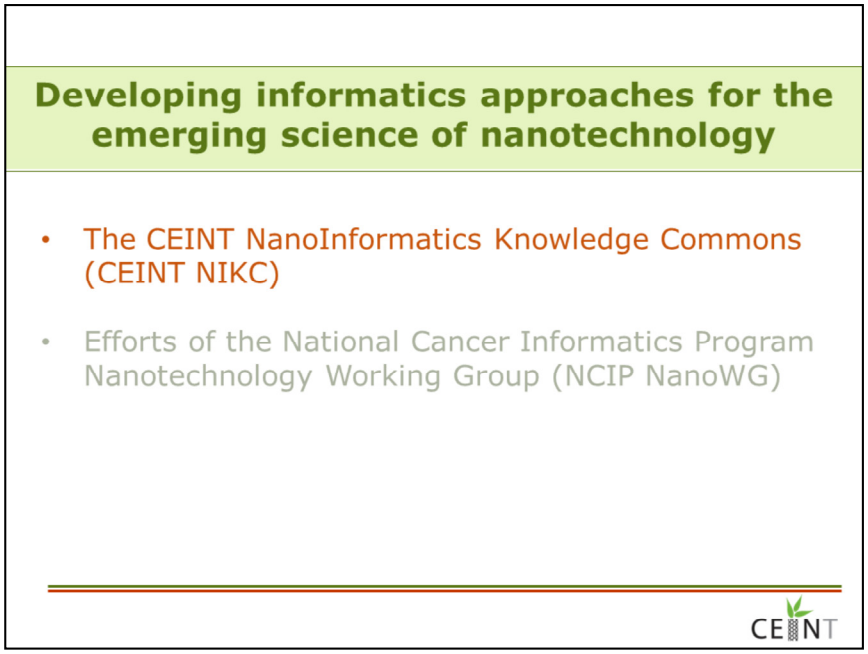


>> Stephen Lehrman: Today's nanoinformatics webinar is sponsored by the Nanotechnology Knowledge Infrastructure, or NKI, Signature Initiative that involves 10 Federal agencies. More information about the NKI Signature Initiative and the Federal resources supporting the development of Nanotechnology Knowledge Infrastructure can be found at www.nano.gov/NKIportal. You are welcome to submit questions via email at webinar@nnco.nano.gov or in the "Submit your questions here" window in the webinar interface. Please note that the views expressed by our panel are their own and do not necessarily represent the positions of Federal agencies participating in the NNI or the NKI Signature Initiative. Now, I am pleased to welcome Dr. Christine Hendren.

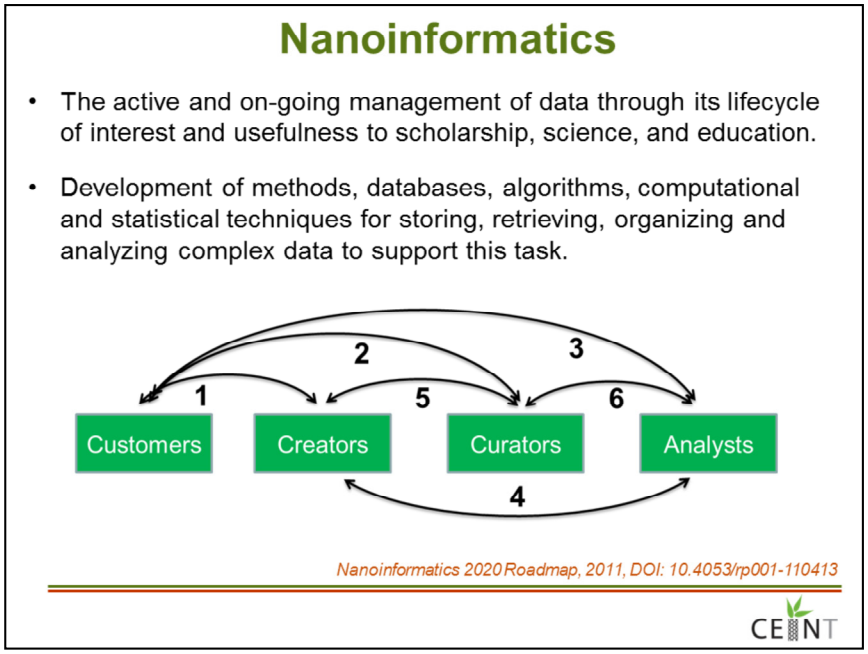
>> Christine Ogilvie Hendren: Good morning, and thank you so much for having me here today. I am going to talk about developing informatics approaches for the emerging science of nanotechnology.



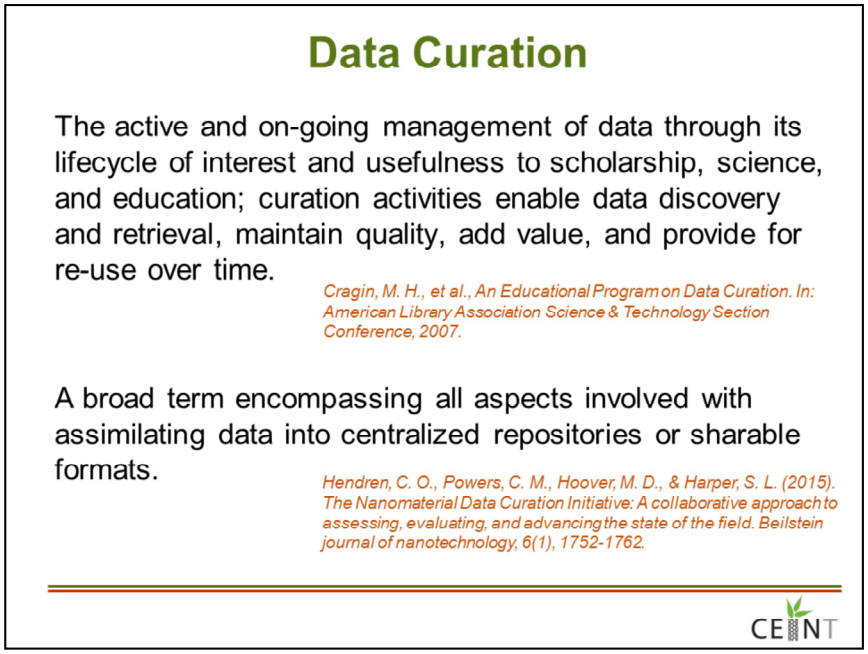
>> Christine Ogilvie Hendren: I'll be talking about nanoinformatics from two different vantage points today. The first is from my role of Executive Director of CEINT, where we're leading a project to develop a NanoInformatics Knowledge Commons, or NIKC. The second is from the efforts of the National Cancer Informatics Program, or NCIP, Working Group. If there's something you would be interested to hear more about later that I can't touch on in detail here, please feel free to reach out at the email address listed in the slide.



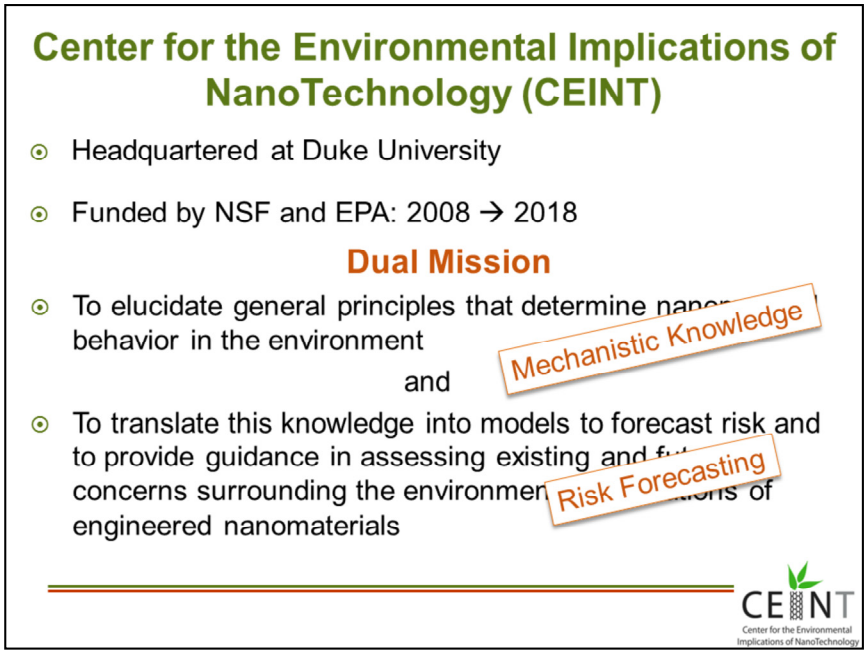
>> Christine Ogilvie Hendren: First let's talk about the CEINT NanoInformatics Knowledge Commons, or CEINT NIKC.



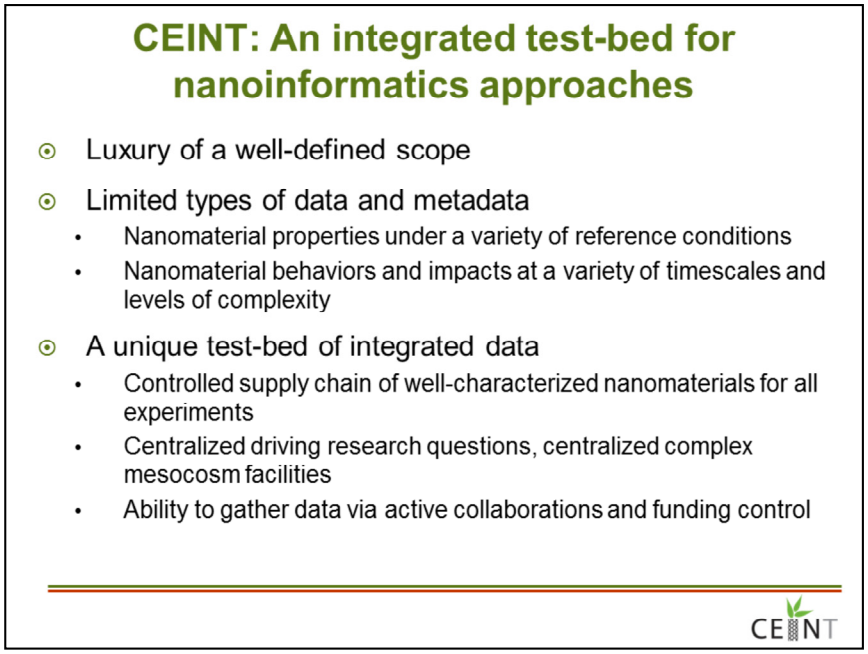
>> Christine Ogilvie Hendren: For our talk today I want to start with a couple of important definitions. The definition you see here is in the Nanoinformatics 2020 Roadmap, and was presented by Mark Hoover in the last nanoinformatics webinar. This diagram shows how we think of nanomaterial data stakeholder roles and their interactions with respect to nanoinformatics activity. This is the term coined for our efforts to use big data and informatics approaches that we have seen in other fields, such as biotechnology, with great success. We then map that to our area of science which is still emerging, and that comes with some challenges.



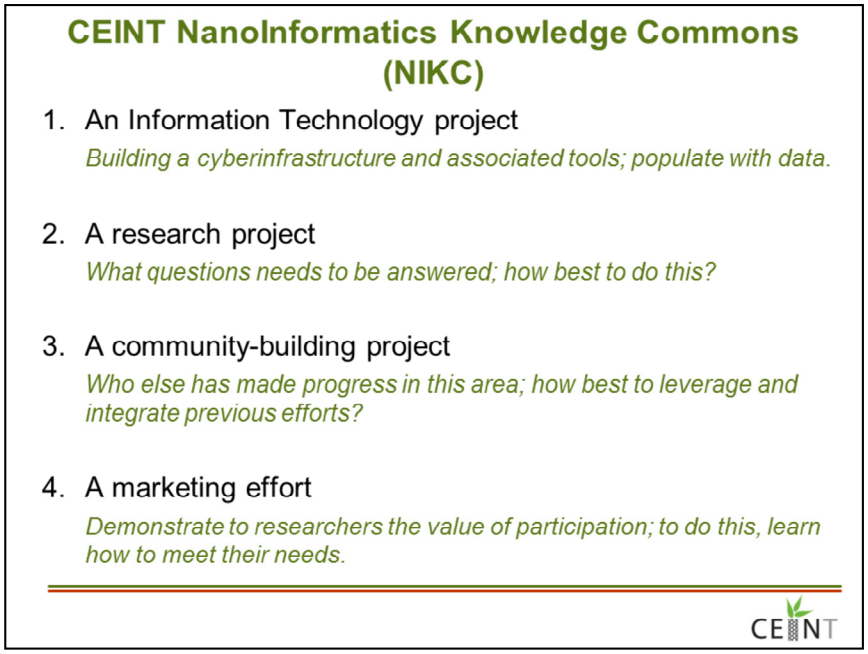
>> Christine Ogilvie Hendren: One of the roles in the diagram you saw was “curator,” and here are two definitions of data curation, which is a unifying aspect across all resources because no matter the purpose of the resource, you have to decide how to get data in there. It's borrowed from the concept of art curation. The important part is it's selected to signify that this process entails more than a series of data management tasks. It also has elements of discernment and judgment inherent in the decisions.



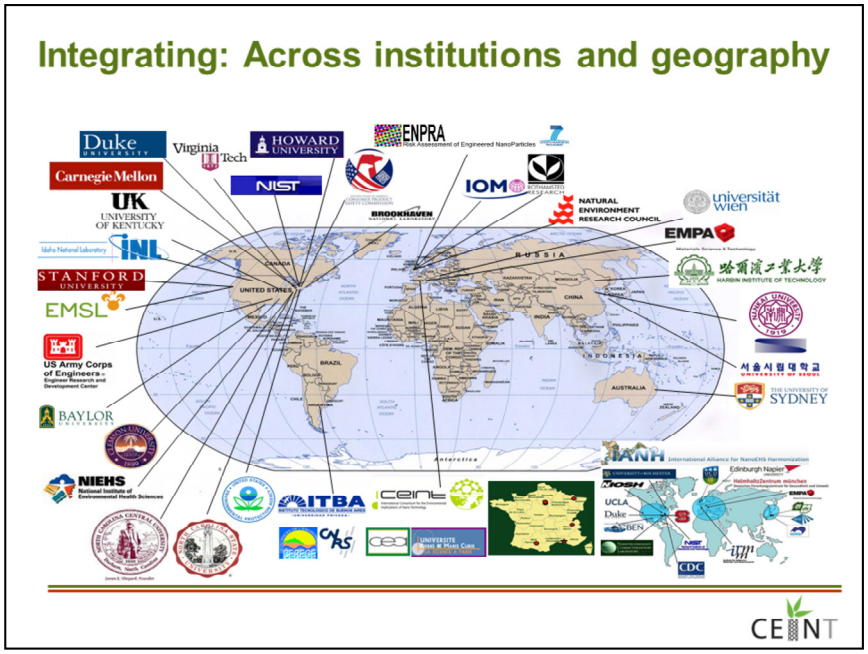
>> Christine Ogilvie Hendren: So at CEINT, headquartered at Duke University, the Director is Mark Wiesner, and Greg Lowry at Carnegie Mellon is the Deputy Director. It's a ten-year contract, funded by EPA and NSF, with a dual mission to elucidate principles of nanomaterial behavior in the environment and to translate these into guidance on decisions surrounding environmental implications of nanomaterials. I mentioned the dual mission because it serves as a compass in navigating the tradeoffs and allocation decisions that I'll talk about in this presentation.



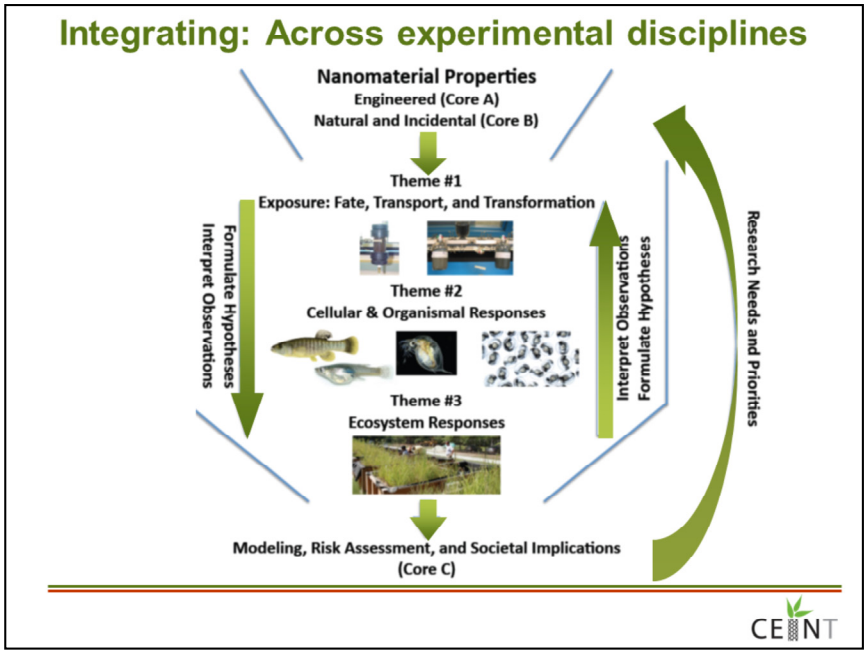
>> Christine Ogilvie Hendren: CEINT is an integrated test bed that makes it a perfect place to start in many ways for nanoinformatics efforts. It is difficult to develop ontologies, controlled vocabularies, cyber infrastructures, and analytical tools that enable the design of things that are uncertain -- queries we haven't even imagined yet, asking questions about parameters we may only now be learning are important. We are potentially measuring with methods and protocols that are still being developed, so a lot of flexibility needs to be built in. CEINT provides a good integrated test bed with built-in constraints that help out. The luxury of our well-defined scope means that we can say definitively, based on our research mission, what will define success for our resource. Not everyone has this combination of the unified scope and integrated test bed of data that's emerged from an intertwined system of projects.



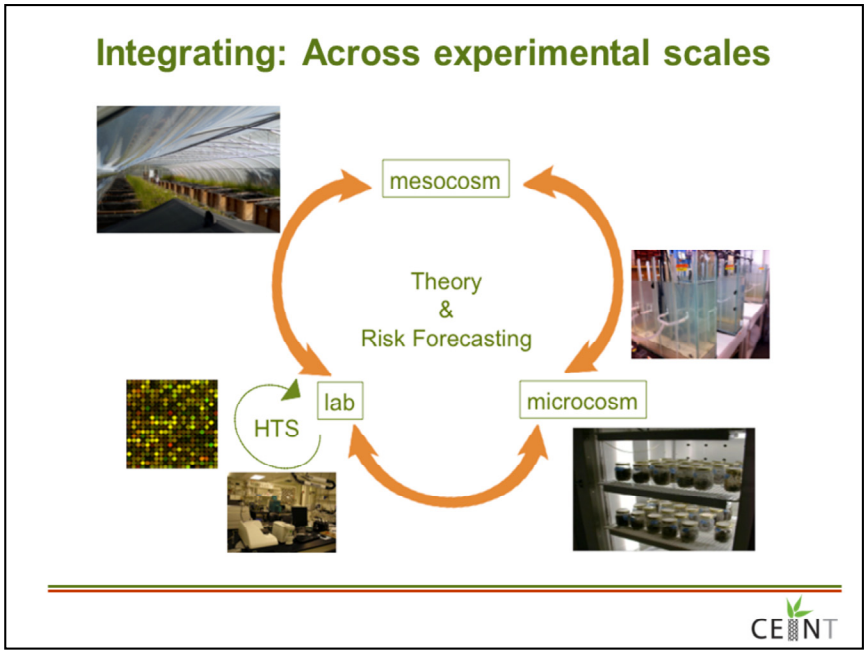
>> Christine Ogilvie Hendren: We set out to build the CEINT NanoInformatics Knowledge Commons with a commitment to advancing the nanoEHS field, but also nanoscience field in a broader sense. At first it seems a nanoinformatics effort would primarily be an IT project, but it also has multiple underlying communications aspects that have really driven our progress and decisions and have also influenced the direction of the NCIP Working Group. This is really also a research project in data science and nanoscience simultaneously, and because of that, I'll frame a bit about CEINT's research questions and how it drives our informatics approach. It's also a community-building project to leverage existing work and to ensure integration down the line. We are happy to follow an existing map if it's the right map leading us where we need to go. Finally, it's a marketing effort to researchers. Really what we have learned is that curation should ultimately be done at the time of data collection. Retro-curation by someone who was not the experimentalist, trying to unpack all the data that were summarized from a paper, is such a bottleneck to the process. To encourage researchers to take the time to curate their own data, we will have to provide them value.



>> Christine Ogilvie Hendren: The next few slides are just intended to illustrate the scope of CEINT, and give a sense of the magnitude of the integration efforts. In addition to seven core universities, we have partners worldwide all generating integrated data.

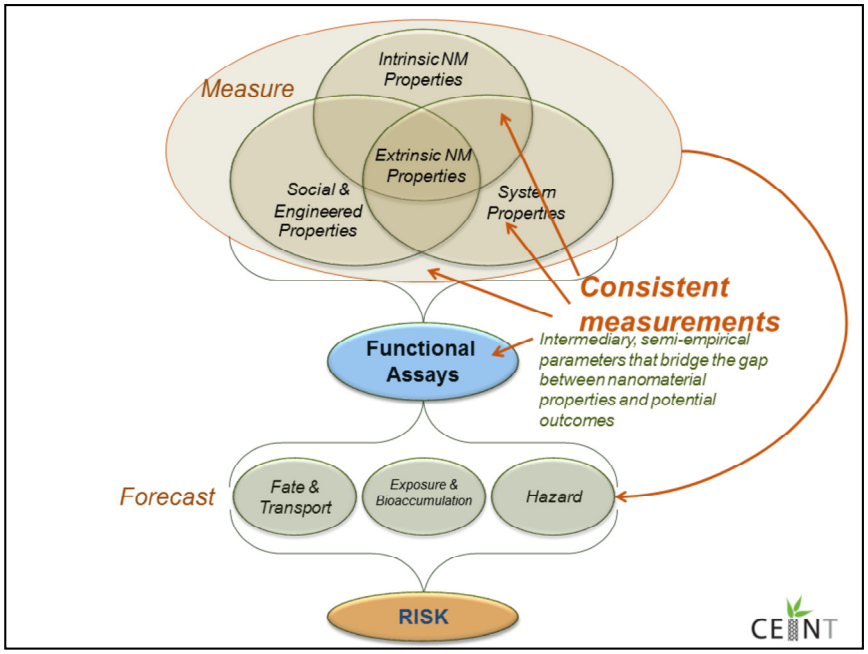


>> Christine Ogilvie Hendren: We are organized into six thrust areas covering all the disciplines needed to go from nanomaterial characterization through their journey in the environment and their ultimate effects, and modeling, risk assessment, and societal implications. Iterative feedback between these disciplines enables relevant hypothesis formulation and experimental design.

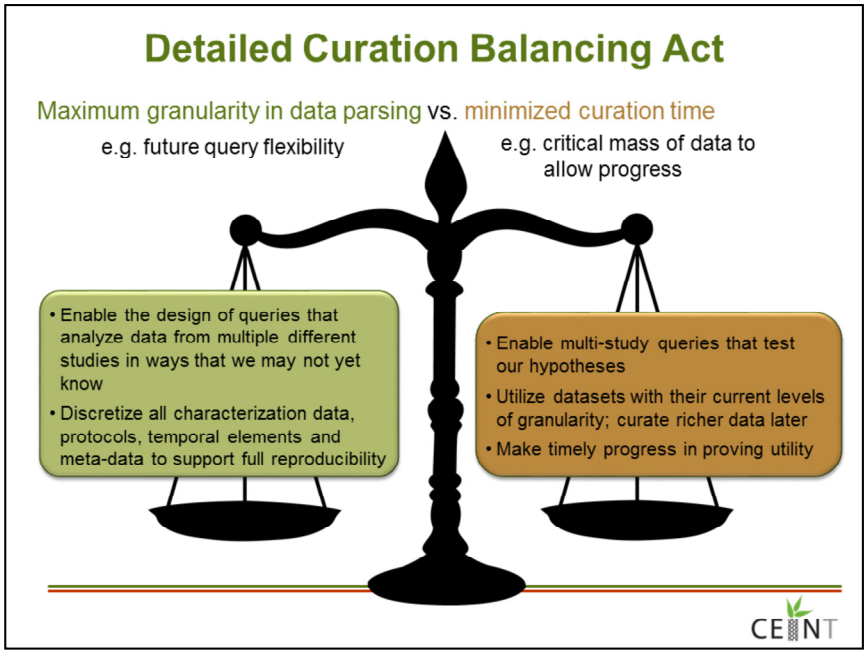


>> Christine Ogilvie Hendren: In addition to integrating across institutions and disciplines, we also work at multiple scales of experimental complexity from controlled laboratories to complex mesocosms, and those inform each other's future directions. All of that feeds into how we have to structure our data to integrate it.

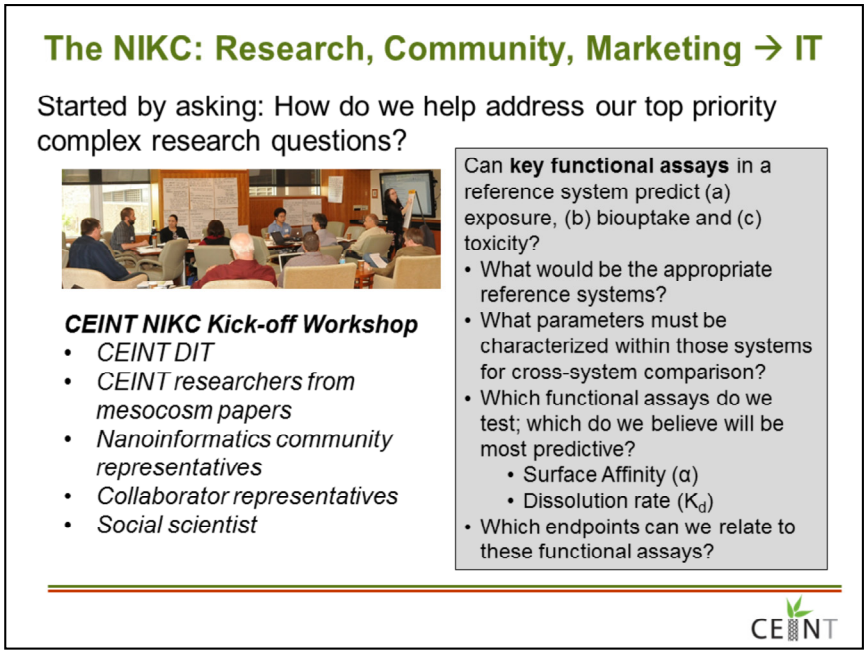
>> Christine Ogilvie Hendren: I'll take a second to talk about the Duke Forest mesocosms because they are the most complex experiments in terms of numbers of parameters and numbers of researchers from different disciplines and institutions, co-designing and executing the experiment, sampling and analyzing the sample. It's worth explaining this in the context of our nanoinformatics work because we have designed the NIKC to accommodate queriable-level detail at the level of this mesocosm data. So that includes characterization of particles before and after dosing, fate and transport throughout aquatic and terrestrial compartments, propagation through the food web, and impacts on biota and nutrient cycling for example. The real kicker is the need to track spatial and temporal components of all types of these measurements for comparison.



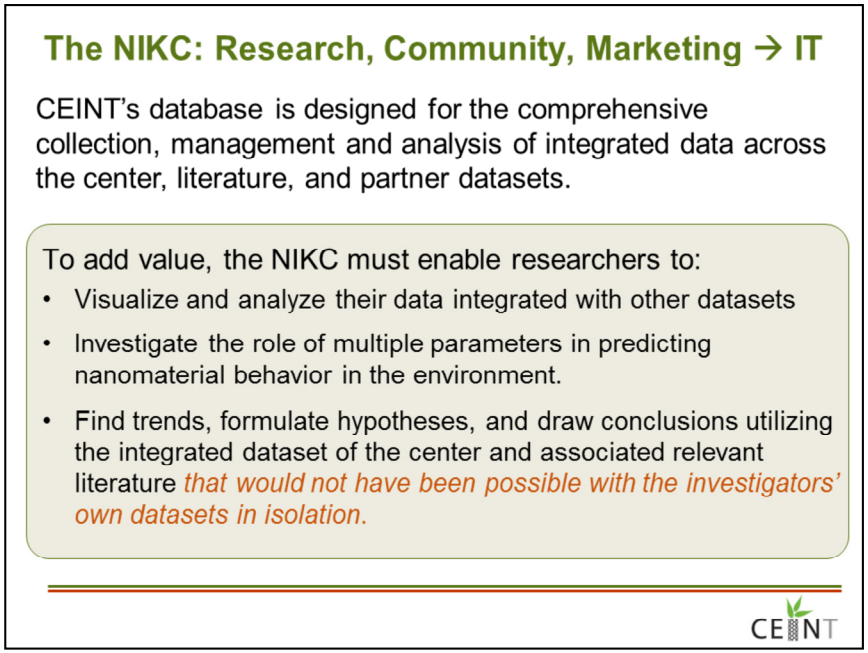
>> Christine Ogilvie Hendren: So, our work in CEINT has moved toward advocating the use of functional assays, which are intermediary, semi-empirical parameters that bridge the gap between the nanomaterial properties and the potential outcomes we would want to predict. Examples of these functional assays currently being tested are surface affinity and dissolution rate. They measure something that's happening in the system, and they automatically, therefore, include phenomena that are a function of all of the individual parameters (intrinsic, extrinsic, environmental, and social, meaning, you know, how much gets out there, what products are they in) that go into a relevant scenario. We test functional assays' ability to predict outcomes of interest to get at the second part of our mission, which is that translation of data into guidance on risk and, really, performance, as well. How can we predict what's going to happen based on what the nanomaterial does in a given system? If we're measuring it consistently with all those pieces, then we're also systematically banking consistent data to enable deep data mining down the line in pursuit of the first part of our mission, which is seeking mechanistic understanding based on first principles. The NIKC had to be built to consistently capture each of these categories, and that did not exist anywhere. So we take these consistent measurements, and then we hope that down the line we can go from those initial material and system properties all the way to the outcomes we care about.



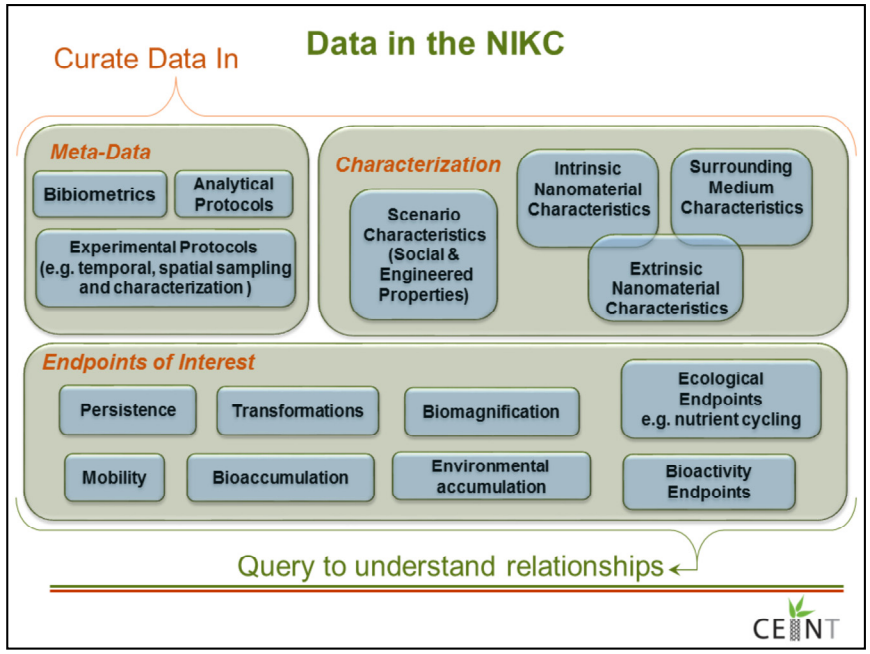
>> Christine Ogilvie Hendren: Now that you know what information CEINT needs, which has driven what we have tried to gather, we come to a non-trivial tradeoff decision that has to be made. Balancing between maximum data parsing and minimized curation time drives a lot of the important decisions about where to dedicate resources in terms of curation, and how to design your resource to meet current needs while anticipating future needs. So we want to enable future flexibility and query design and deep data mining while meeting current needs and making timely progress.



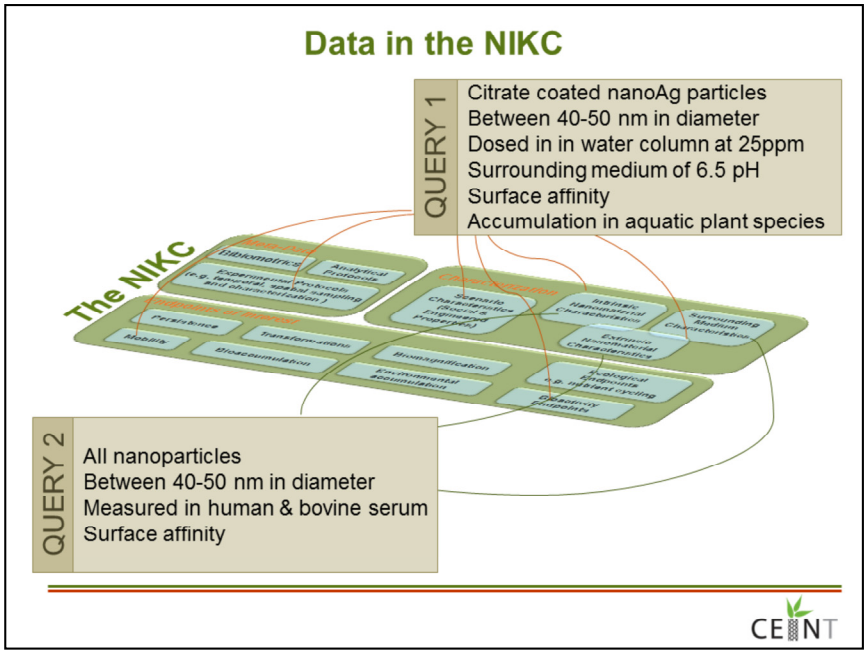
>> Christine Ogilvie Hendren: When attacking the research project with a marketing angle in mind, we started by asking ourselves how we can best address our top priority complex research questions. We held a meeting of NIKC stakeholders to kick it off a couple of years ago to elicit the most important questions around which to orient our cyberinfrastructure and our pilot curation efforts. We knew we had to build a system based around what makes the science better and that we had to be very specific to make generalizable progress. What we talked about at that meeting is, can key functional assays in a reference system predict exposure, biouptake, and toxicity? And then a host of sub-questions about what does that mean for what systems, what parameters, what relationships are we going to be interrogating.



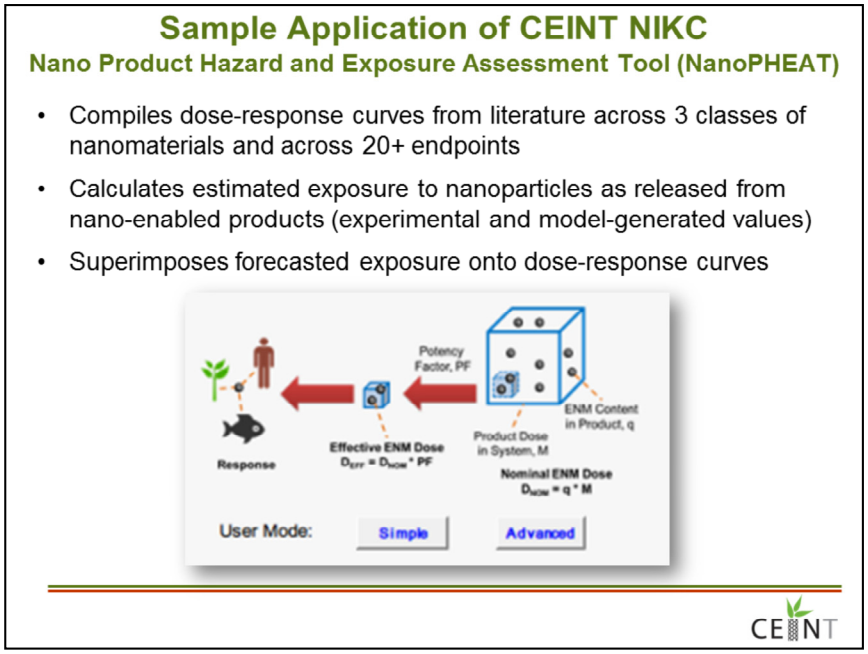
>> Christine Ogilvie Hendren: The NIKC was then, based on all of that, designed to enable flexible analysis across integrated datasets that would support the discovery of trends, hypotheses, and conclusions that would not have been possible without integrated, rich datasets. That's the important part for adding value.



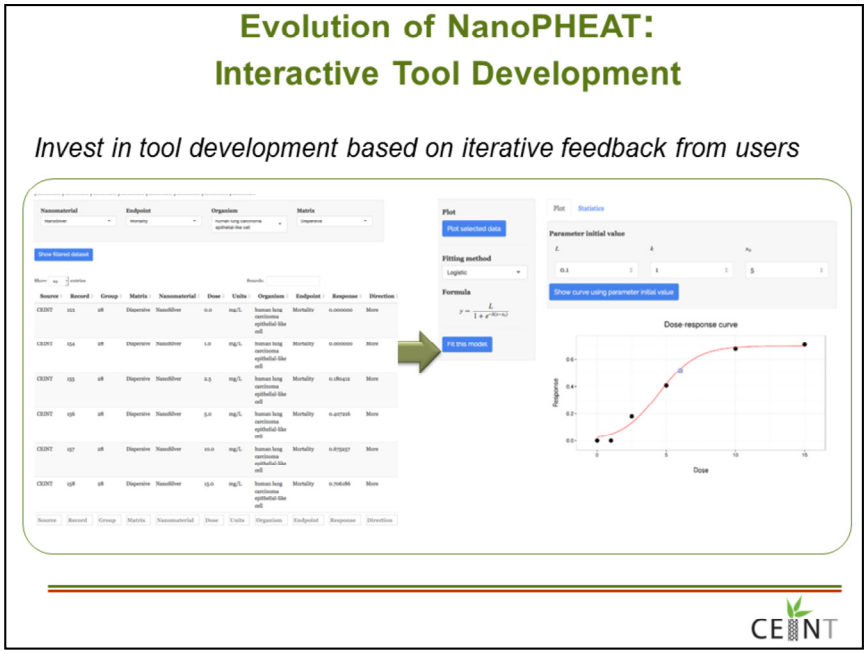
>> Christine Ogilvie Hendren: Data targeted for inclusion in the NIKC, therefore, includes characterization of materials and systems, experimental methods and results, and bibliometrics so we can track things back to where they came from, directly measured values, and single study calculated values at a variety of levels, across all sorts of different endpoints of interest. You curate the data in at the most granular level you can afford to time- and effort-wise, enabling cross-study comparisons through queries on the backend.



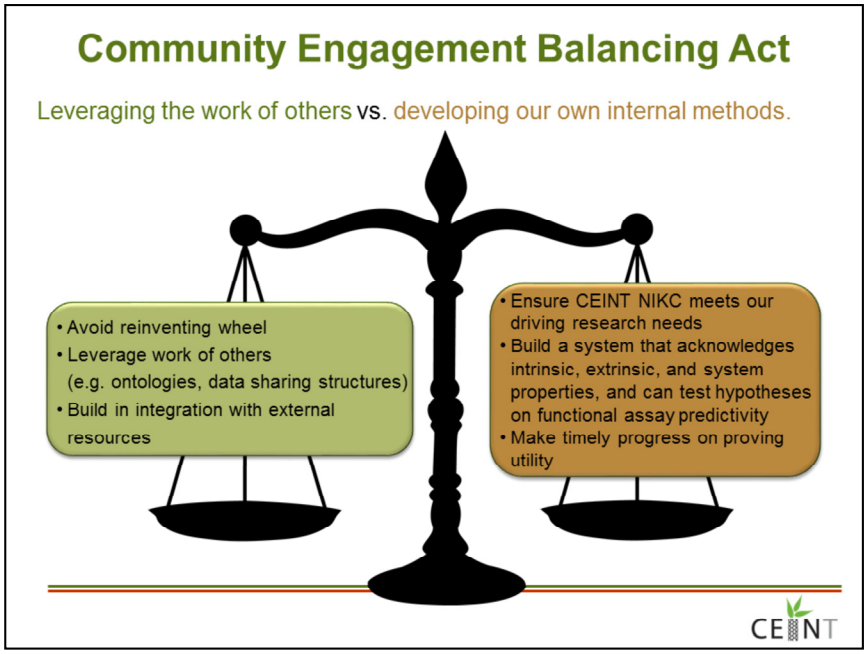
>> Christine Ogilvie Hendren: You see the NIKC on its side there. Designed with these requirements and these balancing acts in mind, the NIKC can support curation and queries at multiple levels of detail. For example, in this query, you can look for the effects of, say, specific intrinsic and extrinsic and social properties of the material, along with environmental system properties on an outcome of interest. This is a pretty complex query. Or, as you can see in the second query, you might look for general trends in values of an extrinsic property across all nanomaterials in a system of interest.



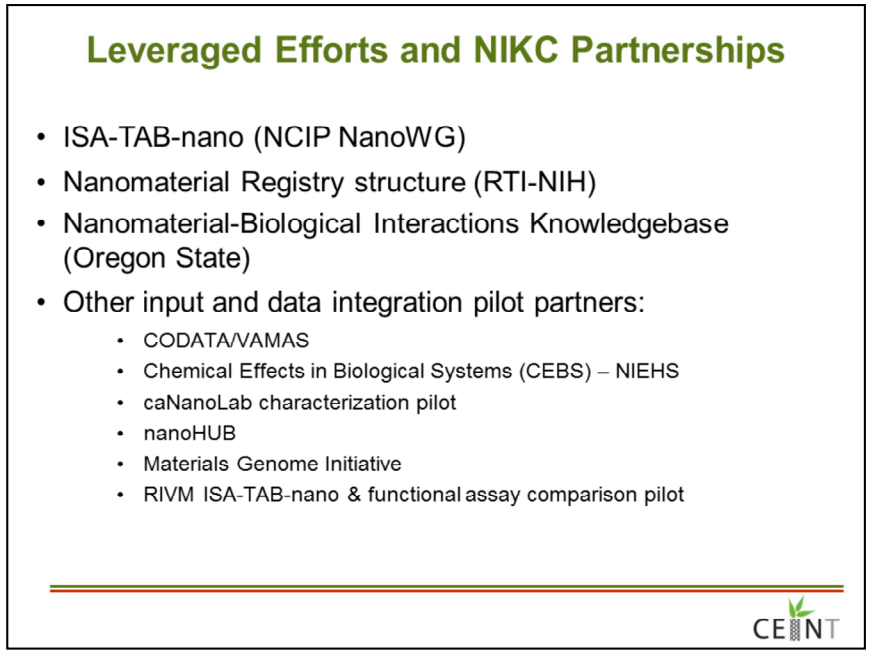
>> Christine Ogilvie Hendren: Here is one example of an application of the NIKC, which I'm going to show to illustrate how a tool can sit on top of this database and draw on otherwise disparate datasets and data types. The NanoPHEAT tool is built to compile dose-response curves from literature, including hundreds of papers, and calculates the estimated exposure to nanoparticles as released from real products, based on some in-house experimental values that we have created and on model-generated values. It superimposes the forecasted real exposure onto dose-response curves from historical data.



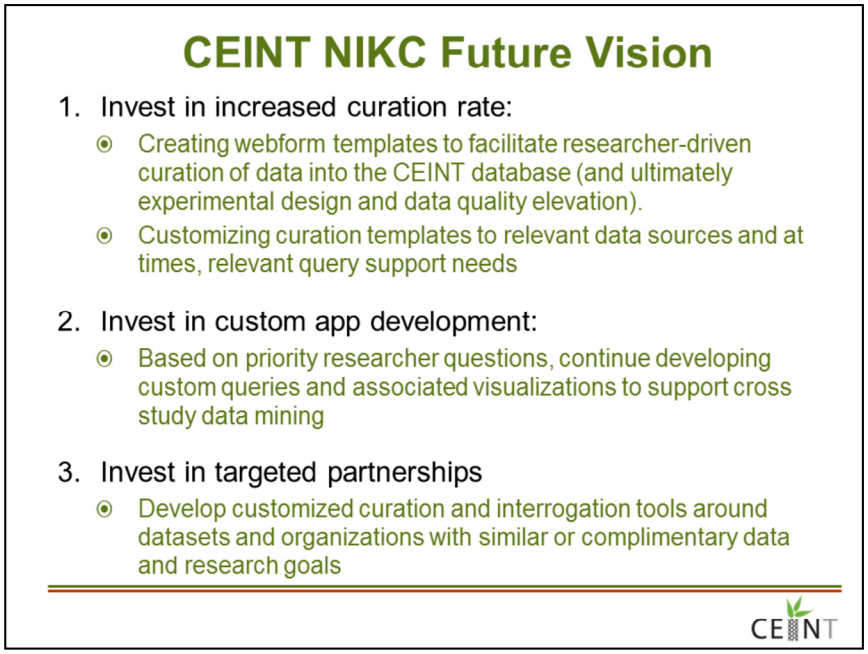
>> Christine Ogilvie Hendren: Here you see the screenshot of where users can select their relevant exposure scenario parameters and their bioactivity endpoint of interest, across a range of over 20 of them. You can see where their exposure is projected to fall in that little blue dot on the dose-response curve, in relation to the dose-response curve that we derived from historical data. We work with our user groups, ourselves or, in some cases, a funding agency that might take a part of this in order to meet what their needs might be.



>> Christine Ogilvie Hendren: As we build all of this, again, we have to navigate some tradeoffs in terms of leveraging the structural and formatting work of others, both to save time and enable future interoperability, while also ensuring that our resource would meet our specific research needs and make timely progress in proving our utility.

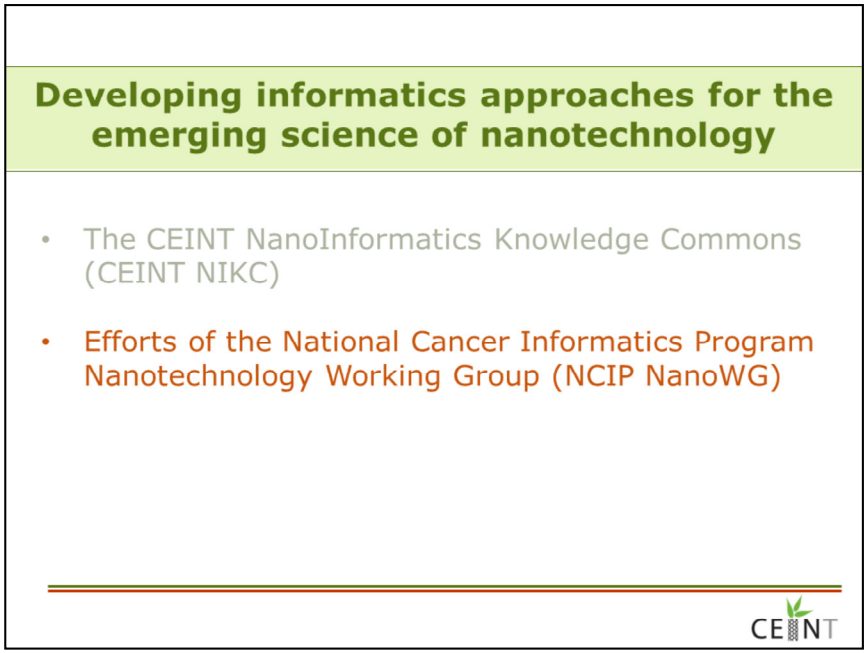


>> Christine Ogilvie Hendren: To do this, in selecting our terminology, structure, and data formatting, we started by learning what had already been done. This was actually our introduction to the Nano Working Group. Beyond input for the NIKC architecture, we're also immersed in the growing nanoinformatics community, knowing that our integrated dataset is a great test bed for a meaningful starting point, but that the idea is to get critical mass way beyond CEINT research. Here I have listed a couple of our pilot integration partners. We consult with a lot of these groups on how they make their decisions in infrastructure and terminology. With some of these groups we trade datasets and say, “How would you put this exact characterization in your resource versus ours and what are some disconnects”. Again saying, we've got to go down to the detail level to make generalizable progress.

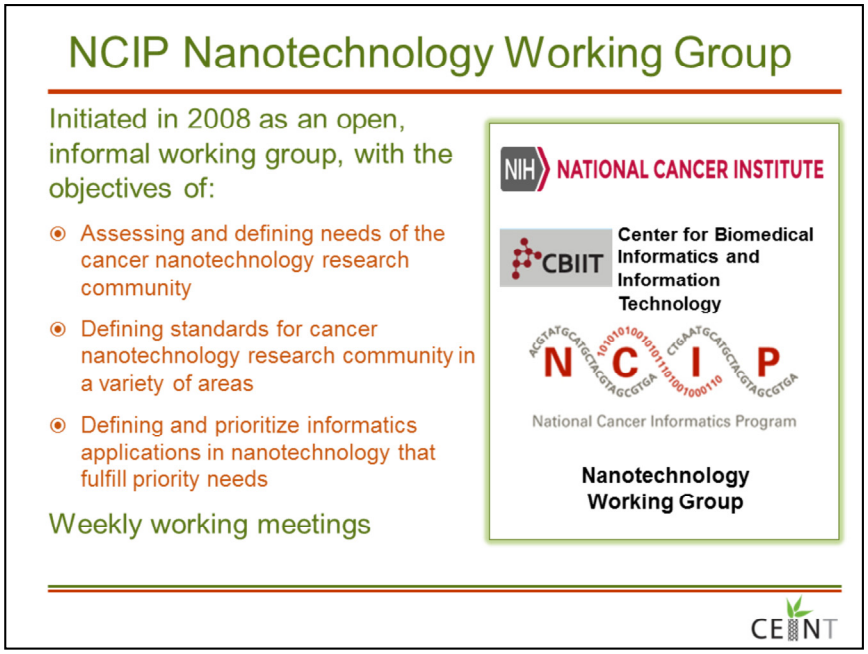


>> Christine Ogilvie Hendren: We've learned a lot through establishing the NIKC that helps us prioritize going forward in terms of the balancing acts I've introduced: how to add value, engage the community, and leverage progress. Areas we know need particular focus are

1. An increase in curation rates. We have got to clear up that bottleneck and raise the quality level, completion level of our data. That's a resource-intensive issue so we do that around targeted applications, targeted webforms that we make customized to particular data relationships.
2. We also invest in custom app developments. That's really about increasing our value. Giving more value in terms of analytical power also increases the engagement on the curation end.
3. Because this is all very resource intensive, we also realize we need to invest in targeted partnerships where we partner with organizations that have similar complementary data and research goals.



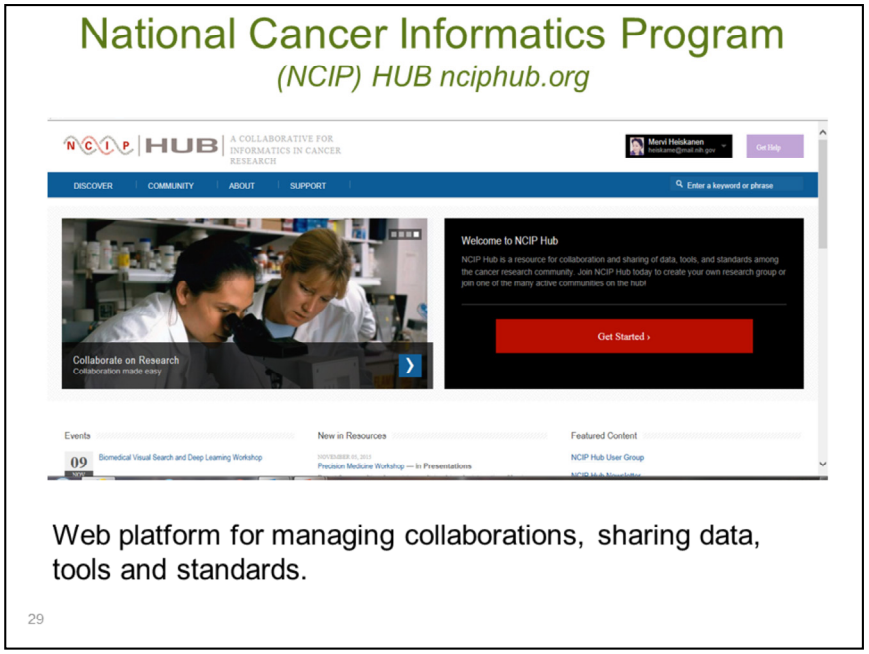
>> Christine Ogilvie Hendren: Now that I've gone through the CEINT aspect of our nanoinformatics work, I'm going to transition to my other role as co-chair of the NCIP Nano Working Group. Coming from the vantage point of CEINT, we have a relatively specific center mission, but as I presented, we have a keen awareness that achieving that mission depends heavily on integration with a much broader community. Many of the balancing acts and judgment calls that I've called out in the first part, described as part of the CEINT experience, are truly universal. Maybe people take different approaches, but they are universal to data sciences, and the Nano Working Group has been a unique and effective place for learning and collectively advancing a number of fields around nanoinformatics.



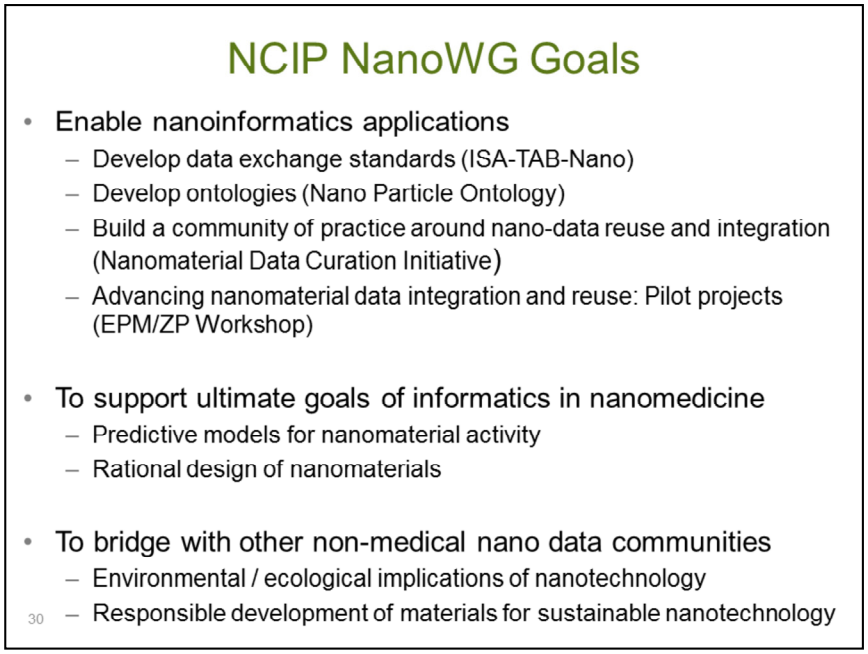
>> Christine Ogilvie Hendren: The Nano Working Group is supported administratively through NIH as part of a significant agency-wide commitment to data science. It was initiated in 2008 as an open, informal working group, with the objective of assessing and defining the needs of the cancer nanotechnology research community and moving forward informatics applications that would help with the cancer and nanomedicine angle. That's originally where it started. But has grown to encompass many other groups, including environmental nanoresearch, ecological endpoints, as well as industry and performance-based sustainable nanotechnology groups. So it's pretty broad. I mentioned we have weekly working meetings which is a pretty intensive schedule, but it has really proven to be a useful way to move a lot of things forward on an all-volunteer basis.

>> Christine Ogilvie Hendren: So who are we? The working group is made up of a broad range of organizations, alliances, and initiatives. While we have a core group estimated around 15 regular members, our open meetings do attract a wide, dynamic range of people. We have different speakers, and we have working meetings, depending on what's going on.

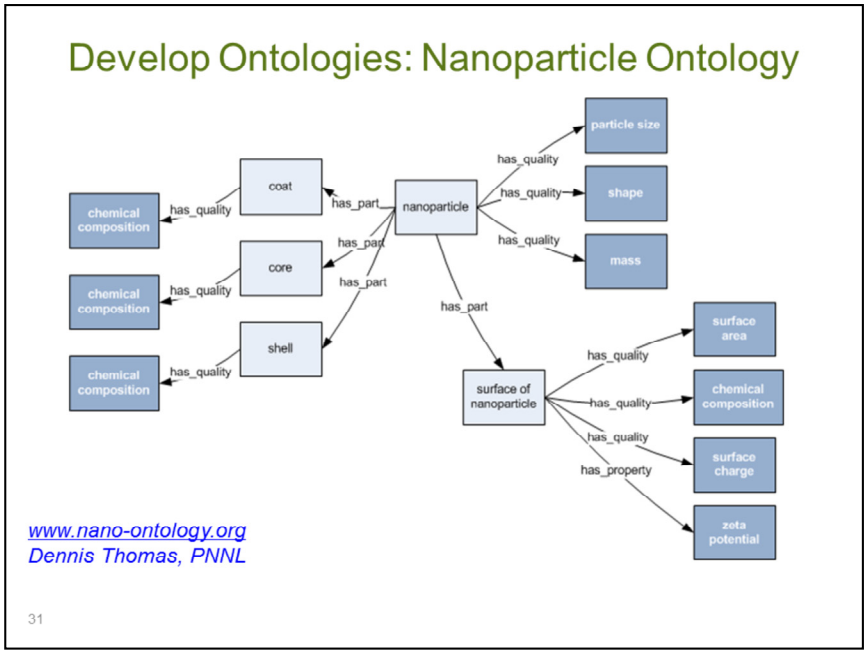
>> Christine Ogilvie Hendren: This is our leadership. You know about me, but I mostly put this up so that I could make sure to call out that Stacey Harper is my co-chair. She's been a member since very early on and contributed to a lot of the progress over the years. She's at Oregon State University and holds a couple of different appointments in different schools there and looks at nano and ecotoxicology and informatics efforts. Mervi Heiskanen is at NCI. She's the Nano Working Group facilitator, also involved in a lot of detailed nanoinformatics mapping projects. Without her we would not be able to accomplish the work of this group; she holds us together.



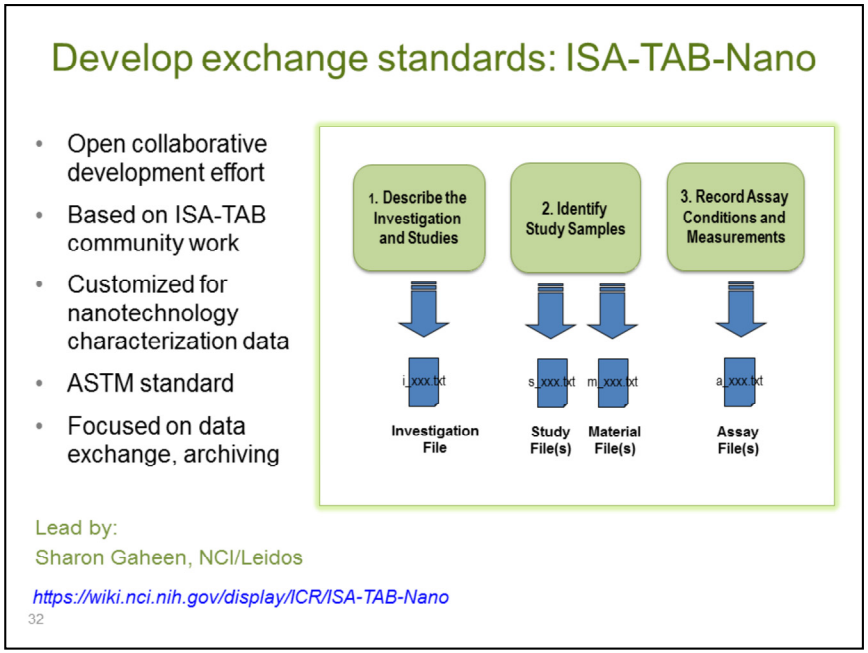
>> Christine Ogilvie Hendren: One thing Mervi does is manage the HUB. It is a web platform for managing collaboration, tools, and standards.



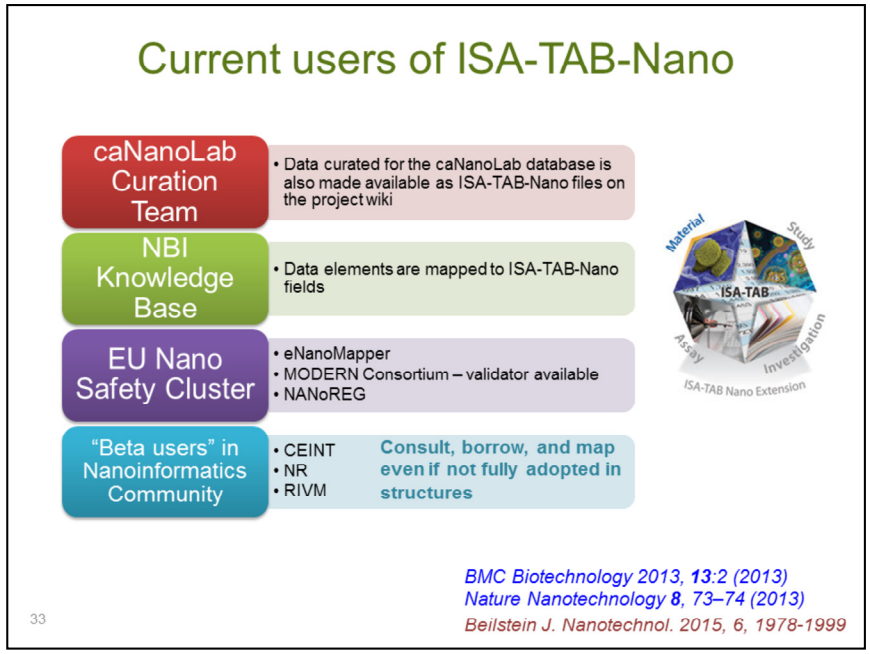
>> Christine Ogilvie Hendren: The goals of the Nano Working Group are really to enable nanoinformatics applications to do the detailed work of making nanoinformatics start to happen. Specific goals I'll talk about are these first four bullet points under that, which are developing data exchange standards, ontologies, a community of practice around integration of nanodata, and advancing nanomaterial data integration through pilot projects. All of this was again, started to support ultimate goals of nanomedicine informatics but also increasingly to bridge with other non-medical nano communities as well.



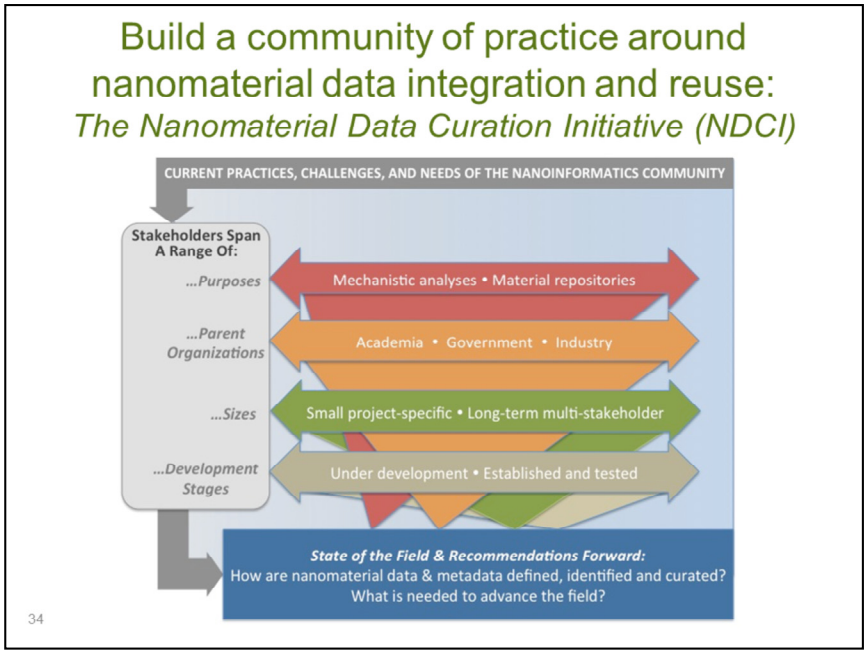
>> Christine Ogilvie Hendren: One of the first things that happened was this came out of PNNL and was led by Dennis Thomas. I should have said Nathan Baker was the originator of the Nano Working Group. He led it from 2008 to 2012 and was also highly involved in leading the NPO and ISA-TAB-Nano that I'll talk about. This goal was to enable nanomedicine data search, sharing, and analysis through ontology development. That was a great starting point.



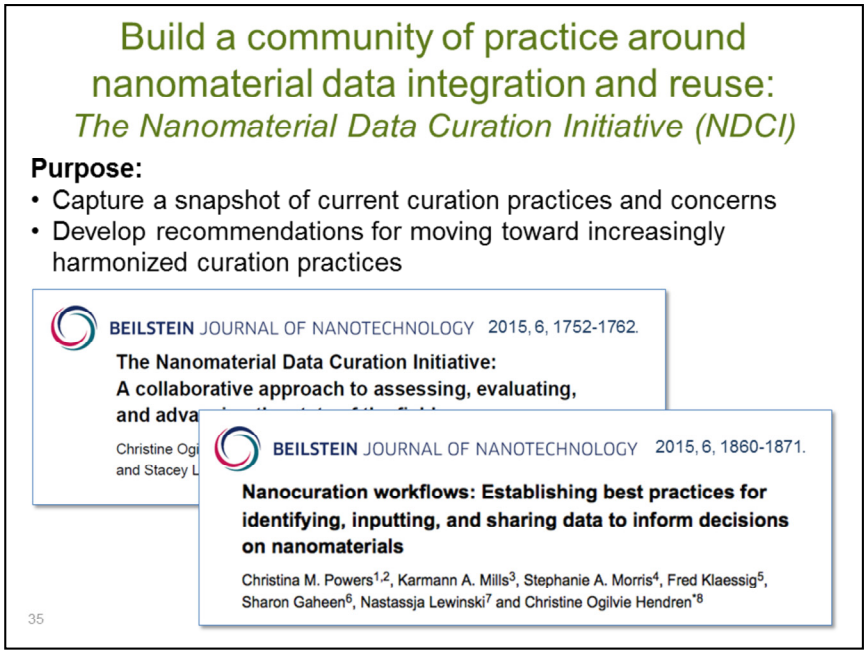
>> Christine Ogilvie Hendren: Then the Nano Working Group moved on to develop a specification that would facilitate the exchange of data on nanomaterials and their characterization. They did this by basing their work on the ISA-TAB community work and customizing the file sharing formats for nanotechnology characterization and data. They shepherded this through until it became an actual ASTM standard, and that effort was led by Sharon Gaheen at NCI. There's a website where you can check out more on this.



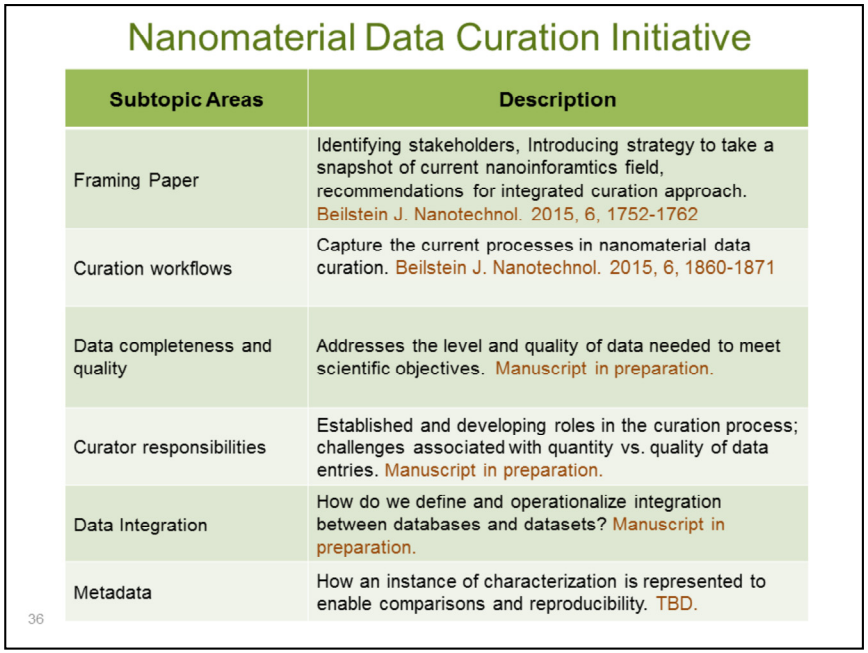
>> Christine Ogilvie Hendren: For a little measure of how successful the ISA-TAB-Nano has been, it is already being used by several teams and we'll say courted by others who realize the importance. That's what I would call the "beta users" in the community, who maybe consult, borrow, and map even if they have not fully developed structures around it. The two papers in blue below describe the ISA-TAB-Nano format in detail, and the one in red is a newer EU perspective -- a really good piece by Richard Marchese Robinson, reflecting on challenges and successes in adopting this format.



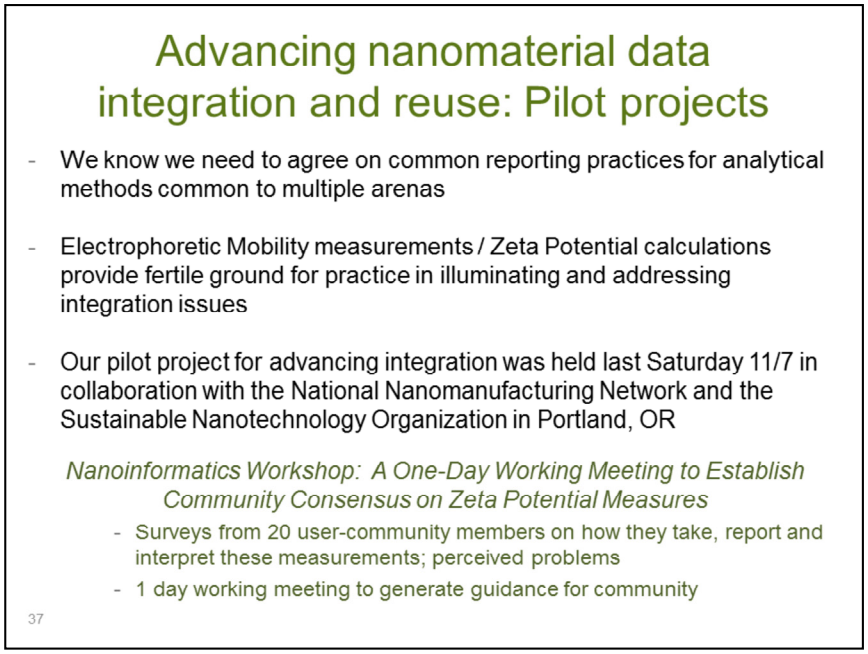
>> Christine Ogilvie Hendren: The next effort is to build a community of practice around nanomaterial data integration and reuse. We're doing that through what we call the “Nanomaterial Data Curation Initiative.” Because we didn't think we had enough acronyms in our lives, we have the NDCI. Its purpose is to capture a snapshot of current curation practices and concerns and secondarily to develop recommendations for moving forward toward increasingly harmonized curation practices. The strategy here is to write a series of consensus papers on multiple specific data curation topics that describe the current status, challenges, and potential solutions or next steps. To do this we assembled a group of nanoinformatics community stakeholders liaisons. At this point, anyone is welcome to serve as one of those to get involved in the project, and we partly just want to identify who is the nanoinformatics community. Then the Working Group leadership surveys stakeholder liaisons on each topic. Sometimes the authors of the papers will do that. But if they are Federal employees then it's inappropriate, and they don't touch that part of it. The authors get the material back from the stakeholder liaisons and develop a manuscript based on the survey results, to sort of take our pulse.



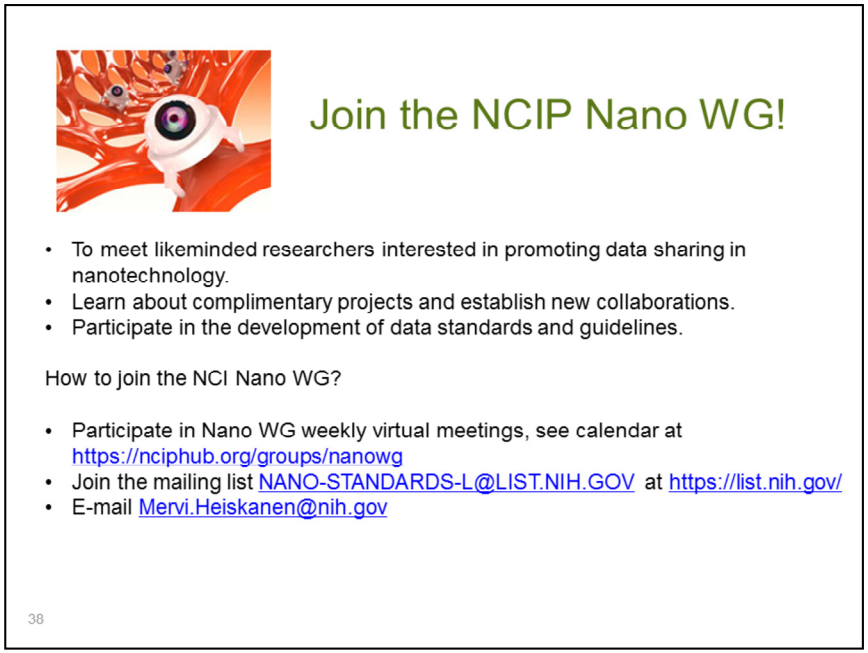
>> Christine Ogilvie Hendren: The first few papers are out. The framing paper is just setting the stage for what we plan to do with this collaborative approach. Then the second one, authored by Christina Powers (Christina Parsons now) at EPA, is about nanocuration workflows. It's been really nice to see those get out there.



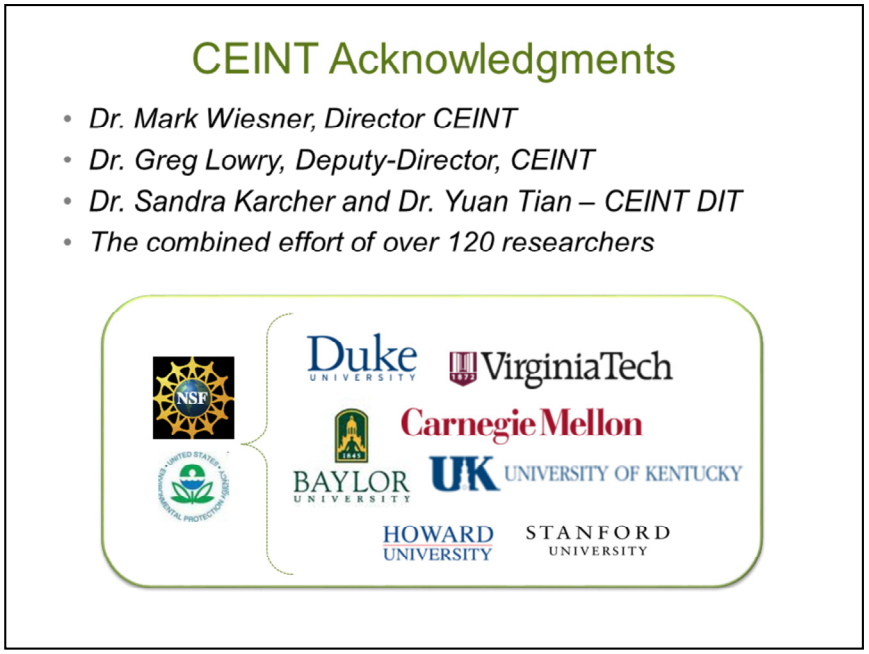
>> Christine Ogilvie Hendren: We have four more papers on the way: one on data completeness and quality; curator responsibilities; and data integration that are all under work; and one on metadata that we're going to figure out the timeline based on what's coming back from the community. We'd really like to build up our stakeholder liaisons bank before taking on that one.



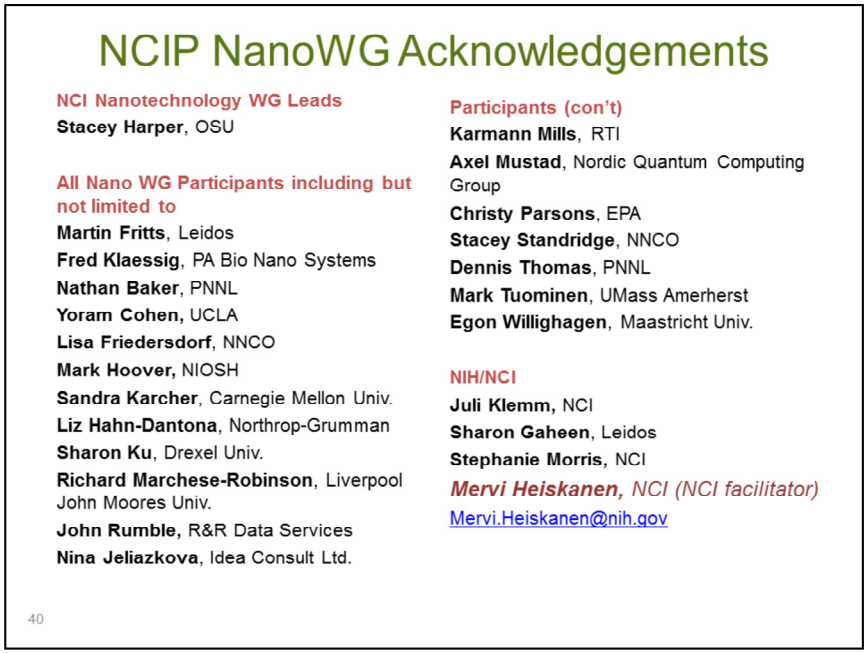
>> Christine Ogilvie Hendren: The final thing is that we want to advance nanomaterial data integration and reuse through pilot projects. Again, really getting into the details. We know we need to agree on common reporting practices. What we decided here was to take just one analytical method that was common to multiple arenas. Since nanotechnology covers many disciplines -- including biomedical, environmental, material science -- all of those use, for example, electrophoretic mobility measurements and associated zeta potential calculations. We thought that provided a fertile ground for practice in illuminating and addressing integration issues. So our pilot project for advancing this was actually held last Saturday. Some of the people on the call were there in fact. That was a collaboration with the National Nanomanufacturing Network (NNN) and the Sustainable Nanotechnology Organization, held in Portland. It was a one-day workshop to establish community consensus on how to measure, interpret, and report zeta potential from electrophoretic mobility measurements. We compiled surveys. We got back 20 different user community member surveys on how they take, report, and interpret these measurements, and the perceived problems. We then held a one-day working meeting to generate guidance for the community on how do we adopt the standards, communicate properly, interpret how to apply the standards, and more generally what is the role of a user community in bridging the gap between the standards communities, which are a separate and established thing, and the real application and true adoption of community-wide standards that will allow interoperability.



>> Christine Ogilvie Hendren: If you're interested in joining the NCIP Nano Working Group either email me if this is going by too fast or email Mervi here or join our mailing list. We have got all kinds of options. It's open. It’s a great place to just get connected with everything that's happening.



>> Christine Ogilvie Hendren: I'd like to acknowledge many people. Very quickly, here are my CEINT acknowledgements. I want to specifically say Dr. Sandra Karcher at CMU and Dr. Yuan Tian at Duke are the core of our CEINT data integration team and have done all the work to create the NIKC as it is.

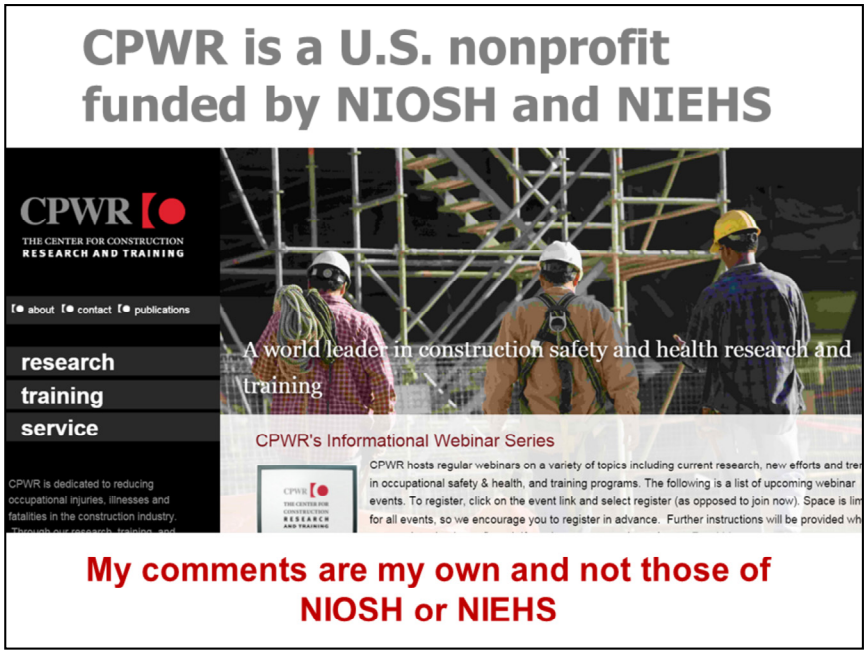


>> Christine Ogilvie Hendren: For the NCIP, there are many, many people listed here, especially Mervi Heiskanen, who helped develop some of the slides and, as I said, holds it all together.

>> Christine Ogilvie Hendren: With that I'm happy to conclude, and thanks again for having me.

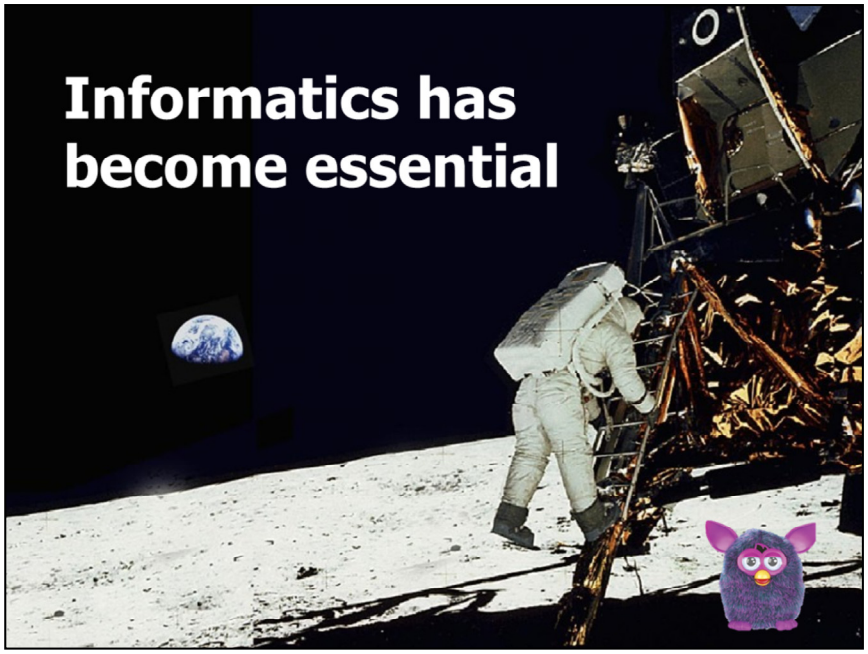
>> Stephen Lehrman: Thank you, Christine. And now, we're going to hear from Dr. Bruce Lippy.

>> Bruce Lippy: Okay. Thank you. That was great, Christine. I'm going to have to change my topic when we talk about construction. That was very well done. I am very pleased to be here. I'm an industrial hygienist. I admit it freely, and I've been doing industrial hygiene since 1978. I want to give recognition to the work NNI is doing. This is the most impressive proactive effort I have ever seen as far as getting ahead of a potential hazard as far as workers. So I'm really very honored to be here. There's my contact information if anybody wants to get in touch afterwards.

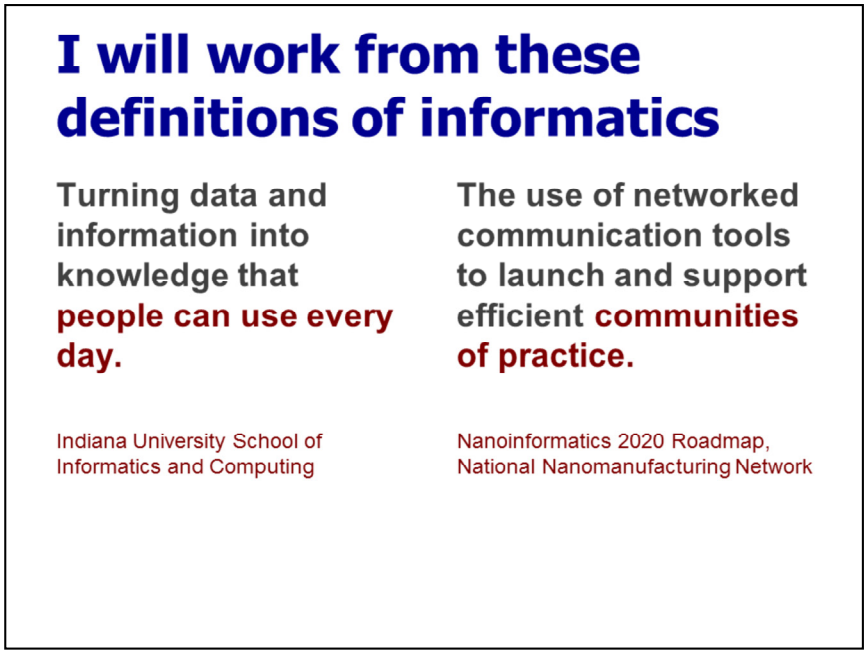


>> Bruce Lippy: I did want to mention that CPWR is a U.S. nonprofit, and we are funded by NIOSH and NIEHS. Our work in nanotechnology is funded by NIOSH. My comments are my own and not those of either NIOSH or NIEHS. We have been the Center for Construction Research for 20 years through NIOSH, and we have just recently started looking at nanomaterials and construction.

>> Bruce Lippy: So quick introductory comments.



>> Bruce Lippy: One is that I want to emphasize I truly believe informatics has become essential. This is obviously the 1969 shot of the moon landing. That's Buzz Aldrin stepping down, a very impressive and historic occasion for the U.S. This is a picture of a toy introduced in 1998. It's called a Furby. It was a little domestic robot, and that toy, which sold around 20 million, has more computing power than the entire NASA mission that successfully got people to the moon. So we have an abundance of data, even in construction.



>> Bruce Lippy: I will work from these definitions of informatics. I like them. One is turning data and information into knowledge that people can use every day. That's from the Indiana University of School of Informatics. This one is the use of networked communication tools to launch and support efficient communities of practice. I heard some great stuff that Christine has been doing with communities of practice. We're not that far along in construction, but there's hope. That's from the nanoinformatics roadmap.

>> Bruce Lippy: Let me say upfront that nanomaterials in construction can make a huge difference. Buildings consume 40% of energy globally. It's important to understand that construction materials represent the most easily available medium to distribute photoactive substances over the widest surface area. We have surfaces. That's where change can occur. So nano in construction can make a big difference in climate change, for instance.

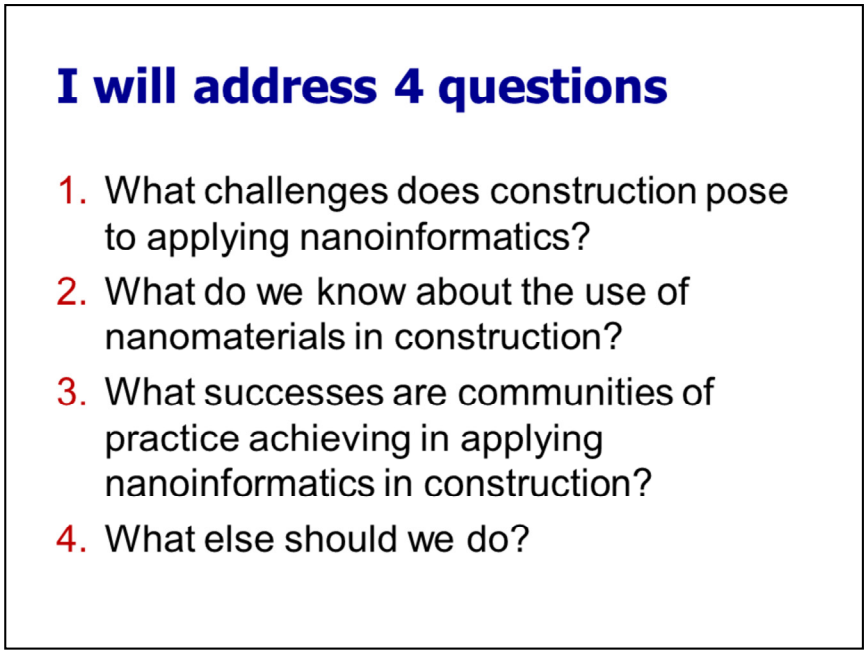
>> Bruce Lippy: There's work done with carbon nanotubes to be able to reinforce cement at a nanoscale with 100 times the tensile strength of steel and just a small part of the weight. So we're seeing a lot of very interesting work being done.

>> Bruce Lippy: What I just wanted to point out is that it's gone from the laboratory to the road surface. This is Eden Energy's test of their EdenCrete, done in August of 2015 working with the Department of Transportation in Georgia, and NIOSH participated. It had been a problem as far as cost to use carbon nanotubes in concrete. The company now says this is not an issue, and so the test is underway. We may have road surfaces that last a whole lot longer, much greater flexure strength and compression. So the question of course is, do the carbon nanotubes stay in the concrete?

The S&H challenge: Protect nano workers *without* being seen as Groucho

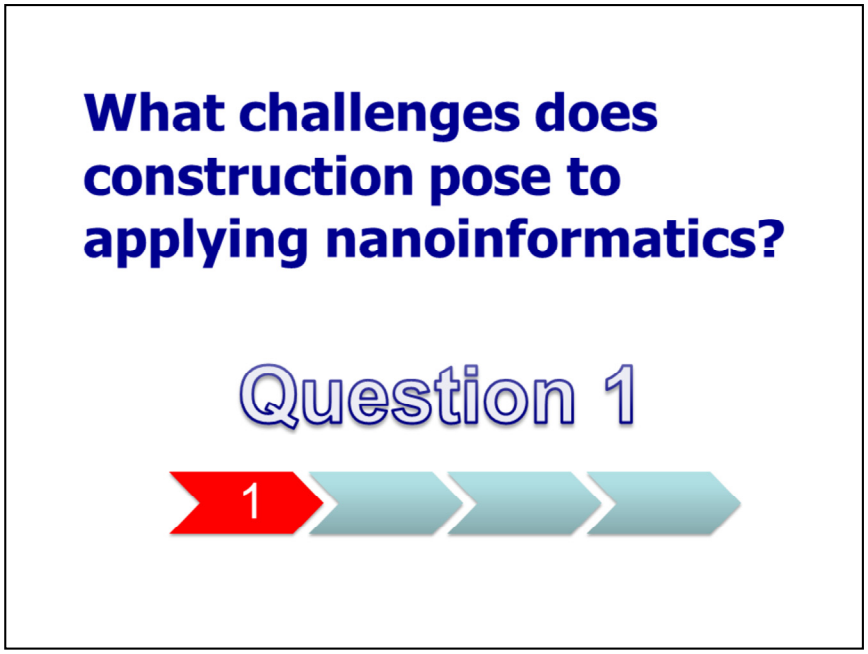
"Whatever it is, I'm against it. Even if I'm the one who commenced it, I'm against it."

>> Bruce Lippy: I would say our challenge is to protect nanoworkers without being seen as Groucho. This is from one of his films where he sings, "Whatever it is, I'm against it. Even if I'm the one who commenced it, I'm against it." I fear sometimes we're seen in that role, but I think the safety and health community fully supports the idea that there are enormous societal benefits from nanomaterials. We just don't want to see the risk being disproportionately placed on workers.

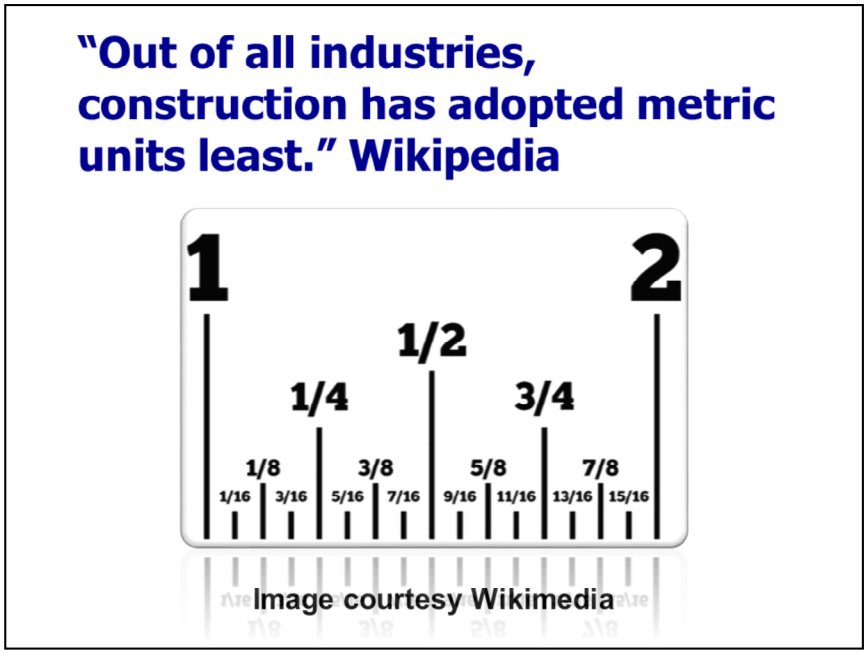


>> Bruce Lippy: So I'm going to look at four questions:

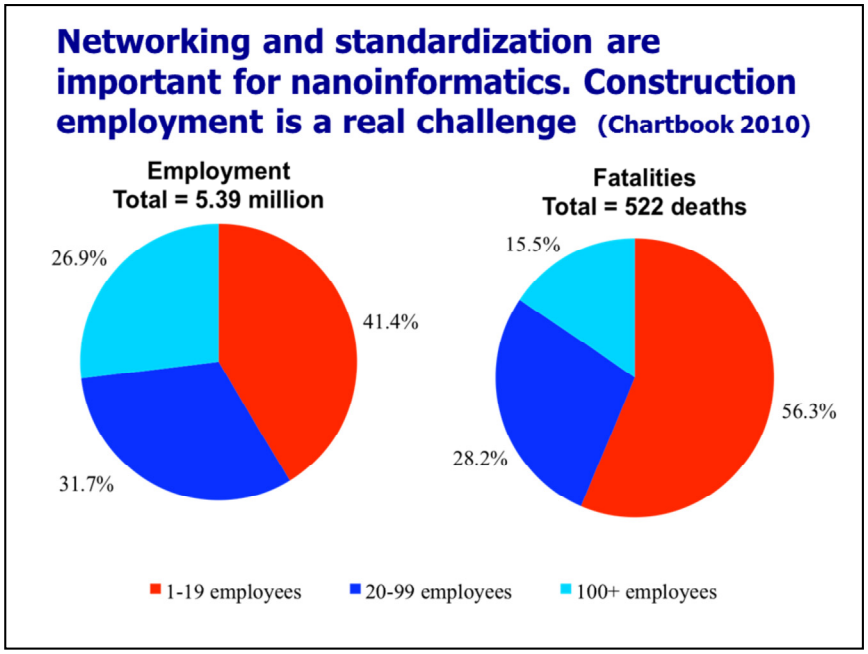
- What challenges does construction pose to applying nanoinformatics?
- What do we know about the use of nanomaterials in construction?
- What successes are communities of practice achieving in applying nanoinformatics?
- And what else should we be doing?



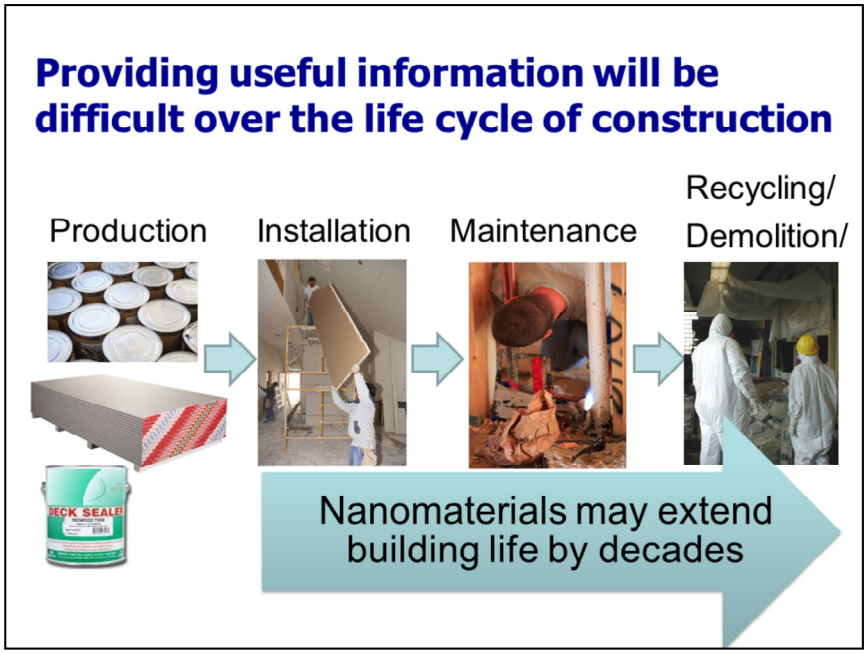
>> Bruce Lippy: Let's take the first one: what challenges does construction pose to applying nanoinformatics?



>> Bruce Lippy: I may be the only speaker at the National Science Foundation who is quoting Wikipedia, but this is true. Out of all industries, construction has adopted metric units the least. Back when Furbys were just hitting their strides, I served on the National Building Sciences Consultative Council, and we were all flushed with the idea that construction would end up using the metric system. That's gone the way of the Furby. We are not doing that.



>> Bruce Lippy: Here is part of the reason why. First off, networking and standardization are going to be the key important parts for nanoinformatics, but we've got real challenges in employment. If you look at these graphs from CPWR's Chartbook, a large portion, 41% of the firms out there in construction have less than 20 employees and represent a disproportionate number of the fatalities being experienced in construction today. So we have this situation of employment where it's very tough to do networking. We have a hard time reaching out and providing health information to these small firms.



>> Bruce Lippy: The other big issue in construction is providing useful information. It's going to be extremely difficult over the lifecycle of construction, from installation to maintenance, way down the road with recycling and demolition. The irony is that nanomaterials are going to be able to extend building life by decades. You can see the term “500 years” for a building in some of the literature. So how do we possibly keep any nanoinformatics moving all the way to the end of the process? How do we let demolition workers know that this material contains carbon nanotubes or contains titanium dioxide?

CPWR surveyed 79 worker-trainers from 22 trades with an average of 30 years in the trade

(2013-2014)

Survey Respondent Characteristics	N	Mean	SD	Range
Years in trade	78	30.5	9.4	9-55
Years as a trainer	79	13.3	7.8	1-34

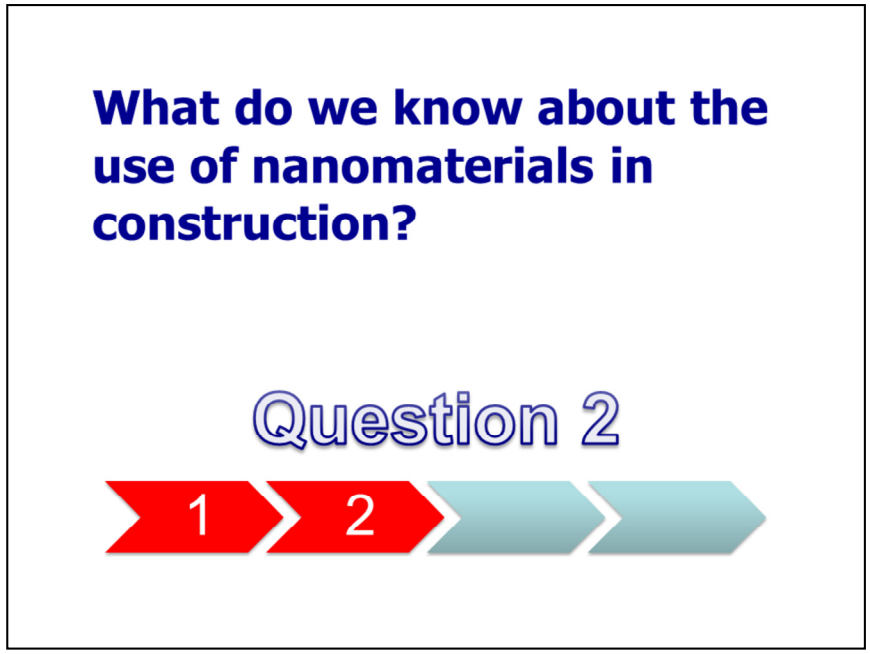
>> Bruce Lippy: The truth is workers don't know. We did a survey of 79 worker trainers. These folks came from 22 trades, had an average of 30 years in their profession, and had served about 13 years on average as trainers. So these are seasoned workers.

Nearly half were not aware that nano had been applied to construction materials

	Yes	No
Aware that nanotechnology has been applied to construction materials?	41 (52%)	38 (48%)
Aware that construction products containing nanomaterials are commercially available in the USA?	38 (48%)	41 (52%)

>> Bruce Lippy: Nearly half are not aware that nano has been applied to construction materials, and over half didn't know that these materials are commercially available in the U.S.

>> Bruce Lippy: Another issue is that there's a lot of great work being done in monitoring the levels of nanomaterials, but it's a challenge for real-time particle counters. This is a test we conducted with a sprayed-on zinc oxide coating that goes on the wood. If you look at the little plastic box there, inside that is a scanning mobility particle sizer and an optical particle sizer. We had to protect it from the materials. Now, the unfortunate thing is we need these instruments, and the manufacturer says they are designed for clean room use. That's very nice, but we can use them, too. We have to figure out how to make these instruments more robust so we can deal with the environmental issues and the large amounts of airborne materials in construction.

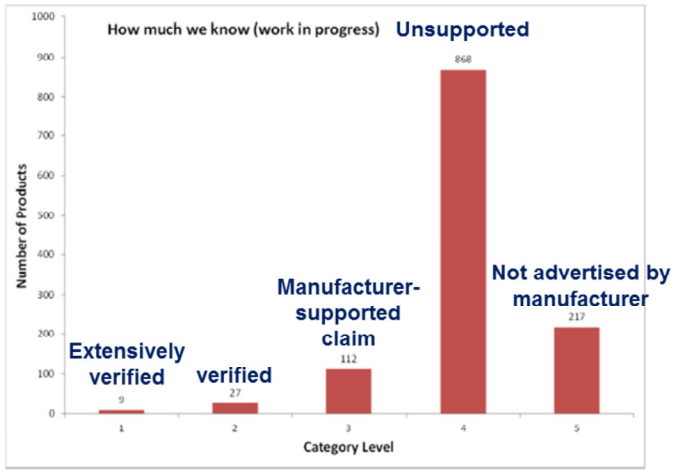


>> Bruce Lippy: What do we know about the use of nanomaterials in construction?

>> Bruce Lippy: One prediction is by 2025, 50% of the building materials will contain some type of nanomaterial. Now we're a long way from there according to my colleague Wendy Jones. We work with Wendy and Alistair Gibb out of Loughborough. They are doing similar types of work with construction materials in Europe, and they are great to work with.

>> Bruce Lippy: Most everyone knows about the Wilson Center Project for Emerging Nanotechnology, which has about 2,000 consumer products in their inventory.

PEN assigns confidence to entries



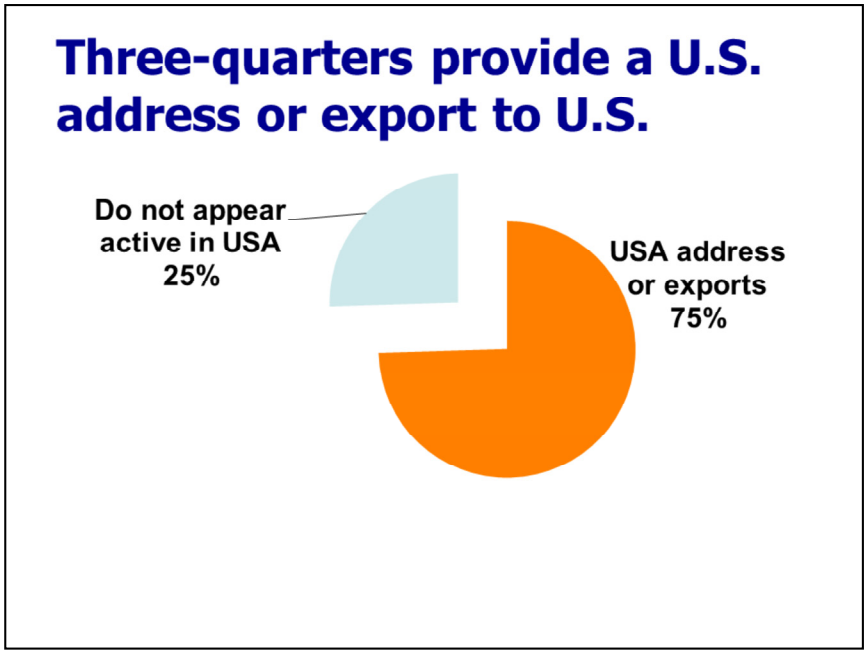
From Todd Kuiken's presentation at NanoSafe2014

>> Bruce Lippy: What they do that's very impressive is they try to assign confidence to their entries: how much do they really believe that this material definitely contains a nanoparticle or nanomaterial? As you can see, very few are extensively verified, and the overwhelming number are unsupported. This is what we have experienced, too.

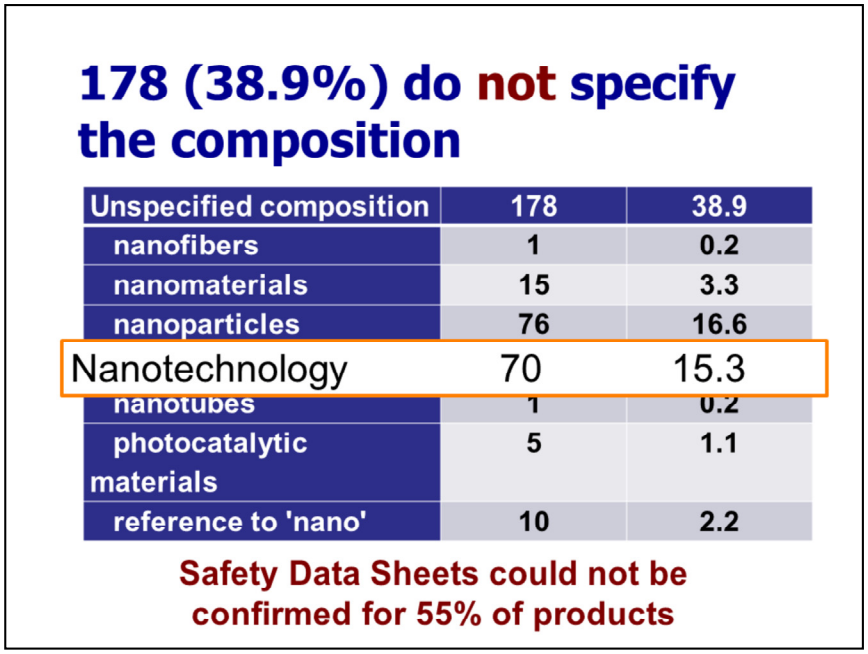
>> Bruce Lippy: I manage this site, ELCOSH, Electronic Library of Construction Occupational Safety & Health, for CPWR. We have just added since last October a site called ELCOSHNANO, which is an inventory of construction products that we are finding on the web that we think have nanomaterials. I would also say if you're going to talk informatics for construction, you better be talking Spanish, too. We have a button that you can click on and flip over and look at everything we have in Spanish. That's an important aspect of any hazard communication in construction today.

>> Bruce Lippy: On our site, and there is the website for it, we have about 487 products. These are commercially available, and they are reported to be nano-enabled. I want to emphasize we're in the same boat as the folks at the Woodrow Wilson Center with their inventory.

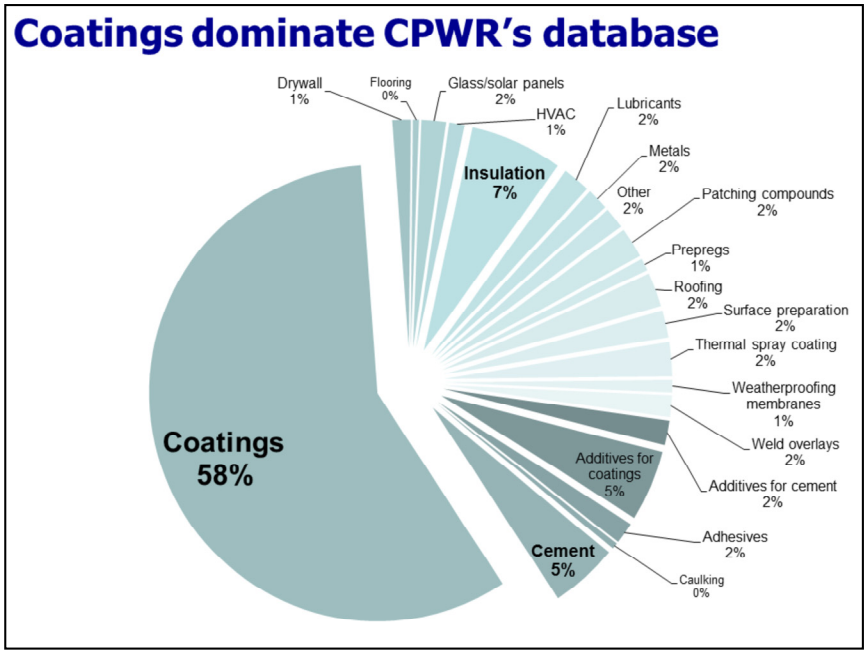
>> Bruce Lippy: We do extensive web-based searches. That is listservs, RSS feeds, construction trade publications, and media articles. We look at peer-reviewed literature and check social media. My colleague Gavin West has done a great job.



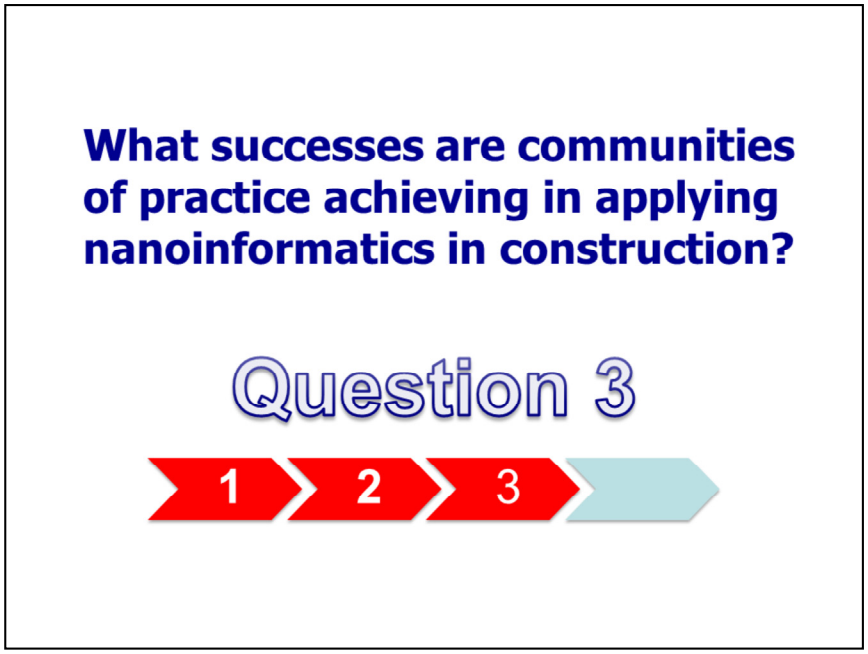
>> Bruce Lippy: We believe about three-quarters of these products are available in the U.S.



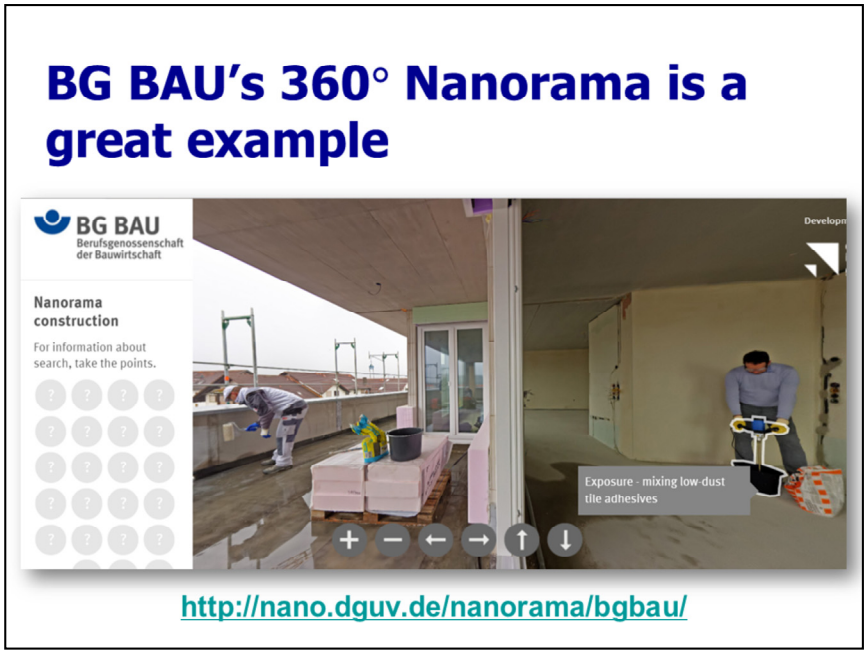
>> Bruce Lippy: But 38% did not specify the composition of the material. Here is an example. It says nanotechnology. Well that's just not particularly useful. In fact, we could not find Safety Data Sheets for 55% of the products in our inventory.



>> Bruce Lippy: If you look at the inventory broken down by what kinds of products, coatings dominate. 58% of our materials are coatings. Then we see cement and insulation as other big areas.

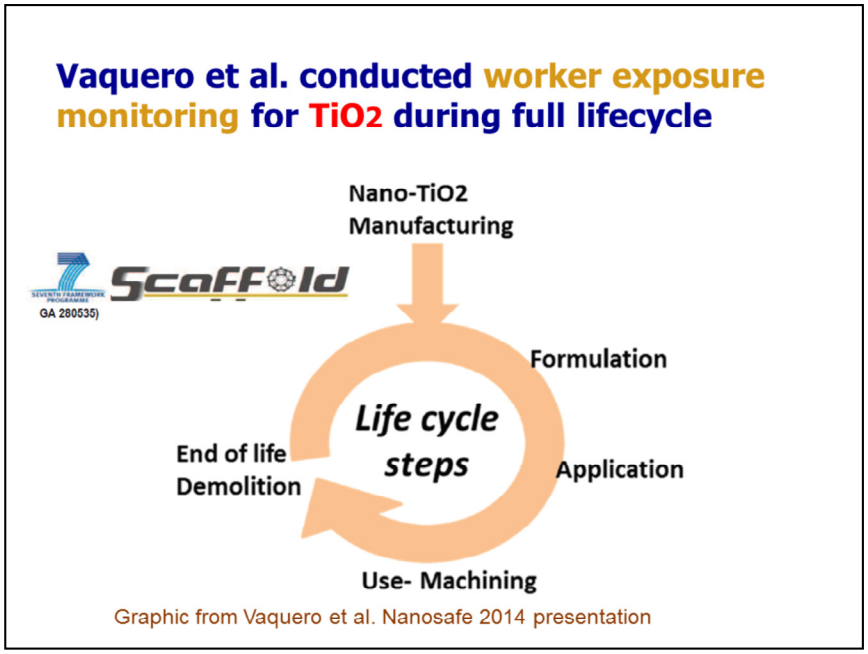


>> Bruce Lippy: So the third question is, what successes are communities of practice achieving in applying nanoinformatics in construction?



>> Bruce Lippy: One of the interesting sites, this is the German Federal Government, the BG BAU site has what's called "Nanorama." It's a site where you can spin around on a construction job site, and focus on individual products -- like this material here that the gentleman is mixing up on the right. It will tell you what the product is. It will tell you what some of the issues are as far as potential health risks. It also actually has a game format which is very interesting.

>> Bruce Lippy: The Europeans really have been pushing ahead, and they are coordinating nano release research under the SCAFFOLD Project, which I think just concluded. This is Grenoble, France. I attended the NanoSafe 2014 meeting where we heard a lot of about SCAFFOLD.



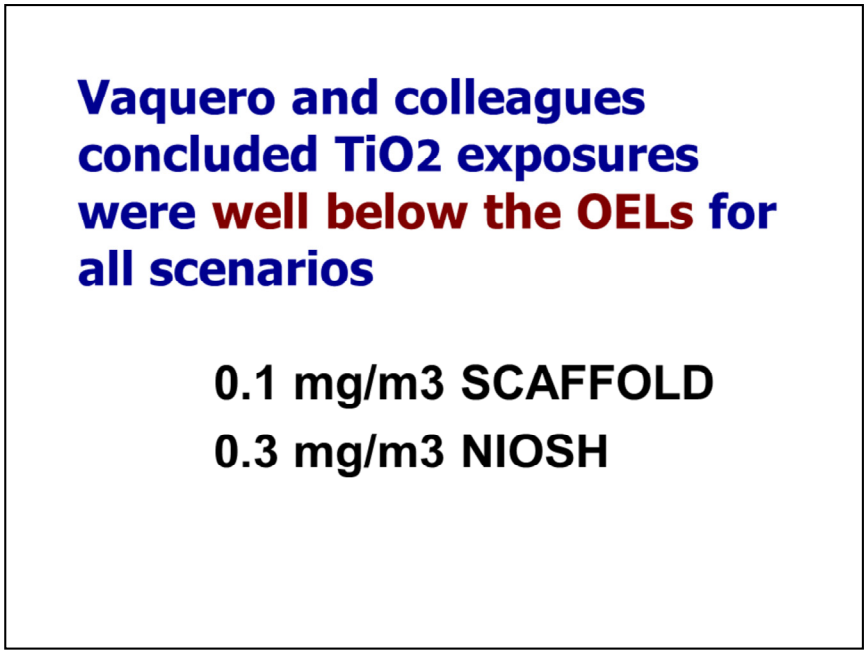
>> Bruce Lippy: I just want to show you a little bit from work done by Celina Vaquero and her colleagues in Spain, where they looked at actual worker exposure monitoring for titanium dioxide, and they looked at the full cycle from manufacturing to machining to demolition.

Sampled during manufacturing of 1 ton of each of 3 types of mortar

Photos from Vaquero et al. Nanosafe 2014 presentation

>> Bruce Lippy: It was serious work. They sampled during manufacturing, 1 ton of each of three different types of their mortars.

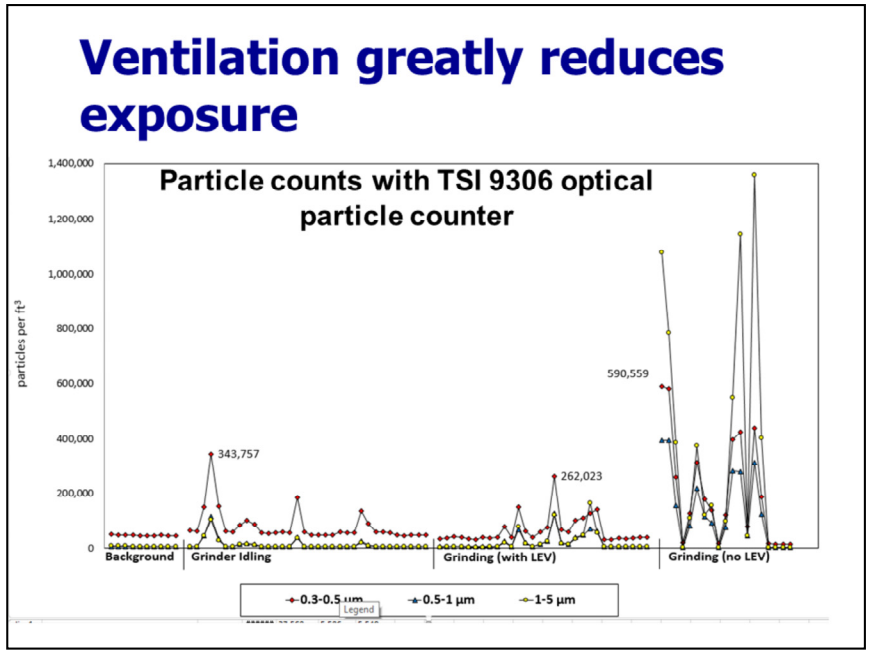
>> Bruce Lippy: Then they sampled worker exposures during drilling and also final demolition of materials that contain the titanium dioxide.



>> Bruce Lippy: They concluded from their work that the exposures were well below the occupational exposure limits for all scenarios that they looked at. They were using a lower level of 0.1 milligram per cubic meter than NIOSH has set in its recommended exposure limit of 0.3. That was good news.

>> Bruce Lippy: We conducted a range of sampling with cutting, drilling, and nailing of tiles.

>> Bruce Lippy: These tiles are photocatalytic. They are called smog-eating tiles produced by a company called Boral. The titanium dioxide coating is on the surface. It is actually a concrete tile.

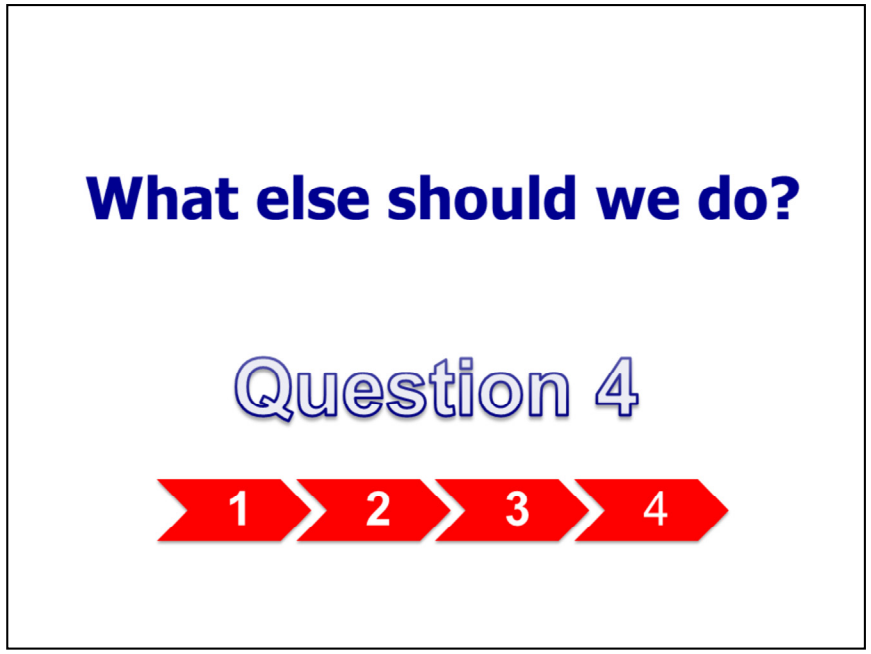


>> Bruce Lippy: What we found, as have a number of other researchers including Mark Methner and folks from NIOSH, is that ventilation, local exhaust, really greatly reduces exposures. As you can see this is particle counting with a device that looks at the smallest level to be 300 nanometers - those are the red dots. If you look at the far right, you'll see when you're grinding without LEV (local exhaust ventilation), you've got tremendous spikes. Whereas when you use the local exhaust ventilation, it drops it very dramatically. I will also say we saw higher numbers of small particles with the grinder idling when it wasn't even cutting in.

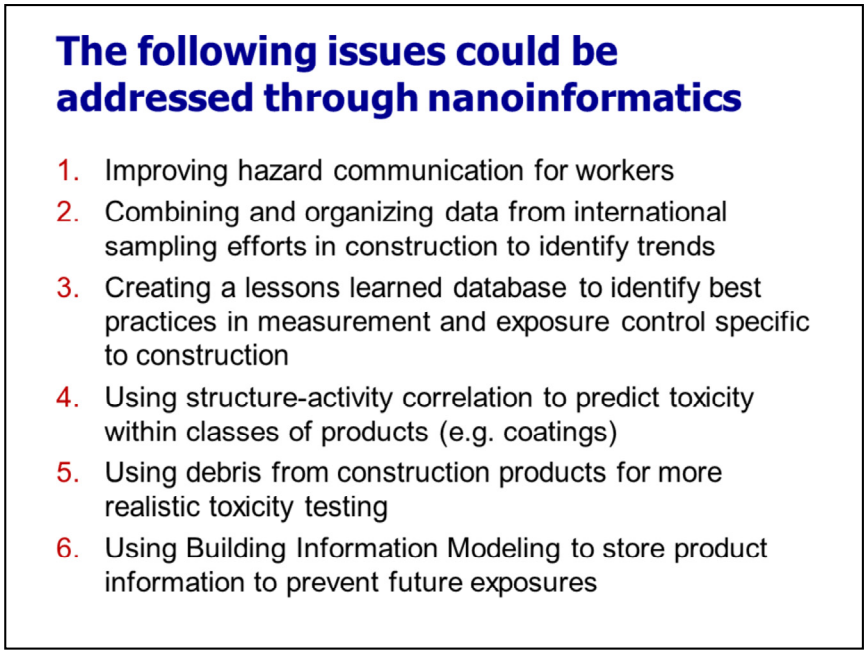
Most results were encouraging

- All measurements were below the NIOSH REL for ultrafine TiO_2 of 0.3 mg/m^3
- Ventilation on the tool reduced *respirable* dust by roughly 50% (88 – 97% in chamber)

>> Bruce Lippy: We did personal measures, too, and all of those were below the NIOSH REL for titanium dioxide that I just mentioned. Outside, we found that the ventilation on the tool you see on the right reduced dust by roughly 50%, and inside in the environmental chamber there was up to 97% reduction. This does work.

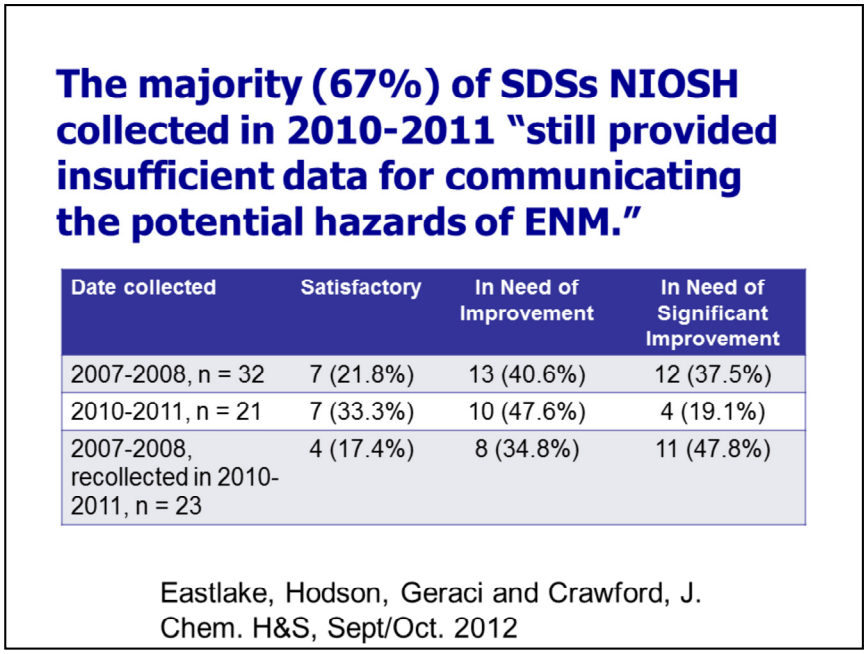


>> Bruce Lippy: Where else do we go? What else should we do?

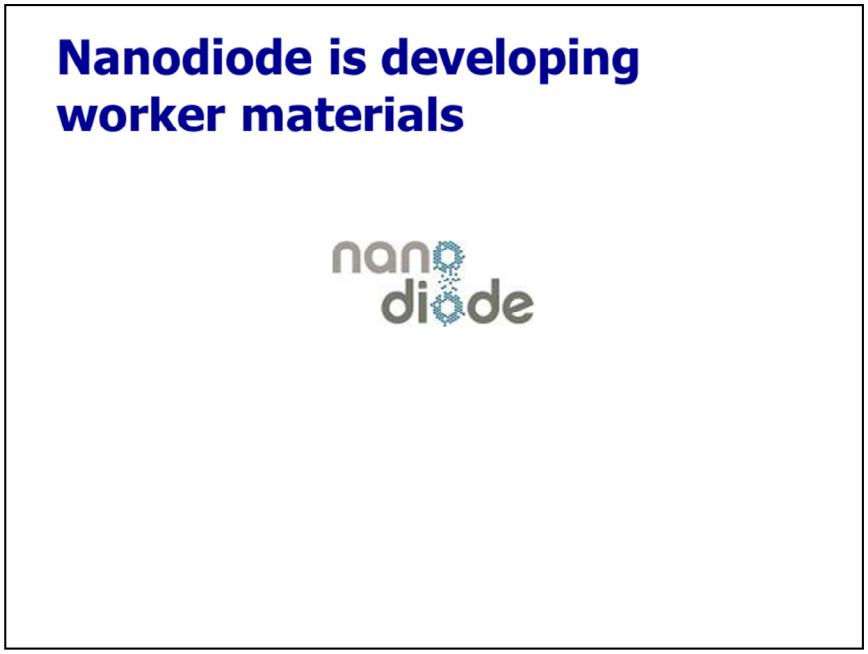


>> Bruce Lippy: Here are the issues I think we should be addressing through nanoinformatics for construction:

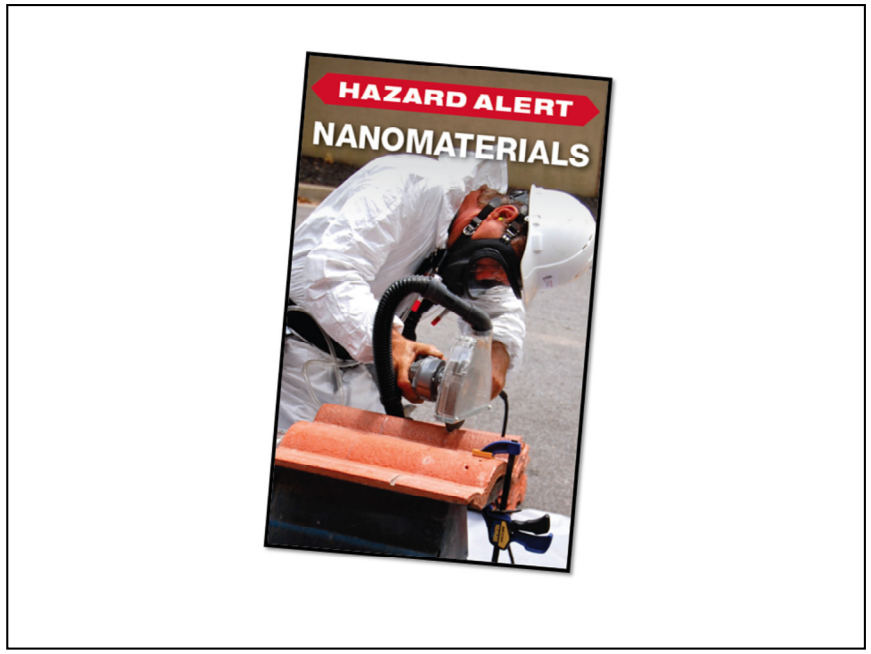
- Number 1 is improving hazard communication for workers. It is just not there.
- Combining and organizing data from international sampling efforts in construction to identify trends and try to understand what we should be doing as far as these exposures.
- And I suggest a lessons learned database. My colleague Dr. Dan Marsick thought it was a great idea to identify best practices, measurements, and exposure controls specific to construction so we can get around the delicate nature of some of the real-time instrumentation, and also understand how best to control exposures.
- Then I think we can use the structure-activity correlation work that's been done elsewhere to try to predict toxicity within classes of products. If there's an overwhelming number of coatings, what does that mean as far as really trying to identify where some toxicity work might cover a number of different products?
- I would like to see using debris from construction products for more realistic toxicity testing. We have been testing the basic nanomaterial. We in construction deal with debris. It would be nice to see how that affects toxicity testing.
- And then using building information modeling. BIM is a very cutting-edge, neat way to keep track of information, and we could store product information on nanomaterials for exposures way down the road.



>> Bruce Lippy: I just want to point out that this is from the NIOSH work on Safety Data Sheets. We have a serious problem with Safety Data Sheets. NIOSH said in 2010 and 2011 that Safety Data Sheets were still providing insufficient data for communicating the potential hazards of engineered nanomaterials. They had looked at them in 2007 and 2008, and they didn't see much improvement.



>> Bruce Lippy: I wanted to also shout-out that there's a project in Europe called NanoDiode, and they are developing materials for workers, which I think this is going to go a long way because we just haven't gotten the information down to the shop floor as far as talking about hazards.



>> Bruce Lippy: CPWR just produced this hazard alert on nanomaterials.

What are Nanomaterials?

There are many kinds of nanomaterials, but they all share a remarkably small size (roughly 100,000 times thinner than a human hair). At this size, they can add new properties to many construction products.

Nanoparticles exist in nature and in man-made combustion sources, but this alert is about manufactured nanomaterials that are added to products. These products are called nano-enabled.

A carbon nanotube laying across a human hair

PROTECT YOURSELF

1 Learn about nanomaterials in your trade

CPWR maintains a website called **eLCOSH Nano** that features over 450 products that may be nano-enabled.

www.nano.elcosh.org

Construction products that may contain nanomaterials include:

- **Coatings**
- **Lubricants**
- **Cements**
- **Adhesives**
- **Insulation**
- **Patching compounds**

2 Control dust

NIOSH and CPWR have demonstrated that dust collection systems attached to tools will reduce the number of nanoparticles along with normal dust. Wet methods will work, too.

Worker with full protective gear conducting CPWR test inside a special chamber using a dust collection system

3 Wear a respirator

Testing shows that nanoparticles do **NOT** get through high efficiency respirator filters. Reduce dust first with a dust collection system or water. If dust levels are still high, use a respirator.

What are the risks?

Some nanomaterials may be safe, but others have been shown to be toxic in the lab. Of particular concern are respiratory exposures to long, thin fibers, such as carbon nanotubes (CNTs). Certain types of CNTs cause lung problems in rodents, similar to asbestos. Nanoparticles don't seem to penetrate healthy skin but may get through damaged skin. Nanomaterials can be released from nano-enabled products, but the risks are not well understood.

The key is to limit exposure.

Are nanomaterials regulated?

OSHA does not have a regulation or Permissible Exposure Limit for any specific nanomaterial, but there are many existing OSHA standards, like the respirator standard, that would still apply.

NIOSH has set Recommended Exposure Limits for carbon nanotubes and nano-sized titanium dioxide that employers should follow. EPA has reporting requirements for nanoparticles under TSCA.

Learn more

- OSHA Respiratory Protection Standard (29 CFR 1926.103): http://tinyurl.com/OSHA1926-103
- OSHA Nanotechnology: http://tinyurl.com/OSHAnano
- NIOSH Nanotechnology: http://tinyurl.com/NIOSHnano
- EPA TSCA Regulations for Nanoscale

If you think you are in danger:

Contact your supervisor.
Contact your union.
Call OSHA
1-800-321-6742

Find out more about construction hazards.

To receive copies of this Hazard Alert and cards on other topics
call **301-578-8500**

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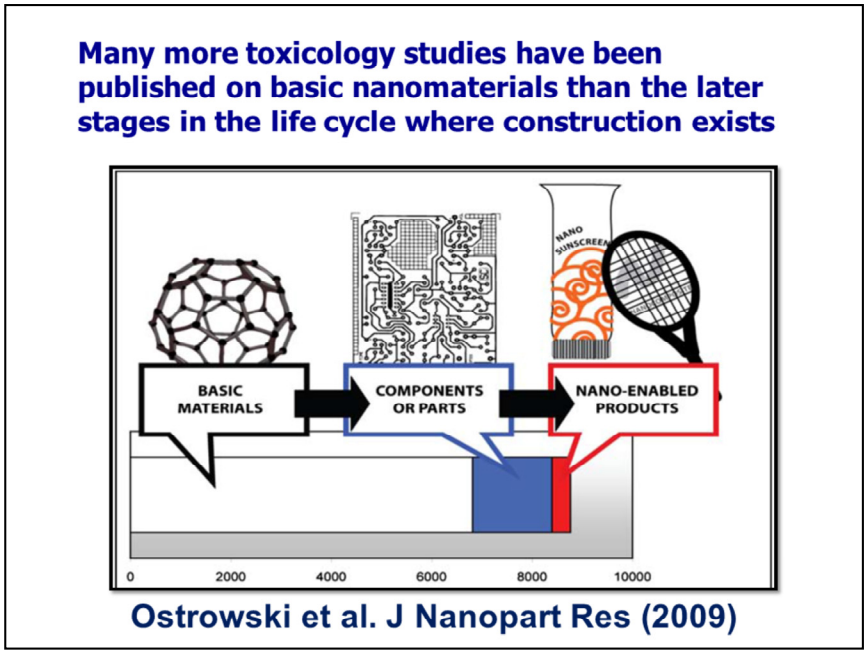
HAZARD ALERT

NANOMATERIALS

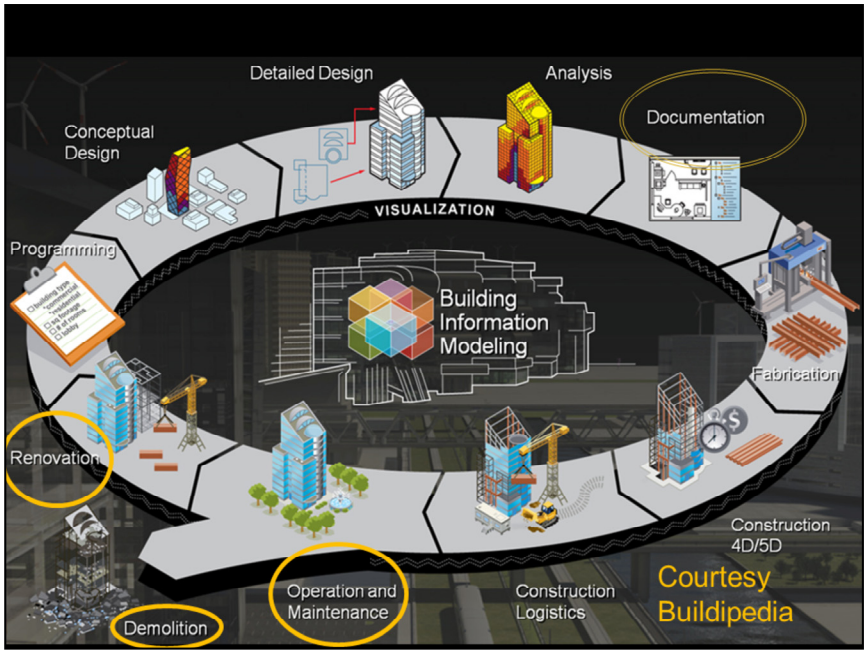
>> Bruce Lippy: We try to keep it aimed for workers. Simple things like 1, 2, 3 steps: learn about the nanomaterials in your trade; control dust; and wear a respirator. Then we tell them what the risks are. We tell them there aren't really nanomaterial regulations for specific particles, but that OSHA regulations still are in effect for things like respirators and other control of dust.

>> Bruce Lippy: We've produced it in Spanish. As I said, with the Latino population in construction, it's absolutely essential.

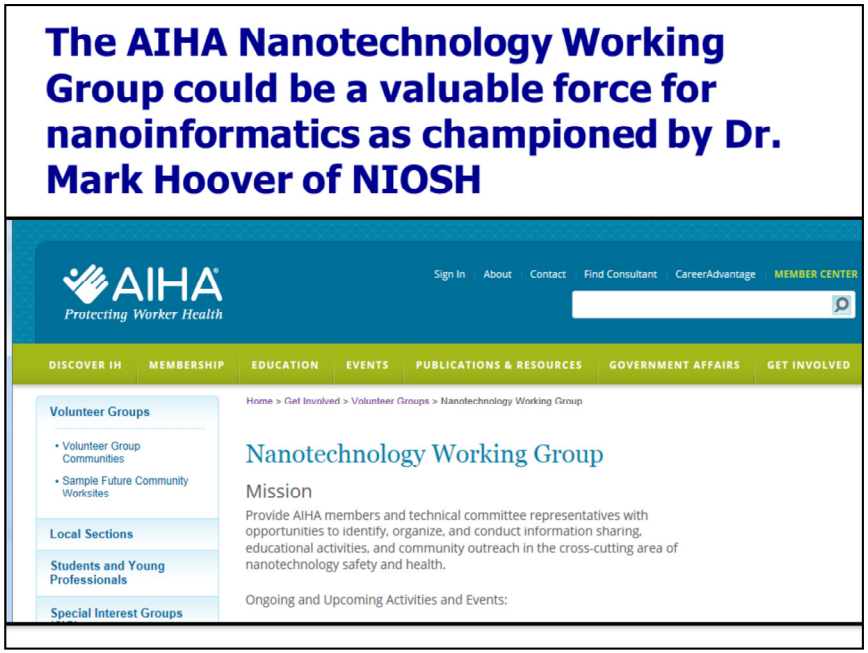


>> Bruce Lippy: I would also say that with the toxicology studies, so much more has been published on basic nanomaterials than the final product. These nano-enabled products -- the little red bar at the end -- that's where we exist in construction, and that's where we want to see toxicology studies.

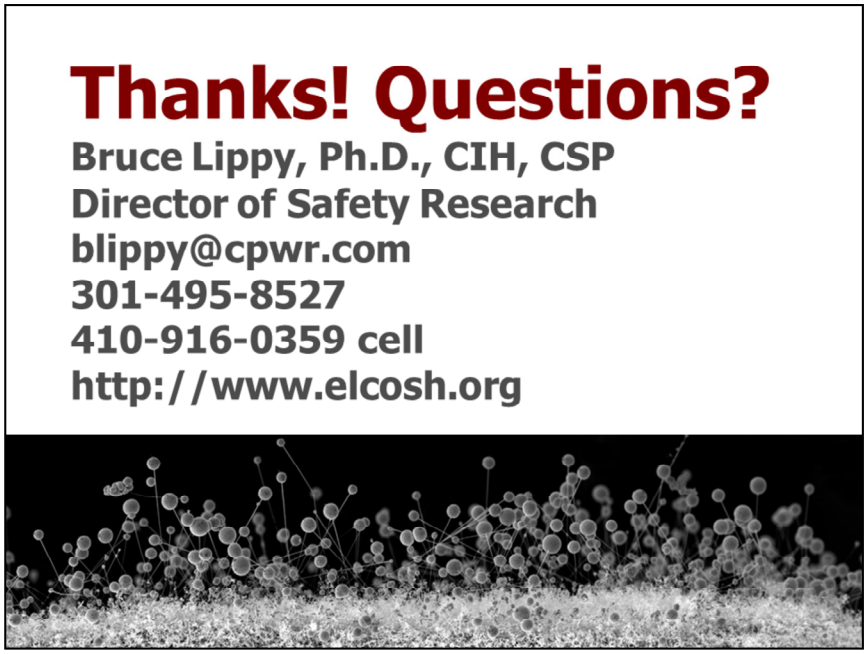
>> Bruce Lippy: NIOSH is doing the work. This is a shot in our environmental chamber where we work with an organization called Environmental Profiles. We looked at nano zinc oxide. You can see the team from NIOSH setting this up with a MOUDI cascade impactor there. They then are going to take this dust, and they have already started to do some *in vivo* testing.



>> Bruce Lippy: This is just a shot of BIM. I want to point out that in BIM (building information modeling), you can see I've circled documentation. That's really part of the whole deal, they keep the documents on the construction. Then when you get down to operations and maintenance, demolition, and renovation, you will know -- however long it is down the road, decades potentially -- what materials have been applied and what were the nanomaterials as part of that.

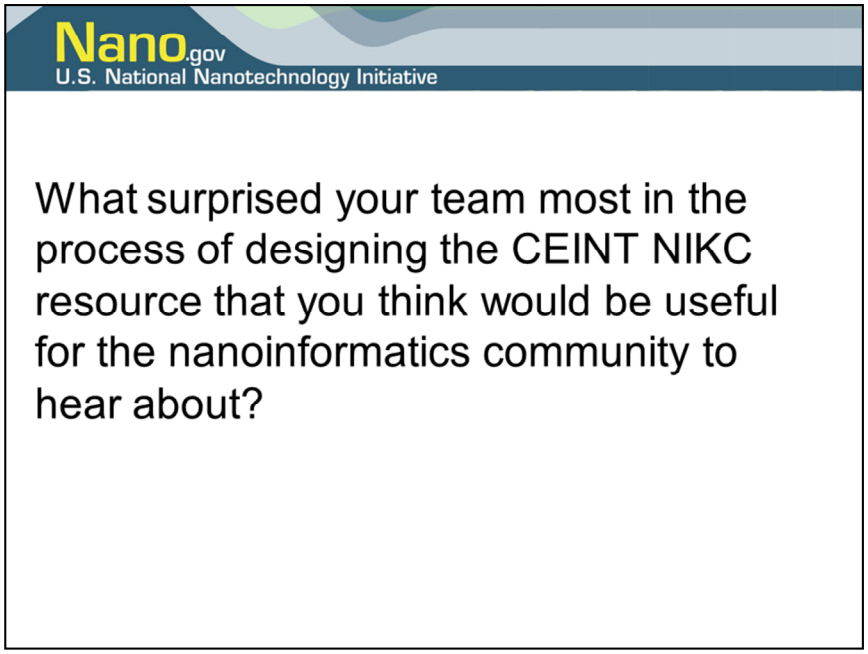


>> Bruce Lippy: I want to give a shout-out also to the AIHA Nanotechnology Working Group. I think it can be and has been very valuable for us in nanoinformatics as championed by Dr. Mark Hoover. I serve on this, and I would say to the people on the phone, certainly consider reaching out to us if we can be of assistance.



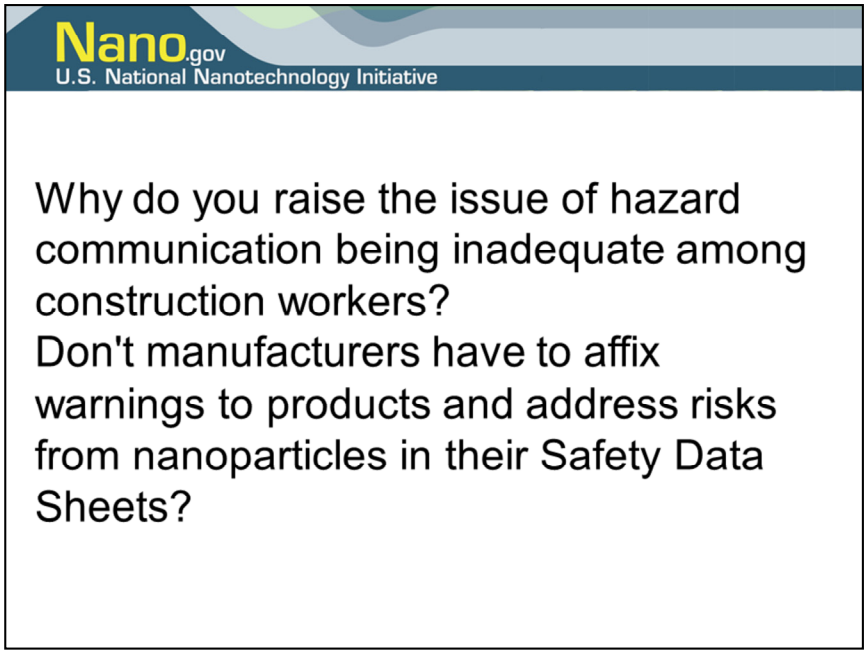
>> Bruce Lippy: I thank you, and I think it's time to open up to questions.

>> Stephen Lehrman: Bruce, thank you. Thanks to both of our panelists, Christine Hendren and Bruce Lippy, for great presentations. Now we have a few minutes for some questions and for answers. I remind you that you can go to the "Submit your question here" window and type in a question, or you can send it to webinar@nnco.nano.gov.



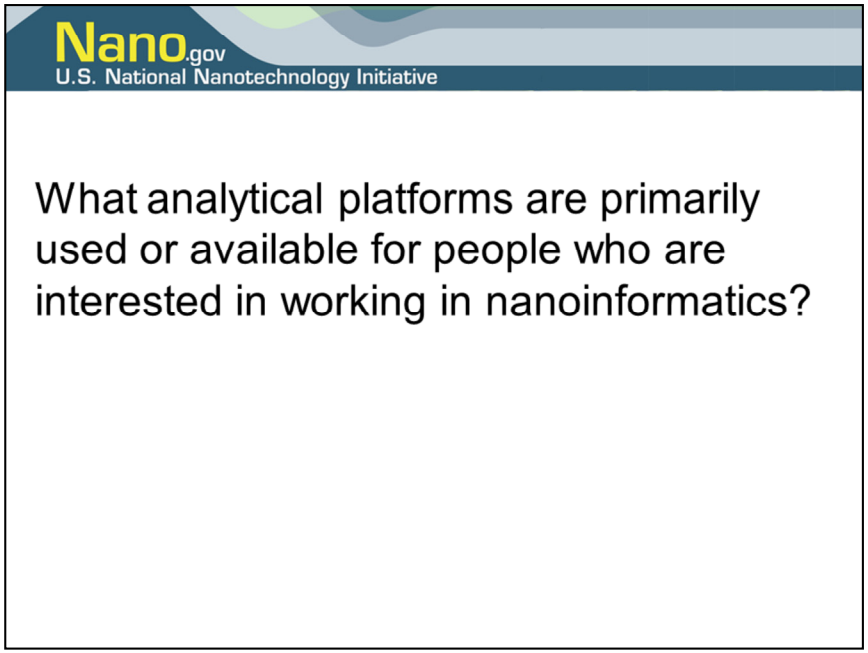
>> Stephen Lehrman: Our first question is for Christine. What surprised your team most in the process of designing the CEINT NIKC resource that you think would be useful for the nanoinformatics community to hear about?

>> Christine Ogilvie Hendren: Thank you. So I think that I would say that it's the fact that a lot of the things that are not the IT aspects of the process are the first place to put one's attention and figure out how to prioritize. It surprised us that it was so difficult to fit an IT project. I do have an IT corporate background before all of this academia world. Fitting an IT project into a research environment was really difficult in terms of tasks and timelines. I think what's useful to know, is knowing your priorities: Do you want to get a lot of data in ahead of time? Do you want to create a very, very detailed infrastructure? Do you want to enable the widest possible range of queries? I think realizing those upfront decisions and the way you navigate those tradeoffs that I talked about are really the determinants for how quickly you move and in what direction.



>> Stephen Lehrman: Okay, thanks Christine. Our next question is for Bruce. Why do you raise the issue of hazard communication being inadequate among construction workers? Don't manufacturers have to affix warnings to products and address risks from nanoparticles in their Safety Data Sheets?

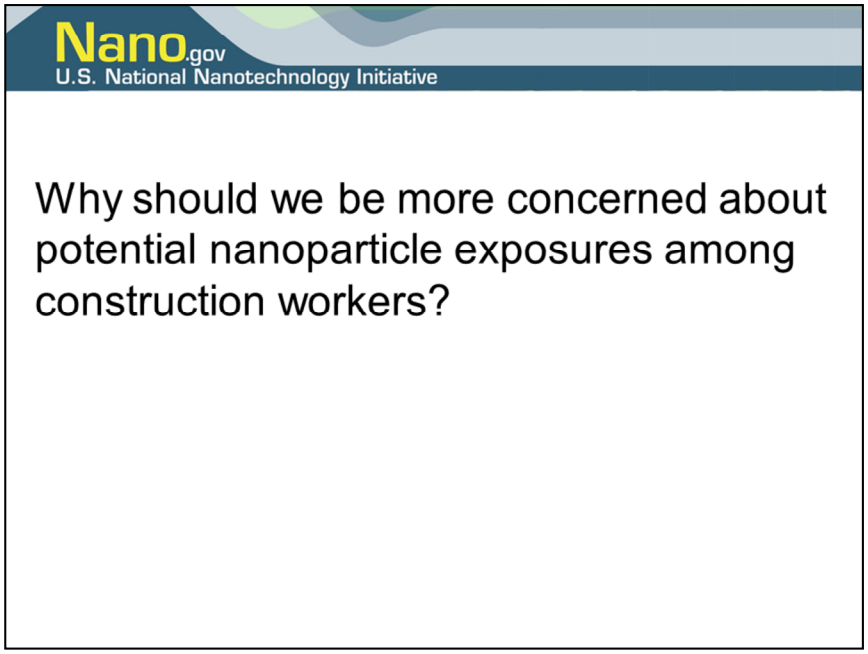
>> Bruce Lippy: Thank you. No, to both. There is no requirement that manufacturers specifically spell out that a material is in a nanoform inside their product. Not in a warning label nor in a Safety Data Sheet. They have to identify the components, but they don't have to say this particular form of carbon is in a nanosize, which is a real failing in my estimation as far as hazard communication.



>> Stephen Lehrman: Okay. Our next question is for Christine, as we alternate back and forth. Christine, in your presentation you talked about some of the different data collection tools available, and you mentioned nanoHUB. What analytical platforms are primarily used or available for people who are interested in working in nanoinformatics?

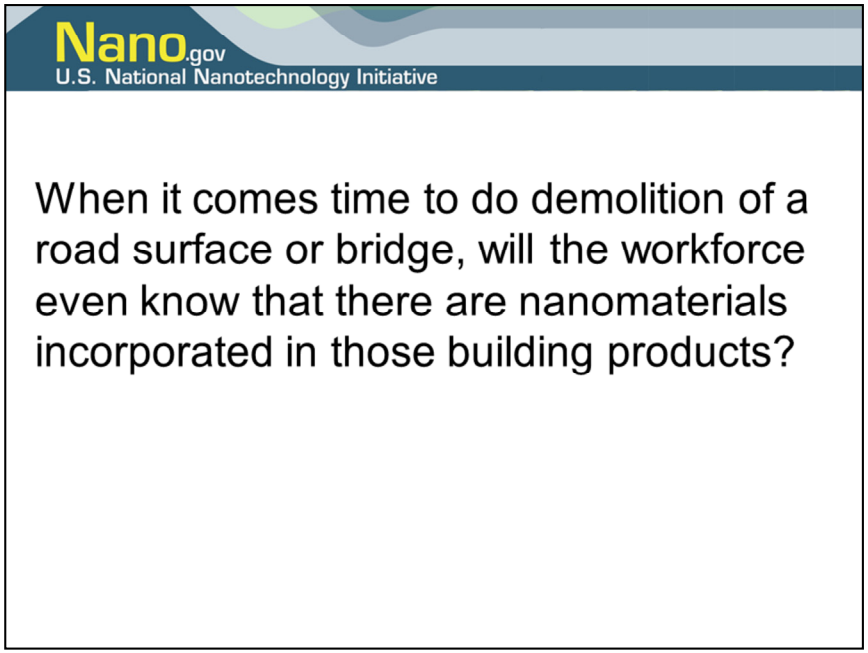
>> Christine Ogilvie Hendren: So I will attempt an answer, and then I would love to hear if it is addressing the basis of the question. There really is not a common platform. I would say ours and others that I know of are built in MySQL. But every application built on top of any resource is pretty much custom. So often it's coded in. I mean we've done a lot of research to figure out what is the most common, so that we can be as interoperable as possible. But nanoHUB has all sorts of different technologies on top of that. We do Django and Python development for web-enabled tools, and we do some things in R. I guess our take-away is that you really have to be ready to interface with a whole host of tool platforms.

>> Stephen Lehrman: I will mention in our first NKI webinar, Introduction to Nanoinformatics, Dr. Daryl Hess from the National Science Foundation talked about some of the modeling tools that are available. So if you want to go back to the www.nano.gov/publicwebinars page and look at the transcript and the presentations from the first webinar, you can see some additional information there.



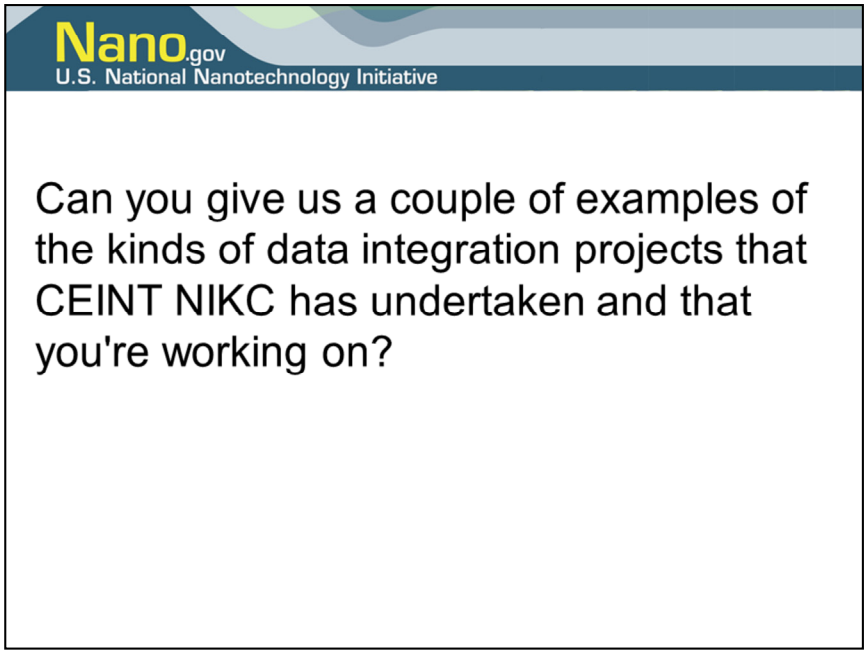
>> Stephen Lehrman: Our next question is for Bruce. Bruce, why should we be more concerned about potential nanoparticle exposures among construction workers?

>> Bruce Lippy: One of the things is that construction applies a great deal more energy to products than you would find potentially in a factory setting where they are manufacturing this. So when you are grinding or drilling or sawing or jackhammering, you are putting a tremendous amount of energy into it. The chance of release is much greater. Construction workers are not just exposed to one item a day where they would be concerned about a particular nanoparticle. There are lots of exposures in construction. Vapors and gases and dust combining in ways that we don't fully appreciate as far as the health effects. That would be my concern. Plus an aging workforce in construction. We are seeing older workers being exposed longer. All of that adds to concern.



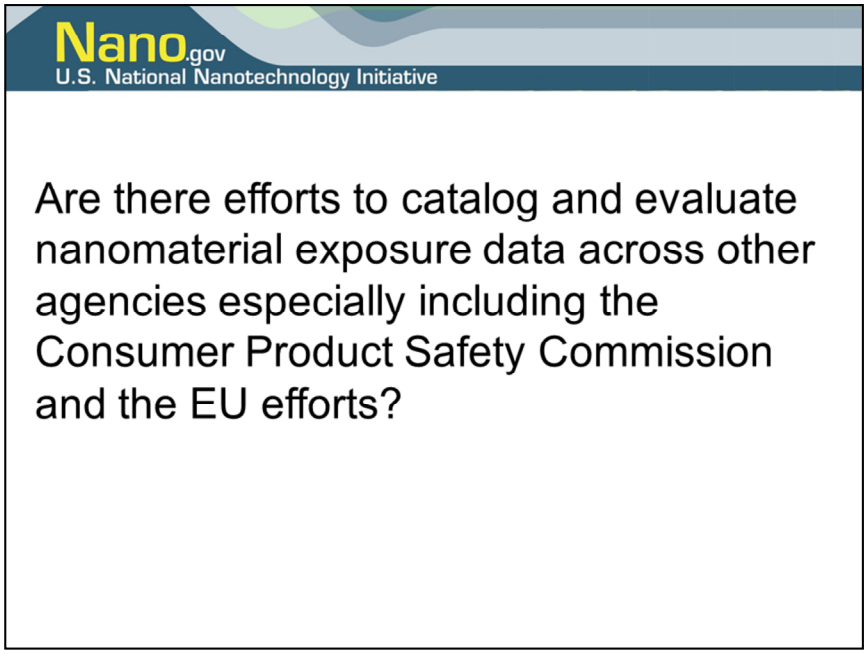
>> Stephen Lehrman: You raised a really interesting point about how nanomaterials are being incorporated into construction materials, which can have lifetimes of 40 or 50 years or sometimes even longer. Then when it comes time to do demolition of that road surface or bridge, will the workforce even know that there are nanomaterials incorporated in those building products?

>> Bruce Lippy: See, that's the major question for us as far as hazard communication. How do we get it downstream that long for such a timeframe? It's a real problem.



>> Stephen Lehrman: We have one more question for Christine. Christine, can you give us a couple of examples of the kinds of data integration projects that CEINT NIKC has undertaken and that you're working on? You gave a really good example of the work that the Nano Working Group is doing in terms of pilot projects going in and looking at zeta potential. I think our audience would be very interested in learning about more examples of pilot projects or activities that CEINT NIKC is working on.

>> Christine Ogilvie Hendren: Sure. We've got a couple in the mix. I'll talk about one in particular that is interesting because it overlaps in a number of fronts, and therefore, kind of presented itself as an obvious good use of resources. So we have been working long-term with the Nanomaterial Registry to map as much of our information as will fit into there, knowing that they are the ultimate repository that has been invested in by NIH to capture all of the data. Well, they were also working with RIVM, which is the Netherlands equivalent of the EPA. They created an introduction for us, thanks to Karmann Mills, which showed us that the folks at RIVM are trying to do the zeta potential measurements and functional assay measurements that I talked about, including dissolution rates and surface affinities using ISA-TAB-Nano data sharing formats. This checked all of the boxes of what we're trying to do, and we are embarking on a task of just trying to say, what are our data on this topic and what are yours? How can we integrate them so that we can investigate these functional assays and their predictive abilities using this ISA-TAB-Nano format introduced by this nanoinformatics community? So that's the kind of an example that checks a lot of different boxes for what can happen and what we're looking to put our energy towards.



>> Stephen Lehrman: All right, great. We have time for one final question to Bruce. Bruce, are there efforts to catalog and evaluate nanomaterial exposure data across other agencies, especially including the Consumer Product Safety Commission and the EU efforts?

>> Bruce Lippy: Thank you, Steve. One of the things I would point to that's very helpful is that we had an EU-OSHA Conference in Fort Worth a month or so ago. We tried to present and show the data being collected. I don't think we're even close to the point at which Christine is discussing as far as integration of data. But the first step is sharing, and that is happening. I'm comfortable that as we go along, we can learn from efforts like the CEINT effort and do a better job. But it is starting.

>> Stephen Lehrman: Wonderful. Well, we are in our final minute. We would certainly like to thank both of our speakers today, Dr. Christine Hendren and Dr. Bruce Lippy, for their excellent presentations, and also to our audience for attending this webinar. In a few weeks we will post the transcript and the presentation slides from the webinar on the nano.gov website. The next Nanotechnology Signature Initiative webinar, titled All Hands on Deck for Improving Data Quality, is scheduled for Friday, December 11th, from 2 to 3 p.m. We hope to virtually see all of you there. More information on this webinar, including registration information is available at www.nano.gov/publicwebinars. With that, thank you, again, and this concludes today's webinar.