“Advancing Nanotechnology through Informatics and Modelling”

Bilateral US-EU Workshop
Wicklow Hall 2a
Thursday 20 June 2013, 14:15

Background

EU-US Science and Technology Agreement

- Mutual interests in the economic, environmental & security fields.
- Strategic partnership.
- Research and innovation cooperation: an enabler of reinforced economic partnership

➢ **EU-US** Science and Technology Agreement: **enhancing cooperation**
science, technology and innovation can play in developing the knowledge and technologies that can foster economic growth, create jobs and help solve shared challenges

➢ Annual Meetings of the EU-U.S. Joint Consultative Group to identify **areas of common interest for leveraging and cooperation**

Background

EU-U.S. Joint Consultative Group Meeting 2013

- **Transatlantic marine, maritime and Arctic research**, which impacts our understanding of oceans and how coastal resources are sustainably managed and the potential for the rapid expansion of joint work on ocean observation and forecasting, including seabed and habitat mapping was discussed.
- **Transport research**, concentrating on the development of highway infrastructures, road safety, traffic management, freight logistics and other areas.
- **Health research**, joining forces to develop new methods to prevent and treat diseases like HIV/AIDS, malaria and tuberculosis and working together to strengthen science capacity in developing regions of the world.
- **Materials science**, critical raw materials research and *advanced materials*, particularly in the field of computational modeling.

Background

EU-U.S. Joint Consultative Group Meeting 2010

Bilateral cooperation in R&D focused on:

- how to prioritize global challenges in food security, global health, sustainable energy, and climate change.
- infotech, energy, biomedicine, cyber infrastructure, homeland security, and Earth-observing systems; **Nanotechnology** and in particular the environmental and health impacts of nanomaterials (**nanoEHS or nanosafety**)

✓ **Nanosafety research**, a common challenge:
a necessity for safe commercialization,
a tool for converging regulatory approaches
→ removing obstacles to innovation and trade

Background

US Agencies and EC services working on modalities for cooperation:

Workshops, networking, **Communities of Research**, joint calls for research proposals

Players

- E.U. FP7 & H2020 – Framework Programme - http://ec.europa.eu/research
  Industrial Technologies for research projects in Nanotechnologies, materials and production technologies (NMP) - http://ec.europa.eu/research/industrial_technologies

- U.S. 18 Federal Agencies and Departments – see individual websites
  - White House Office of Science and Technology Policy (OSTP) provides advice on R&D budget, shapes priorities across agencies, and coordinates interagency research initiatives - http://www.whitehouse.gov/administration/eop/ostp
  - National Nanotechnology Initiative & NNCO - http://www.nano.gov/
  - Nanotechnology Signature Initiatives - http://nano.gov/signatureinitiatives

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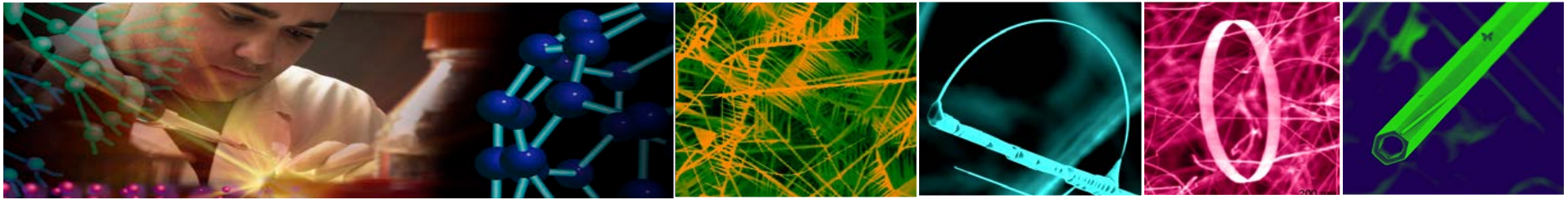
bridging research efforts

Communities of Research (CORs)

- groups of **people**: US-EU scientists
- share a **significant interest:** nanoEHS
- develop a **shared repertoire of resources**: experiences, tools, ways of addressing recurring questions, challenges and research needs
- **regular contact:** use wikis, webcasts, conference calls, annual US-EU meeting.



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Communities of Research (CORs)


Exposure through the Life Cycle


Ecotoxicity Testing


Predictive Modeling for Human Health


Databases & Ontologies


Risk Assessment


Risk Management & Control

3 CORs announced at Society of Toxicology Annual Meeting
Mar 15, 2012

3 CORs announced at NanoSafety Cluster Meeting
May 31, 2012

EuroNanoForum
Jun 18, 2013

2011 | Mar | Aug | Jan 2012 | Jun | Nov | Apr 2013 | Sep | 2013

Mar 11, 2011
CORs proposed at first U.S.- EU workshop

Oct 25, 2012
First in-person meeting of all CORs at second EU-U.S. workshop

Dec 3, 2013
In-person COR meetings at third U.S.-EU workhsop

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CORs Selected Activities

Databases & Ontologies

Working to publish a special issue of *Computational Science & Discovery*

Building a list existing databases and resources

Risk Assessment

Building a list of relevant resources (*i.e.,* papers, reports, etc.)

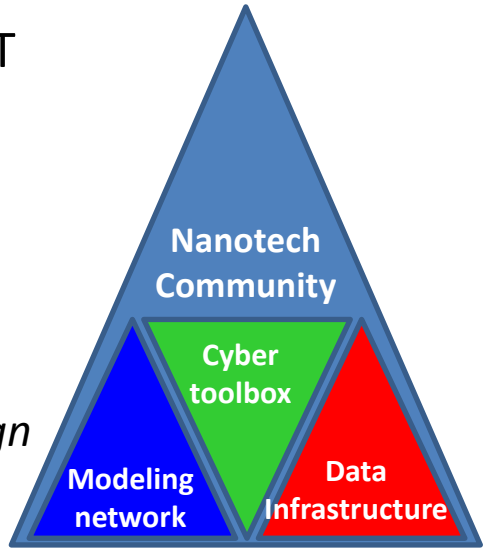
Exposure through the Life Cycle

Developing a database of methodologies to characterize NMs in a variety of media

For More Information: http://us-eu.org/

Workshop scope

- Build on efforts in nanosafety and extend to other fields, prepare the ground for H2020
- Modelling and IT infrastructures seen as key for advancing NT
  - *NNI signature on "Nanotechnology Knowledge Infrastructure: Enabling National Leadership in Sustainable Design"* *http://nano.gov/node/825*
  - *Increasing number of EC FP7 projects addressing modelling NMP.2013.1.4-1 "Development of an integrated multi-scale modelling environment for nanomaterials and systems by design*



- Goals:
  - Identify specific needs & areas of common interest for leveraging/cooperation
  - Identify Groups and Points of Contact around identified areas

- **14.30 Panel Session 1: Collaborative Informatics Infrastructure**
  - *Nathan Baker (PNNL, US)*
  - *Marty Fritts (SAIC, US)*
  - *Roy Chantrell (Univ. of York UK, EU)*
- ***15.00 Panel Session 2: Modelling and Simulation***
  - *Robert Rallo (URV, Spain, EU)*
  - *Curt Breneman (RPI, US)*
  - *Pablo Ordejon (CIN, Spain, EU)*
- ***15.30 Mechanisms for US-EU cooperation***
- ***15.40 Conclude***

Next steps ?

- Interest sign-up sheet
- Short report
- Follow-up workshop ?

  Together or after the nanoEHS COR meeting on 3-4 December, Arlington (2013 NSF Nanoscale Science and Engineering Grantees Meeting on 4-6 December)

needs for databases?

Common vocabulary

Common data sharing format

Framework Data Curation/Sharing Workflows

Sector specific? Links between sectors?

Sharing & Reuse of Scientific Data

*Integrating **nanomaterial property data** into a shareable database for model development and validation*

Many separate codes, few open sources) - develop an environment capable of linking all lengthscales and creating mesoscopic models with specific materials parameters

- Code Standards - Interoperability - Libraries of too - I/O standards - Passing info between scales
- Defining protocols for databases, and sharing contents of computed materials properties
- Exploiting Petascale and future (?) Exascale computers

Flexible approach, producing linking structures independent of CPU platform; Applicable to Local, National and Cloud-based systems

Collaborative environment for software development linking formalisms (open source and commercial) Need to develop user community via workshops

*Establishing a joint initiative for linking different length scale modelling methods in a **multi-functional webtool***

- Areas for multipurpose modeling platform: Structural and dielectric Materials
- Sectors: Energy, ICT, Environment and Safety (Nanoparticles, chemicals), Health