"Enabling and Investigative Tools in Nanotechnology: Measuring, Modeling and Computer Simulation Methods"

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Nanonoscience and Nanotechnoly are general terms that are employed to describe scientific and technological developments dealing with the synthesis, characterization, properties assessment and modelling as well as fabrication of functional nanomaterials, nanostructures, nanodevices and nanosystems. It is the promise of radical new applications, amongst them energy storage, medical diagnostics, measurement and testing, nanotools analysis and drug delivery, robotics and prosthetics, where Nanoscience and Nonotechnolgy will potentially prove disruptive to existing products and market. Industrial sectors that can benefit from the advancements of Nanoscience and Nanotechnology include: Transport, Chemical / Biochemical Industry, Construction and Housing, Consumer and Household Goods, Defence and Security, Electronics and Information Technologies, Energy, Environment, Water, Food and Drink, Life Sciences and Healthcare, etc.

Nanotechnology is the ability to understand, control, and manipulate matter at the level of individual atoms and molecules, as well as at the “supramolecular” level involving clusters of molecules. Its goal is to create materials, devices, and systems with essentially new properties and functions because of their small structure.

The largest barrier to rational design and controlled synthesis of nanomaterials with predefined properties is the lack of fundamental understanding of thermodynamic and kinetic processes at the nanoscale. The lack of basic scientific knowledge regarding the physics, chemistry and biology limits the ability to predict a priori structure-property- processing relationships. Thus, R&D is needed for the elucidation of kinetic and thermodynamic rules for synthesis and assembly that can be applied to rational design of nanomaterials at commercial scales, including hierarchical nanomaterials, from first principles.

Observing, correlating and understanding structure and function at the nanoscale is essential to developing reproducible Nanomaterials. To do this, analytical tool capabilities must move from static measurements of quenched samples to dynamic, real-time measurements. Chemical, physical, and temporal properties at the nanoscale must be monitored as reactions occur and as systems evolve (including living systems). Accurate and precise three-dimensional (3-D) characterization tools providing this capability are essential to the advancement of R&D in fundamentals and synthesis, manufacturing, and modeling as well as commercial production.

This new generation of nanotools can be categorized according to their purpose as follows:

Imaging. Chemists, physicists, engineers and biologists want better methods for seeing things at the nanoscale. For instance, imaging of cells and tissues in the body could potentially be done on a finer scale using nanoparticles as contrast agents. The detailed structures of nanomaterials and of single proteins, and even the catalytic sites of enzymes, might be better visualized using new kinds of optical probes and microscopy.

Measuring. The researchers have noted that anyone who aims to manipulate a material must understand its physical – and sometimes biological – properties. Nanomaterials can behave in unexpected ways, so it is important to understand them well before they are widely used in products. To fully characterize these materials new kinds of probes are needed to measure electrical conduction, surface reactivity, strength, magnetic properties and so on. Other measurement tools that exploit nanoscience, such as “lab-on-a-chip” devices, hold promise for detecting and quantifying specific molecules of interest in water and blood. Likewise, devices with nanopores could enable rapid and cheap sequencing of DNA.

Integrating. Combining two or more tools within a single device. These could allow researchers to integrate multiple kinds of data and to get a fuller picture of the nanoworld in 3-D and in real time. Such tools would be essential for understanding complex nanosystems, measuring changes in nanostructures and observing molecular interactions. For example, new methods for “nanotomography” (similar to computed axial tomography, or CAT scanning) might combine an optical probe with a physical probe with a physical probe to make a “movie” of how molecules interact with one another.

Manipulating. To work at the nanoscale, scientists will need tools for putting atoms where they want them to go. Adaptations of scanning probing microscopy and new lithography methods for creating nanoscale patterns hold promise, as do nanotweezers and nanosize machines for moving around atoms. But once researchers develop more advanced methods for manipulating atoms, they will still need additional tools to do this efficiently on a larger scale. Such tools for nanomanufacturing are of particular interest to computer chip makers, but eventually all kinds of nano-enhanced industries will need them.

Nanomaterials and products containing nanomaterials (e.g., nanotubes, inorganic powders, organic films, and coatings) are manufactured today with traditional manufacturing techniques and unit operations. These nanomaterials are prohibitively expensive for many applications due to high capital costs and low production volumes. However, researchers are not focused on the requirements posed by scalable, cost-effective manufacturing. Thus, robust and reliable production methods – consistently and correctly controlled at the atomic scale – are needed to significantly expand the commercial use of nanomaterials. In addition, production must be accomplished in a safe, environmentally friendly manner.

Finally, robust, high-confidence models and simulations are needed to predict the properties and behaviours of new nanomaterials and assembled systems across scales – from synthesis of particles through their integration into devices, and finally, to their performance in final products. Models and simulations will aid the development of synthesis and assembly protocols that impart and preserve required functional properties across scales. At the application level, they will define the functional needs and probable designs of nanostructures.

The ability to develop accurate predictive models will depend on theoretical understanding of chemistry and physics fundamentals, methods that bridge time and spatial scales, data protocols and standards, and an a priori focus on the requirements of manufacturing during model development.

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Costas Kiparissides is a Professor at the Chemical Engineering Department of Aristotle University of Thessaloniki since 1981. During the period 2001-2006, he was Director of Chemical Process Engineering Research Institute (CPERI) at CERTH and in the period 2005-2010 Director of Centre for Research & Technology Hellas (CERTH). In 1971, he received his diploma Degree in Chemical Engineering from NTUA. In 1978, he received his Ph.D. Degree from McMaster University in Canada. From 1978-1983, he taught as an assistant and associate Professor at University of Alberta in Canada. He has also been a visiting Professor of University of Newcastle in U.K. and Queen’s University in Canada. He is member of the Expert Advisory Group (EAG) of the NMP programme, member of the Mirror Group of the European Technology Platform for Sustainable Chemistry, member of the Ad-hoc Advisory Group on Industrial Nanotechnologies, vice-chair of the working group: Nanopharmaceutics of the European Nanomedicine Technology Platform, etc. He has supervised more than fifty Ph.D. graduate students, 160 diploma theses and has presented more than three hundred invited seminars and lectures at international scientific conferences, industrial research centres, institutes and universities in Europe and North America. In addition he has published 200 papers in refereed journals, 350 conference papers and 6 books. His published work has received more than 3000 citations. His current research interests are in the areas of advanced multi-scale modelling of chemical and biological systems, functional materials, sustainable bioprocesses, nanotechnology applications in targeted delivery systems, nanodiagnostics and regenerative medicine and in virtual physiological human.