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ABSTRACTS



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Direct optical absorption in cylindrical quantum dot with rectangular infinitely high confinement potential

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In given article direct optical absorption in cylindrical quantum dot with rectangular infinitely high confinement potential is theoretically investigated. According to [1] absorption coefficient is defined by the formula

$$K = A \sum_{\substack{NN' \\ mm' \\ nn'}} \left| \int \psi_{Nmm}^e \psi_{N'm'n'}^h d\vec{r} \right|^2 \delta(\Delta - E^e - E^h),$$

where $\Delta = \hbar\omega - E_g$ (E_g is the width of forbidden band), ω is the frequency of incident light, e index refers to electron, h index refers to the hole, A is a quantity, proportional to the square of dipole momentum matrix element modulus, taken on Bloch functions.

The corresponding selection rules for optical transitions are defined. The expressions for absorption threshold frequencies are found. The obtained results are compared with the case of light direct optical absorption in spherical quantum dot.

[1] A.I.L. Efros, A.L. Efros, *Semiconductors*, **16**, 1209 (1982).

Exfoliation in NanoComposites: An Alternative Use of Acetone

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Nanoclay filled polymeric systems have been studied for many researchers who concluded that polymeric systems' mechanical and thermal properties are greatly enhanced with the addition of small amounts of nanoclay. However, the exfoliation of these particles stills a problem for many polymeric systems, especially for the epoxy systems. In this specific case, as the resin presents high viscosity, to exfoliate the nanoparticles an elevated temperature must be reached. By heating the resin, its viscosity decreases leading to a better exfoliation. However, when the hardener is added at high temperature, in general between 40 and 60 °C, the polymerization reaction is so fast that can cause the nanoparticles precipitation or a non-uniform exfoliation. To avoid it, an investigation using acetone as an exfoliation vehicle is conducted. The epoxy system employed is the ARALDITE 2000 (resin XR 1553/hardener HY 1246) from Huntsman and the nanoclay used is montmorillonite clay (NANOMER I 30) from Nanocor. Different dilutions of acetone and I30 were selected. This solution is then exfoliated at ARALDITE matrix up to 5% in weight. The nanocomposite preparation involves not only the search for the ideal diluted solution nanoclay/acetone, but also of a period of low heating and mixing to obtain a homogeneous mixture. After cooling and degassing, the hardener is added and the cure is processed. By controlling the amount of remaining acetone, it is possible to control the nanocomposite toughness and stiffness. Experiments have demonstrated that the presence of acetone associated to nanoclays increases the nanocomposite toughness. Indeed, it was observed that for large concentrations of acetone, the nanocomposites get a rubber-like behavior, while an increase of stiffness is observed for small or quasi-null nanoclay concentrations.

Health and Environmental Implications of Engineered Nanoparticles

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Engineered nanoparticles have recently become commercialized in a number of consumer products, and the types that are being produced in large-scale quantities are increasing dramatically. However, the biological and ecological impacts of these nanoparticles have only begun to be explored experimentally. The public perception, public policy, regulatory, and commercialization issues surrounding this technical area will be discussed. The general approach being employed to address these issues at Rice University's Center for Biological and Environmental Nanotechnology will be described. Buckminsterfullerene, a model hydrophobic nanomaterial, has been found to form a water-soluble nanocrystalline colloid in environmentally relevant concentrations upon contact with water. The interactions of these nanocrystallites with Gram-type positive and Gram-type negative bacteria, tissue cultures, and other organisms will be presented.

A Case for Nanomaterials in the Oil & Gas Exploration & Production Business

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While nanomaterials are frequently associated with alternative energy sources such as solar, fuel cells and the hydrogen economy, their application in the hydrocarbon extraction business is seldom discussed. This paper will highlight the range of materials-related challenges faced by the oil & gas industry and the resulting significant market potential for nanomaterial-based solutions. The need for increased collaboration between the oil industry & nanomaterial developers will be emphasized and critical success factors for successful industry partnerships will be proposed.

Stakeholders in Nanotechnology Policy

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A [Google.com](http://www.google.com) search under the key words “nanotechnology + implications” nets almost 70,000 hits, and a search for “nanotechnology + policy” will find you greater than 300,000 hits. Clearly, people are talking about these issues, but what are they saying that is useful? These discussions have expanded outside scientific journals, are progressing through the more industry specific literature and headed for the popular press.

The beginning of this millennium has seen, government, venture capitalists, and increasingly corporations boosting their investment in Nanoscale Science and Engineering (NSE) research, aggressively promoting this research as the key to the next industrial revolution and a direct path to human betterment. At the same time, starting with Bill Joy’s seminal 2000 article ([Why the Future Doesn’t Need Us](#) April, 2000) other voices of alarm and concern have been calling for preventative actions.

The growing cacophony of voices in the NSE debate thus comes from a variety of sources, ranging from governmental funding agencies, non-governmental organizations and academic research groups. Apart from a few extreme positions, the common theme is that “policy is needed”. Yet no process for connecting an evolving understanding of social, economic, and environmental implications of NSE to the policy process has yet emerged.

In this poster I will map out the positions and details of the major interests and constituencies in the NSE policy world, and their relations to various policy-making fora. The overall picture is one of uncoordinated pursuit of interest group agendas, with little capacity for constructive feedback into the policy process. I will suggest some alternative approaches to organizing both research and policy making to take advantage of what is known about NSE, capture new insights as they emerge, and connect this learning to the policy process through what Guston and Sarewitz (2002) have termed “Real-Time Technology Assessment”.

The Three Orders of Nanotechnology Ethics

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One way that humanity attempts to capture and understand the human condition is through science, and its quest for knowledge of the laws that govern the physical universe. Another is through religion, and its attempt to garner and obey any laws, which might govern the domains of the soul. Ethics, a third attempt to capture the human condition, seeks to identify and understand principles or laws, which might govern human moral choices and behaviors. Or, in the absence of discernable or existing moral laws, to capture and reflect on the way in which human communities construct and agree upon values about how it is they want to live together.

Technological development is not so much concerned with understanding the human condition, but rather, is geared towards solving perceived problems and making improvements to the material conditions in which humans live and function. Nevertheless, in shaping and rearranging the material world, the effects of technology are felt in the social and psychological dimensions of human life, thereby affecting the human condition itself. An ethics of nanotechnology then, seeks to understand the goods and harms which might result from nanotechnology development. It also functions to ascertain how nanotechnology may be shaped by and simultaneously reconstruct the human condition. Ways in which the products and processes of nanotechnology might reflect and express human beliefs, values, and relationships are also subjects of inquiry for nanotechnology ethics.

Nanotechnology ethics is a newly emerging field of scholarly inquiry. It is just beginning to form as a complement other efforts to explore the moral dimensions of scientific and technological transformations in human action. This speech suggests that given the unusual nature of nanotechnology, a multi-dimensional approach to the formulation of nanotechnology ethics is necessary. The speech offers and explains one such approach, *the three orders of nanotechnology ethics*, as named and developed by the speaker. That approach entails looking at increasingly complex layers of inquiry into how nanotechnology might affect the condition of human life. What is it that most consumers of this complex new technology should be able to understand? What is it that most policy makers ought to assure the public? What is it that most business leaders must commit to if nano-technological developments are to be incorporated into the society in healthful and ethical ways? Is there something about nanotechnology, which warrants ethics considerations, as distinct from the general ethics considerations given to any new technological development? Perhaps size will make a difference in terms of ethics in the things we will be able to do. What might nanotechnology mean for human health, to the environment, to the structure of society and the common good? Who may be harmed, and who stands to benefit? What social goods will come as a result? Will fundamental moral or religious beliefs, ontological meanings, or familiar ways of perceiving and engaging the world may be compromised or otherwise altered as a result of its development? The three orders of nanotechnology ethics offer a way to approach the different levels of ethics represented in these questions, through different dimensions of inquiry.

Hydrogen Interaction with Carbon Nanofibers

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Carbon nanofibers of herringbone formation were grown by chemical vapor deposition on different catalysts from a number of hydrocarbon sources. After the removal of the metal oxide particles, which are part of the catalyst system, six samples with several different ratios of Pd/C were obtained by controlled oxidation in air. The hydrogen uptake experiments performed volumetrically in a Sievert-type installation, showed that the quantity of desorbed hydrogen (for pressure intervals ranging from 1 to 100 bars) by the carbon nanostructures free of any metal catalyst particles, was between 0.04 and 0.33 % by weight. For the samples of nanofibers that contained Pd in various Pd/C ratios, palladium revealed catalytic properties and supplied atomic hydrogen at the Pd/C interface by dissociating the H₂ molecules. The results show a direct correlation between the Pd/C ratio and the quantity of hydrogen absorbed by these samples. A saturation value of about 1.5 wt. % was reached for a high ratio of about 1:1 of Pd/C. The surface area of the fibers was measured by BET and found to be 425-455 m²/g.

Spatially Controlled Chemical Reactions At The Molecular Level Using Atomic Force Microscopy

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Atomic force microscope (AFM) probes can be used as tools to initiate chemical and physical changes upon the surfaces with which they come into proximity.

By forming self-assembled monolayers (SAMs) with functionalised terminal groups, and through the controlled modification of atomic force microscope probes, self-assembled monolayers can be altered with a high degree of spatial resolution and specificity to obtain chemically distinct areas.

A variety of reagents have been assembled and characterised in well-defined SAMs. By scanning suitably designed proximal probes across these monolayers under carefully controlled conditions which include temperature and pressure, chemical reactions were carried out.

The results of various spatially-confined reactions initiated with reagent/catalytic AFM probes including those modified with catalytic nanoparticles will be presented.

Biology as nanotechnology solutions to engineering problems

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An increasing number of physical scientists and engineers are beginning to devote considerable attention to biological problems. As more physical/mechanistic understandings of biological systems emerge, we are beginning to develop a deeper, quantitative understanding of how molecular biological systems work. With this understanding, we are beginning to appreciate the extraordinarily clever ways living systems have chosen to solve can be though of as essentially engineering problems. I will present examples of the engineering problems and solutions that life has taken that allow us to hear music and make proteins. Finally, if time permits, I will discuss how nature might give us insights into how we might solve the challenge of realizing a sustainable, CO₂ neutral souce of energy before out fossil fuel is depleted.

The Emerging NanoEconomy: Key Drivers, Challenges and Opportunities

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Can we anticipate and direct the impact of nanoscience on the economy? Will we be ready to develop the economic opportunities and navigate the challenges that nanoscience will bring? This keynote examines a strategic view of the emerging NanoEconomy, focusing on some of the change drivers, key challenges and opportunities that will face the nation in the near future. Though nanoscience is in the early stages of invention, current breakthroughs indicate significant potential. The convergence of other key innovations in information technology and biotechnology, for example, will be accelerators moving nanoscience into mainstream commercial readiness. How might this occur? What other drivers of the nanoeconomy will be relevant? A possible nanoeconomic ecosystem will be reviewed. Attention to the key future-readiness factors that may influence the emerging NanoEconomy will be examined including: entrepreneurship, education, intellectual property, capital, jobs, talent, supply chains, competition and nanoscience product or service offerings. An analysis of future-readiness factors that we need to adopt now, as a nation, to prepare for the coming NanoEconomy, will be identified.

Nanoscience for Information Technology

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For almost 40 years Moore's Law, the doubling of the number of transistors on a single chip every 18 to 24 months, has driven the semiconductor and information technology. Is the end in sight or will there be more of Moore's Law? Scientists in the Research Laboratories of IBM and elsewhere are trying to push Moore's Law to the ultimate limit, i.e. atomic and molecular levels. What is the current status of this research and are there potential alternatives?

Anodized aluminum oxide as a template for fabrication of nano-structures: metal / metal oxide / pores

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Anodic aluminum oxide (AAO) arrays are self-ordered porous structures, which are suitable for many technical applications. These arrays are attractive for design of nanotechnology devices because of the hexagonal pore arrangement, a very high aspect ratio of 1000 (pore length to pore diameter) and a high pore density of 101^{-1} pores/cm².

In this presentation, we describe a novel procedure (Figure 1) for the fabrication of patterned AAO arrays by using a dense barrier aluminum oxide layer as the anodization mask. This fabrication procedure includes the following steps. The aluminum is patterned with a photoresist and then briefly anodized at a high voltage, which produces a dense layer of barrier aluminum oxide. The photoresist is then removed and the aluminum film is again anodized at a low voltage to grow porous aluminum oxide. The dense barrier aluminum oxide acts as an anodization barrier thus leaving the underlying aluminum intact. As a result, fabricated AAO arrays (Figure 2) consist of alternating regions of porous aluminum oxide and aluminum metal perpendicular to the silicon substrate.

AAO arrays are suitable templates for non-lithographic fabrication of an array of nanoelectrodes. The electrodes can be made, for example, by electrodeposition of gold inside the pores of AAO arrays. For the functional array of nanoelectrodes, it is important to deposit continuous columns of gold. Electrodeposition of continuous columns of gold is facilitated by decreasing the thickness of the barrier oxide layer formed during poroustype anodization of aluminum. The thinning of the barrier oxide layer can be accomplished by the voltage reduction method originally implemented for detachment of the AAO membrane from the underlying aluminum support. As a result of this method, the thickness of the barrier oxide layer decreases, because it is linearly proportional to the applied voltage. In the second part of this presentation, we report a procedure aimed at

(1) fabrication of AAO arrays with hexagonally arranged pores, (2) thinning of the barrier oxide layer and (3) electrodeposition of gold into the pores of AAO arrays. The continuous columns of gold are expected to function as an array of nanoelectrodes (Figure 3), which can be utilized for a diverse number of applications in analytical chemistry.

Topic: Nanomaterial

Supramolecular Nanomaterials: Novel Design and Unorthodox Approaches

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Nanomaterials have attracted considerable interest and have been recently investigated in a number of research groups. Nanosized building blocks have been found to be important and versatile synthons both in nanoscience and supramolecular chemistry. The use of these building blocks in conjunction with other molecules such as organic macrocycles and hydrophilic polymers allows designing and developing novel concepts for the synthesis of supramolecular nanomaterials using unorthodox approaches. Such novel and unorthodox design concepts are presented and highlighted both as synthetic approaches and in the context of their applications.

The building blocks can stem from different types of molecule classes including synthetic and semi-synthetic molecules as well as biopolymers. Typical examples are the families of cyclodextrins, calixarenes, and cucurbiturils as well as hydrophilic polyesters, peptides and DNA for macromolecular synthons. Nanosized building blocks include spherical clusters such as different fullerenes with an emphasis on [60]fullerene and also carbon nanotubes. As a further example for the nanoencapsulation of fullerenes the supramolecular interaction with peptides has been studied. A survey of fundamental designs for novel nanomaterials is presented and discussed in view of their potential and perspectives on the basis of recent research examples.

Several model systems with carbon nanotubes have been also studied and examples of interaction products based on different types of reactions and syntheses are given. The nanosized supramolecular conjugates presented are based on the use of single- and multi-walled carbon nanotubes for the supramolecular constructs. The novel nanomaterials are expected to have an application potential in many areas such as the biomedical and electronic areas.

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WIAS-HiTNIHS: Software-Package for simulation in crystal-growth of SiC single crystal

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The numerous technical applications in electronic and optoelectronic devices, such as laser, diodes, and sensors demand high quality silicon carbide (SiC) bulk single crystal for industrial applications. These apparatuses for crystal growth are presented with respect to the thermal processes. We describe the heat equation and the radiation of our thermal processes.

The model is based on the physical vapor transport, also called the modified Lely-method. The main interest is the evolution of the temperature in this growth process, because one could not measure it directly. The simulations are done on a mathematical model for the heat transfer with heat conduction, radiation, and radio frequency.

We simulate the temperature differences between the top and bottom layers and also between the temperature of the Si inside the source and on the source. The information is used to construct an apparatus for the crystal growth. We present different materials for in our model as a flexible application. At the end we discuss our numerical results for the complex processes.

Use of nano-scale phage display selection for the generation of human monoclonal antibodies against breast cancer

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The current goal of cancer drug discovery and development is to identify agents that are effective cancer therapeutics and yet have minimal systemic side effects. Therefore targeted drug design directed towards molecular pathways that underlie the malignant phenotype has been initiated. These therapies are targeted against specific tumor cell receptors or signaling events that are critical to tumor progression while reducing toxicity to normal cells. One way to direct activity against therapeutic targets is to use monoclonal antibodies directed to growth factor receptors, tumor-associated antigens or antigens differentially expressed on cancer cells. We are using very large antibody phage display libraries to isolate and characterize human monoclonal antibody fragment that specifically recognize breast cancer-associated cell surface proteins and which can be used as nanodevices for diagnosis and/or therapy of cancer patients. Our focus is on isolation of antibodies specific for surface proteins associated with high metastatic potential and we have optimized nano-scale selection strategies for antibodies recognizing cell surface molecules central for relevant biological functions, such as cancer cell proliferation, adhesion, migration and invasion. The long-term goal is to conjugate the cloned human antibody fragments and use them as nanodevices for in vivo diagnosis and/or therapy of cancer patients.

Designing new analogs; agonists and antagonists, for the glycoprotein hormones using site directed mutagenesis and gene transfer”

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Thyrotropin (TSH) and the gonadotropins (FSH, LH, hCG) are a family of heterodimeric glycoprotein hormones composed of two noncovalently linked subunits, α and β . The hTSH heterodimer was converted to a biologically active single-peptide chain, by fusing the common α subunit to the carboxyl-terminal end of hTSH β subunit in the absence (hTSH $\beta\alpha$) or presence of a ~30 aminoacid peptide from hCG β (CTP) as a linker (hTSH β CTP α). Ligation of the CTP to the carboxyl-end of hFSH, hCG α subunit and to hTSH resulted in increasing the biological activity and longevity *in vivo*. In the present study, the hTSH β CTP α , was used to investigate the role of the N-linked oligosaccharides of α and β subunits on secretion and function of hTSH. Two deglycosylated variants were prepared: one lacks both oligosaccharide chains on α subunit (hTSH β CTP α_{1+2}), and the other lacks also the oligosaccharide chain on β subunit of the single chain (hTSH β CTP α (deg)). The single-peptide chain variants were expressed in CHO cells and they are secreted into the medium. Absence of the N-linked oligosaccharides on α or β subunits and the O-linked oligosaccharides on the CTP, does not affect the secretion of the variants. These results indicate that the signal for the secretion exists in the single peptide chain is independent of the oligosaccharides. hTSH variants lack of the oligosaccharide chains is less potent than hTSH β CTP α on cAMP accumulation and T₃ secretion in human cultured thyroid follicles. Moreover, both deglycosylated variants compete with normal hTSH and hTSl in a dose dependent manner in *in vitro* and in *in vivo* systems. Thus, this variant, behaves as potential antagonist, who may offer a novel therapeutic strategy in the treatment of Grave's disease, the most common form of hyperthyroidism. Our studies indicated that super agonists with long half-life *in vivo* can be prepared by addition of O-linked oligosaccharides to the protein. On the other hand, antagonists can be prepared by deletion of N-linked oligosaccharide.

Neuroelectronics: Semiconductor Chips with Brain Cells

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Electrical information processing in brains and computers relies on different charge carriers, ions and electrons. It is a challenge to join neuronal networks and computer chips on a microscopic electrical level, with the goal to get better insight of brain dynamics, to develop pharmaceutical sensors and to develop hybrid neuroelectronic processors for medical and technological applications.

On the side of electronics, we have to distinguish two levels, simple silicon chips with elementary microelectronic devices and complex CMOS chips fabricated by very large scale integration. On the biological side, we distinguish three levels, molecular ion channels on the nanometer scale, individual nerve cells on the micrometer scale and brain tissue on the millimeter scale.

Much of our work on the three biological levels was performed on simple silicon chips with capacitors for biostimulation and transistors for biorecording. In particular, we analyzed the nanostructure of the neuron-silicon contact with respect to geometry and electrical features using various luminescent dyes. We incorporated molecular ion channels into the cell-chip contact using recombinant genetic methods and characterized the fundamental physics of signal transmission between electronics and ionics. On that basis, we were able to connect individual nerve cells from snails and rats to silicon chips and to create small hybrid bioelectronic networks. Finally, we succeeded to combine thin tissue layers from rat brain with silicon chips and to establish neuronal learning on a chip.

Recently, we started to combine the three biological levels of ion channels, nerve cells and brain tissue with CMOS chips that were developed with Infineon Technologies. Care was taken that the physics of ionic-electronic interfacing was the same as with simple silicon chips. Arrays of 128x128 sensor transistors provided dynamical electrical maps of excited neuronal networks from snails and of signal propagation and learning in rat brain.

Reference: Peter Fromherz, Neuroelectronic Interfacing: Semiconductor Chips with Ion Channels, Nerve Cells and Brain. In: Nanoelectronics and Information Technology, Ed. R. Waser (Wiley-VCH, Berlin, 2003), pp 781-810.

Supramolecular Nanomaterials: Novel Design and Unorthodox Approaches

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Nanomaterials have attracted considerable interest and have been recently investigated in a number of research groups. Nanosized building blocks have been found to be important and versatile synthons both in nanoscience and supramolecular chemistry. The use of these building blocks in conjunction with other molecules such as organic macrocycles and hydrophilic polymers allows designing and developing novel concepts for the synthesis of supramolecular nanomaterials using unorthodox approaches. Such novel and unorthodox design concepts are presented and highlighted both as synthetic approaches and in the context of their applications.

The building blocks can stem from different types of molecule classes including synthetic and semi-synthetic molecules as well as biopolymers. Typical examples are the families of cyclodextrins, calixarenes, and cucurbiturils as well as hydrophilic polyesters, peptides and DNA for macromolecular synthons. Nanosized building blocks include spherical clusters such as different fullerenes with an emphasis on [60]fullerene and also carbon nanotubes. As a further example for the nanoencapsulation of fullerenes the supramolecular interaction with peptides has been studied. A survey of fundamental designs for novel nanomaterials is presented and discussed in view of their potential and perspectives on the basis of recent research examples.

Several model systems with carbon nanotubes have been also studied and examples of interaction products based on different types of reactions and syntheses are given. The nanosized supramolecular conjugates presented are based on the use of single- and multi-walled carbon nanotubes for the supramolecular constructs. The novel nanomaterials are expected to have an application potential in many areas such as the biomedical and electronic areas.

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Molecular Wiring for Enhanced Photocatalytic Hydrogen Evolution

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A simple photocatalytic hydrogen-evolving system will be described based on intermolecular electron transfer using isolated Photosystem I (PSI) reaction centers as the photoactive element. The system is comprised of platinized PSI covalently-linked to plastocyanin. Water soluble sodium ascorbate is the electron donor. Plastocyanin was attached to PSI by formation of peptide bonds with the cross-linking reagent, 1-ethyl-3,3-dimethyl aminopropyl carbodiimide. Compared to the unlinked proteins, cross-linking of PC and PSI resulted in a substantial increase in light-driven reduction of hexachloroplatinate ions ($\text{PtCl}_6^{2-} + 4e^- \rightarrow \text{Pt}^0 + 6\text{Cl}^-$). Hydrogen photoevolution by platinized cross-linked PC-PSIPt was increased three-fold both in initial rate and total yield. Analysis of the reaction indicates that covalent linkage of PC to PSI results in a greater rate of total electron throughput from sodium ascorbate to light-activated hydrogen evolution. In addition, although photocatalytic hydrogen-evolving activity was easily demonstrated in the cross-linked system, the native pathway of electron flow yielding enzymatic NADP⁺ reduction activity was not observed upon addition of the natural PSI electron-accepting system, ferredoxin+ ferredoxin:NADP⁺ oxidoreductase.

A molecular dynamics study of the role that surface-active phospholipids play in the lubrication of synovial joints: implications for the treatment and prevention of Osteoarthritis

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Using molecular dynamics simulation, the lubricating abilities of surface-active phospholipids (SAPLs) will be accessed. To begin with, an initial simulation will determine if the fatty acid chains collapse when two surfaces containing SAPLs are brought into contact. The dependence of spacing between the two surfaces will be analyzed to determine its impact on how the chains collapse. The significance of how the chains collapse could provide insight into the effectiveness of SAPLs as boundary lubricants. Another issue to be investigated is what role does the double chain fatty acid play in enhancing lubrication. Simulation results from single, double, and triple chain molecules will be compared in an effort to address the issue of why nature forms this double chain molecule and the impact it has on its lubricating abilities. The last issue that will be addressed is the relevance of surface roughness. The surface of articular cartilage is considered relatively rough. Whether or not the surface roughness plays a role in the effectiveness of SAPLs as boundary layer lubricants will be addressed. The simulation results from smooth and rough surfaces will be compared. Hopefully, finding from this research will assist in the prevention and/or treatment of Osteoarthritis. The impact these research results could have on economics alone is outstanding. It has been estimated that the cost of the total arthritis bill for the U.S. is \$50 billion annually. Moreover, it may also prove invaluable to pharmaceutical companies hoping to develop a drug that could one day benefit those suffering from this painful, debilitating disease. Arthritis pharmaceutical companies are projecting as much as \$21 billion in sales by the year 2010.

Sub-100 nanometer Ion Beam Probe for Applications in Biology and Many Other Disciplines[†]

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Focused ion beams (FIB), at sub-100 nanometer scale, have utility for a wide range of applications in both basic and applied science covering geology, materials science, microelectronics and biology. An example of current interests is imaging by FIB-SIMS (Secondary Ion Mass Spectrometry). In biology and medicine its utility is recognized [1-2] due to the relevance of SIMS to study fundamental problems, for example mapping distributions of targeted chemical species in tissues. The critical role of ion beams is realized in ion beam milling and diagnostics instruments including in-line inspection of semiconductor devices for defect management.

While significant progress has been made to design an efficient ion-optical column, the critical issues to achieve a high-resolution ion beam probe with target beam intensity of about 1 A/cm^2 are governed by beam characteristics from the ion source, namely, virtual source size, beam brightness, and energy spread. An acute need prevails to advance the state-of-the art of sources so that desirable beam characteristics for a variety of beam species, especially, for hydrogen, oxygen, argon, and many complex molecular ions, can be achieved.

This article especially focuses on developing high-brightness negative ion beams and coupling the beams to an ion-optical column. The goal is to achieve a sub-100 nm ion beam probe. Negative ions have unique merits for applications involving beam-materials interactions. When negative ions strike a surface, especially an electrically isolated surface, the surface charging voltage does not exceed a few volts, and the charging voltage is independent of the beam energy [3]. Figure 1 shows an example of the charging voltage of an isolated alumina surface due to irradiation by H^- beams [4]. This property can be effectively utilized to circumvent problems due to surface charging that can cause device or sample damage and ion-beam defocusing.

A compact plasma source, with the capability to produce negative as well as positive ion beams, is developed. Intense ion beams, including H^- , O^- and Ar^+ , have been generated. The unnormalized beam brightness for 10 keV H^- beams is $\sim 10^5 \text{ Acm}^{-2}\text{sr}^{-1}$ [5]. Figure 2 shows an example of H^- beam spot when the beam is focused using a simple einzel lens with magnification of about 0.1. This spot size of about $2 \mu\text{m}$ suggests that a focused spot size of about 20 nm is achievable by an additional magnification of 0.01. The results of ion-optical calculations, in Fig. 3, for a three-lens column show the required beam focusing for sub-100 nm spot size [4]. Experiments on measurements of beam characteristics, design and development of ion-optical column and application goals will be discussed.

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Active Transport by Biomolecular Motors: A New Tool for Nanotechnology

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Biomolecular motors are unique nanoscale machines, which convert chemical energy into mechanical work by hydrolyzing ATP. In nature, motors like kinesins and myosins perform a wide variety of functions, ranging from active transport of nanoscale objects within cells to the contraction of muscles.

Inspired by these diverse biological applications, we have integrated biomolecular motors into synthetic devices in order to explore the potential of molecular motors in nanotechnology [1]. Examples for this approach are the “molecular shuttle” [2], a nanoscale transport system, “Monte-Carlo imaging” [3], a surface imaging method based on the random sampling of a surface by self-propelled nanoscale probes, and a piconewton forcemeter for the measurement of the strength of intermolecular bonds [4]. These hybrid devices are fabricated by combining protein-patterning, soft- lithography, and microfluidics with biomolecular techniques.

Our most recent progress includes the design of complex track structures for molecular shuttles based on kinesin motors and microtubules [5, 6], and an investigation of the compatibility of materials frequently used in micro- and nanofabrication with the stringent requirements of motor proteins, and the ensuing effects on device lifetime [7].

The utilization of molecular motors in nanotechnology is an emerging area of research, and I will discuss our vision regarding the future of this exciting field.

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On the calibration of frictional forces in atomic force microscopy

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A new method is proposed for the calibration of frictional forces in atomic force microscopy. An angle conversion factor is defined using the relationship between torsional angle and frictional signal. Once the factor is obtained from a cantilever, it can be applied to others without additional experiments. Moment balance equations on the flat surface and the top edge of a commercial step grating are used to obtain the angle conversion factor. The proposed method is verified through another step grating test and frictional behaviors of Mica.

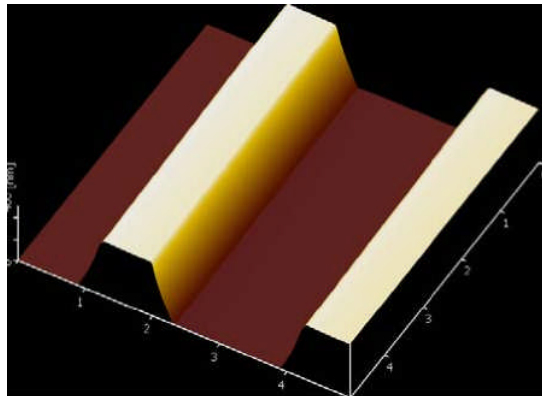


FIG. 1. An AFM image of a commercial step grating.

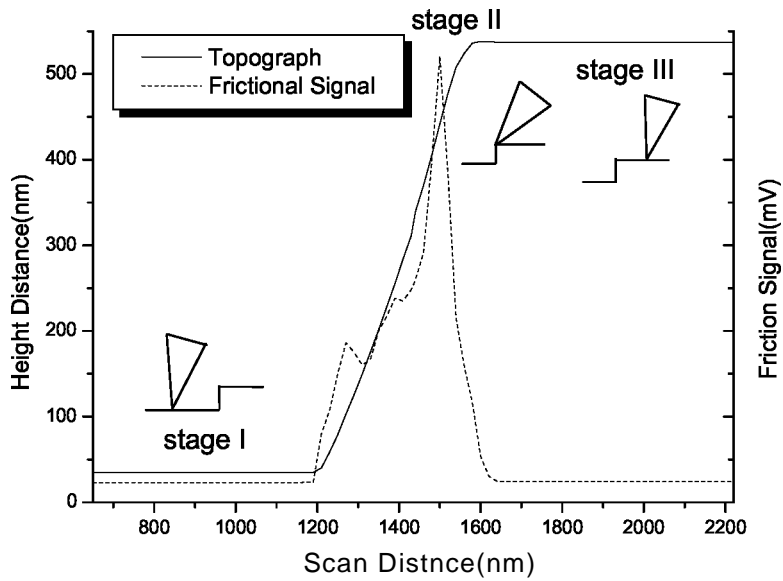


FIG. 2. The frictional signal and the topography at each location.

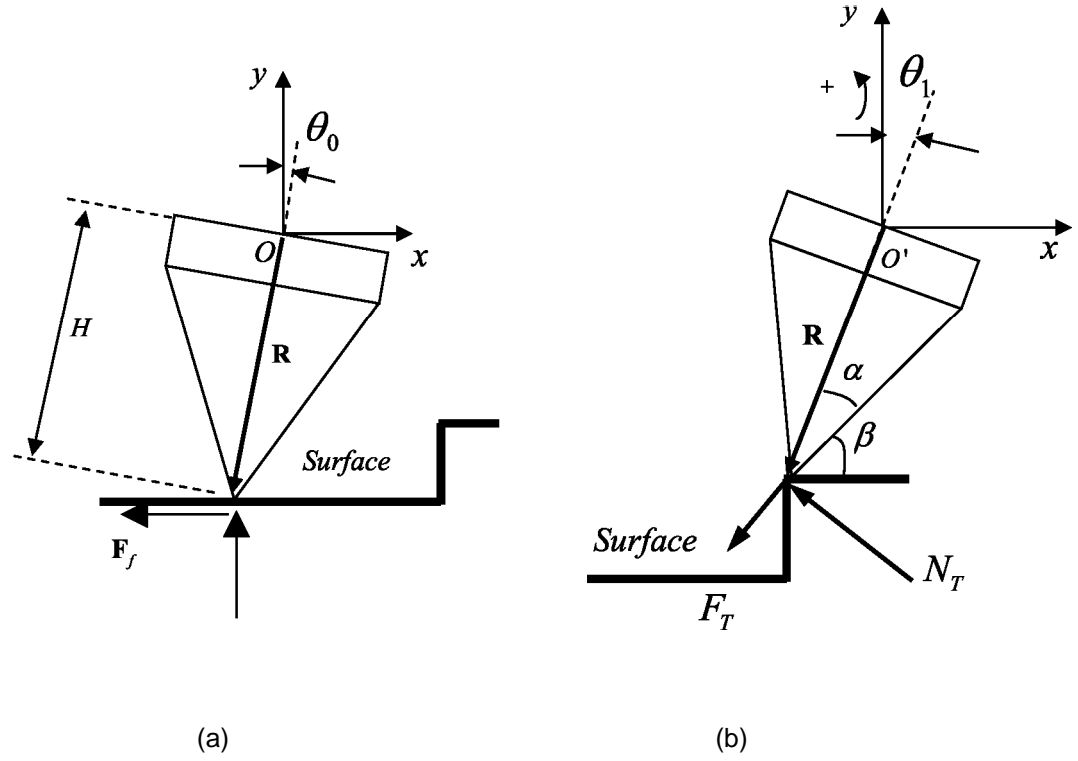


FIG. 3. The orientation of the tip for a cantilever (a) on the flat surface and (b) on the top edge of the step grating. θ_0 is the torsional angle caused by the frictional force and the normal force between the tip and the surface, and θ_1 is the torsional angle caused by the frictional force and the normal force between the end of the tip and the top edge of the step grating.

Dielectric Properties of the Hybrid Board of Polytetrafluoroethylene/ Nano-scale SiO₂ Powder

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The dielectric properties (dielectric constant, dielectric loss factor) of the hybrid board of polytetrafluoroethylene(PTFE) emulsion/ nano-scale SiO₂ powder are studied. The process parameters of board fabrication including powder add-on (1-3%), rotational speed (1200-3200 rpm), temperature (30-345°C), stage of sintering and cooling (1-16) and calendering times (1-12) are altered. The impacts of these parameters on the dielectric properties of the hybrid board are studied.

The experimental proceeded as follows: 60% solid content PTFE emulsion was blended and mixed with nano-scale SiO₂ powder and coupling agent in a blender. During the mixing, the fabrications of PTFE were formed and impacted by the rotational speed of the blender. After mixing, the viscosity of mixed solution was increased and became to a gel (semi-solid) state. The gel was proceeded with moulding and calendaring in order to release bubble and increase surface uniformity. Then, the gel was solidified by sintering and cooling to hybrid board. The temperature and stage of sintering and cooling plays an important roll for the solidification of hybrid board.

Both dielectric constant and dielectric loss factor are decreased with addition of SiO₂ powder. Both dielectric constant and dielectric loss factor are decreased with increased rotational speed and reach a maximal, in this study 3000 rpm, and then increased. The temperature and stage of sintering and cooling plays the most important rolls for both dielectric constant and dielectric loss factor.

From Small Carbon Fragments To Self-Assembled Fullerenes In Quantum Chemical Molecular Dynamics Simulations

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Keywords: Self-Assembly, Fullerene Formation, Quantum Chemical Molecular Dynamics Simulations

Abstract: We present an analysis of our fully quantum chemical molecular dynamics simulations for the formation of fullerene molecules from ensembles of C_2 and C_6 molecules *without assuming a designed reaction pathway*. The importance of electronic

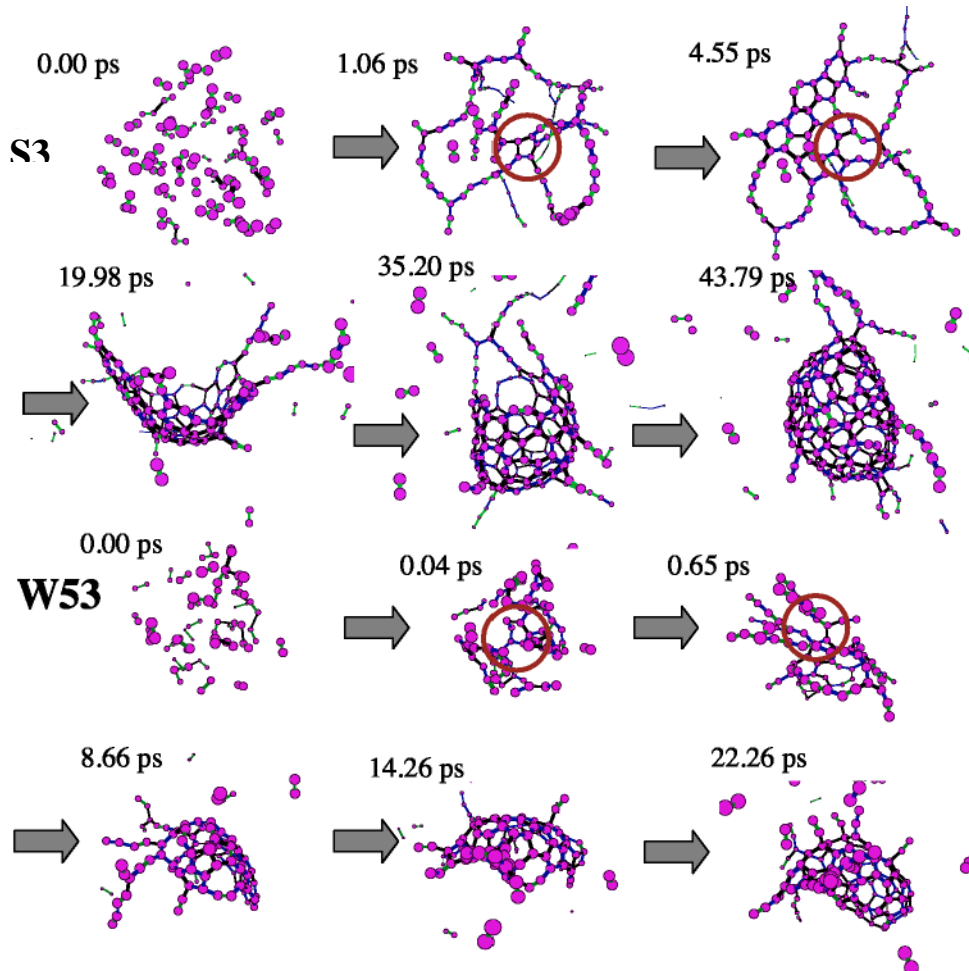


Figure 1. Snapshots for two successful trajectories for fullerene formation from C_2 molecules using different carbon densities. The **S3** trajectory starts at 0.09 g/cm^{-3} and leads to a C_{146} cage, **W53** starts at 0.20 g/cm^{-3} and leads to a C_{82} cage.

structure and non-equilibrium dynamics of these systems is discussed by analyzing trajectories at 2000 and 3000 K, in which periodically further batches of randomly oriented small carbon fragments are added. In several trajectories self-assembly of fullerene molecules is observed within less than 100 ps, their size and formation time being dependent on initial carbon density. Three distinct stages can be identified: *nucleation* of polycyclic structures by entangled linear carbon chains, *growth* by ring condensation of attached chains, and *cage closure* (see Figure 1). Giant fullerenes are obtained in this “size-up” approach, and a “size-down” roadmap is discussed based on prolonged heating of these large carbon cages. In “size-down” simulations of giant fullerenes, C₂ elimination at a rate of approximately 1/2 C₂/ps is observed, leading eventually to more rigid and kinetically more stable smaller fullerene cages like Buckminsterfullerene C₆₀. Simulated annealing leads to the formation of its famous, perfectly I_h-symmetric soccerball structure.

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Synthesis of Au Nanoparticles with Multipod Shape for the Use in Nanocircuits

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Control of size and shape of nanostructured materials is an important issue, because optical, electrical and magnetic properties change with their morphologies. This field has rapidly progressed in the past years, with the synthesis of rods, triangular platelet, hexagonal platelet, disks, cubes, and multipods. An important application of these nanoparticles is nanocircuits by 'bottom-up' self-assembly approach. Nanorods and multipods can be used for wire and interconnection, respectively, in the nanocircuits. In this study, we report the synthesis of multipod nanocrystals via wet-colloidal chemistry. In the synthesis, Au precursor was added to a cetyltrimethylammonium bromide (CTAB) solution. Au-CTAB mixed solution changed from orange to colorless by the addition of L-ascorbic acid. The directional growth was initiated by adding shape-directional seeds. Reaction temperature and CTAB concentration were manipulated for the control of size and shape of nanoparticles. Increasing in reaction temperature has caused drastical increase in the size of multipod, but the shape had little change, while the nanoparticles of sphere, rods, triangular platelet, multipod and their mixture were observed by the change of CTAB concentration. Results showed that the shape of Au nanoparticles was able to be controlled by reaction temperature and surfactant concentration. These results indicate that the directional growth condition and surface activity of each facets can be controlled by temperature and surfactant.

Shape-dependence of Gold Nanoparticle in Enhanced Sensitivity of Surface Plasmon Resonance Sensing.

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Surface plasmon resonance (SPR) spectroscopy is an effective method for the detection of biochemical changes occurred at the surface of a thin noble metal film. However, sensitivity of SPR is limited by small shifts in both angle and reflectance. The coupling of SPR with gold (Au) nanoparticles has been proposed in order to enhance the sensitivity of SPR. It is well known that the curved surface of nanoparticles has their own localized surface plasmons (LSP) due to the collective oscillations of free electrons. Therefore, additional surface plasmon polaritons (Au film) – LSP (Au nanoparticle) interactions result in the enhancement (large perturbation) in the sensitivity of SPR measurements. To our knowledge, however, no clear proof about the geometrical effect (shape-dependence) of Au nanoparticles has been reported so far. In this study, shape-dependence of Au nanoparticles coated on the thin film for the amplified surface plasmon resonance response is reported.

Spherical and rod-like nanoparticles were prepared by Frensz method and seed-mediated method, respectively. SPR substrate was prepared by the sequential thermal evaporation of a thin adhesion layer of Cr (5 nm) and Au (50 nm) layer. Au films were modified with 1,6-hexanedithiol (HDT), which produced a self-assembled monolayer. An Au coated substrate with the HDT monolayer was immersed for 12 hr into the spherical Au nanoparticle solution and rod-like particle solutions. SPR measurements were carried out using a home-made instrument.

Adsorption of Au nanoparticles on the surface of Au film result in dramatic and shape-dependent shifts in surface plasmon angle and minimum reflectance. The extent of this enhancement is largely dependent on the particle geometry. From the in situ SPR kinetics measurements of nanoparticle adsorption, it is observed that the shape of Au nanoparticles has a critical role in the kinetics of signal change. These results indicate that the selection of nanoparticle shape improves both sensitivity and kinetics of SPR.

Nanofabrication of Molecular Level Detector via AFM Lithography: Application to Copper Ion Detection

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New inventions of submicron- or nanometer-scale fabrication methods are crucial to create advanced sensors and devices. Traditional photolithography has proven to be useful in patterning large surface, but has limitations with respect to ultimate resolution ($\sim 1 \mu\text{m}$) due to the beam diameter and proximity effects by beam scattering. However, scanning-probe-based lithography (SPL) is capable of producing small features ($<100 \text{ nm}$) with high spatial precision. Among the several SPL techniques, AFM anodic oxidation is a promising method for creating nanoscale structures. In this study, the island-type gold electrode with nanoscale was prepared and applied to metal ion detection. The island-type SiO_2 pattern was fabricated on the surface of derivatized (3-mercaptopropyl)trimethoxysilane (MPTMS) p-type Si(110) by AFM oxidation based on a pre-programmed voltage. Monolayer of MPTMS was coated on the surface by a self-assembly and used to link gold nanoparticles (ca. 14 nm). In addition, acetic anhydride was used to protect amine groups of (aminopropyl)triethoxysilane (APTES). Temporary modified amine groups (APTES^o) are easily regenerated by treatment of HCl. In this invention, no metal lining or lead line was required, because the conductive Ti-Pt tip as a mobile electrode was directly in contact with gold-deposited mesa part. Surface conductivity of the fresh metal ion detector was approximately 8 nS, and the conductivity (or resistivity, capacitance) was changed with the amount of adsorbed copper ions due to the change of current field between mobile (tip) and surface electrodes (gold). When the other types of silanes are used as active sites, a variety of molecules as well as metal ions could be detected at a molecular level with short response time and high sensitivity.

Keywords: AFM, APTES, Detector, Lithography, Metal ions, MPTMS, Protection of amine, Self-assembly
Topic: Nanoelectronics

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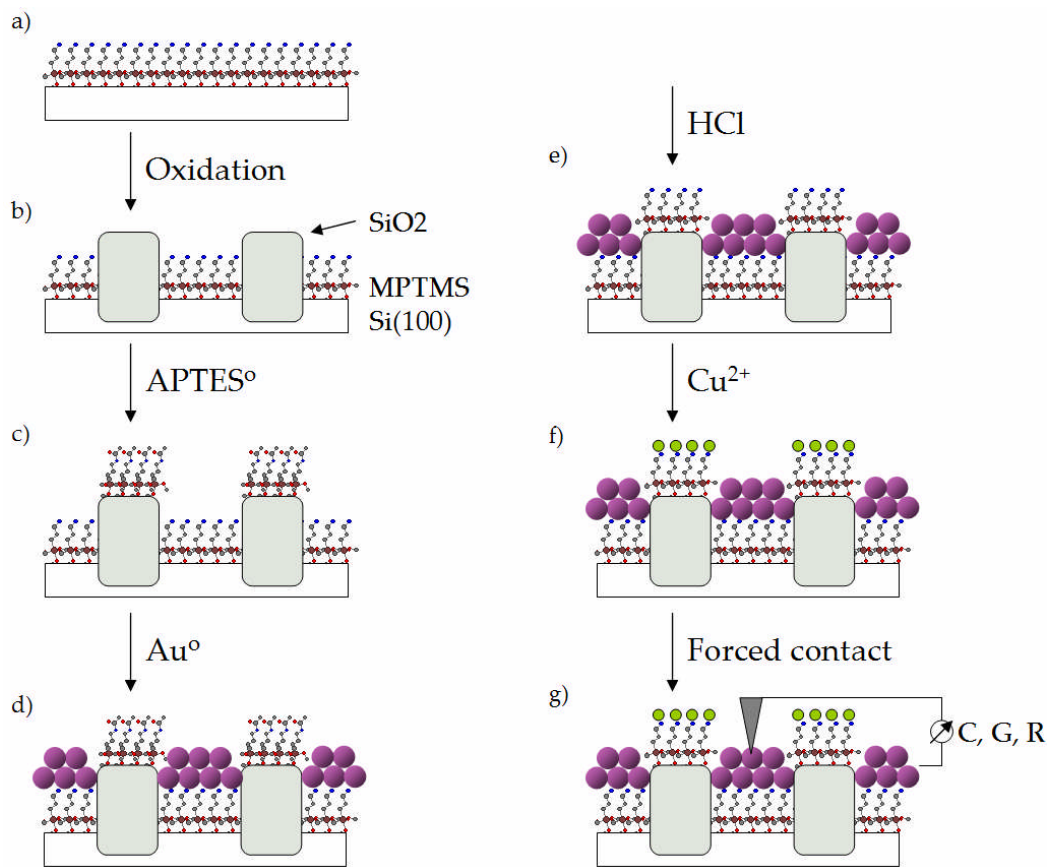


Figure 1. Schematics of metal ion detector via AFM lithography and self-assembly of silane

Environmental Perspectives Of Nanotechnology

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Nanoscience and Nanoengineering are the exciting breakthrough to manufacture structures and materials on molecular level. In the next few generation its applications will be in bioengineering, material science and electronics. Nanostructured particles will develop new environmental cleaning agents for chemical detection, creation of biological organs, development of nanoelectronic mechanical systems(NMS) and ultra dense high speed optical circuits. Challenges in Nanotechnology development should preserve our environment for future generations. Implement more ecologically sustainable Nanotechnology practices to achieve economic prosperity. The issue associated with Nanotechnology should involve legal, regulatory, economic, Business and social considerations. Potential impacts of nanostructured particle and devices on environment will pose high profile concern due to non biodegradability in the environment. Nanostructured heavy metals could provide high ionic mobility it might transport into underground water. However our recent research (Ilangovan & Ranjani 2002, US Patent Pending) showed that nanostructured particles of aluminosilicates can be used in waste treatment and as result of treatment the nanostructured particles after reaction reverse to micro scale by which micro particle penetration and transportation into the environment can be avoided. In recent years little known literatures are available to ascertain the possible effect of nanostructured particles in biological system and environment. Disposal of nanostructured particles in to the environment could attach toxic elements (inorganic & organic) and find the way to slip into the environment (Biota, water, soil and air) that could potentially create benign or harmful substances into the environment.

Development of new nanoparticles could provide structural similarities (Asbestos, Silica and Nanotubes etc) could speculate certain physiological effects in the biological system. Risk posed by the nanotech based products to biological and environment has not yet been assessed. Nanotechnology could substantially benefit the environment through reduced waste and improved energy efficiency, environmentally benign composite structures, waste remediation and energy conservation. Before the release of nanotech products into the environment there should be fundamental understanding of complex processes in the environment in terms of size, shape and surface chemistry. Strategic and holistic approaches with objective of social, environmental and cultural impacts should be focused on nanotech based products for economic sustainability. The process and product should integrate environmental impact assessment. Implement Life cycle analysis to ensure that all the nanostructured particles are safe and benign as possible. The recent technology development should minimize depletion of the natural resources, to achieve sustainability and improve natural ecosystem. Advances in Biotechnology have significantly improved the quality of life style in human history and we presume that the new developments in nanotechnology will improve possible template of changes in environment with in 2020. Hence protection of environment for future generation we must develop through implementation of environmental nanotechnology to achieve global sustainable environment. Geometric growth rate of nanotech based products introduction and adoption by the society will continue to decrease product cycle and each cycle deliver more functional and less expensive version of existing or new products and this emerging nanotechnology could make older technology obsolete at an increasing rate. The society will face human-machine-nature interface .Skills are required to use and adopt new technologies. To have better environment, a properly designed principles of regulatory regime such as Transparency, Consistency, Accountability, proportionality and targeting will help to achieve producers/users from developed and underdeveloped nations to keep sustainable environment for the economic prosperity.

Electrodeposition of Gold Nanoparticles on Electrodes Toward Improvement of Impedance Sensing of Interfacial DNA-Drug Interactions

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The interfacial interactions between immobilized DNA probes and the DNA specific sequence binding drugs were investigated using electrochemical impedance spectroscopy towards the development of a novel biosensor device. The electrochemical deposition of gold nanoparticles on a gold electrodes surface showed a significant improvement in the sensitivity over existing approaches, in which a self-assembled monolayer of DNA was formed on the flat gold surface. DNA-capped gold particles on electrodes act as selective sensing interfaces with controlled porosity and tunable sensitivity due to higher amounts of DNA probes and the concentric orientation of DNA self-assembled monolayer. The processes of gold nanoparticle deposition, DNA immobilization, as well as drug-DNA interaction were analyzed by electrochemical impedance spectroscopy (EIS). In the analysis the measurements of interfacial electron transfer resistance and atomic force microscopy (AFM) directly reflected the changes of surface topography upon gold nanoparticles deposition and DNA immobilization. The specificity of the interactions of two classical minor groove binders, mythramycin, a G-C specific DNA binding anticancer drug, netropsin, an A-T specific DNA binding drug and an intercalator, nogalamycin at poly (AT) DNA modified substrate and poly (GC) DNA modified substrate are compared. Using gold nanoparticle deposited substrates, the impedance spectroscopy resulted in 20-40 fold increase in the detection limits. Arrays of deposited gold nanoparticles on gold electrodes offered a convenient tool to subtly control of probe immobilization to ensure suitable adsorbed DNA orientation and accessibility of other binding molecules. The experimental approach described in this study may be applicable to fast analysis of other interfacial molecular interactions between DNA-binding molecules and selected target DNA sequences.

Problems of the creation of nanoreactors for the synthesis of metallic nanoparticles in carbon shells

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Abstract

For the synthesis of metallic nanoparticles and nanowires in carbon shells, it is expedient to use the metal ions that can be reduced in nanoreactors by the interaction with the negatively charged walls of nanoreactors. The synthesis is a reduction-oxidation process, therefore aromatic hydrocarbons or organic polymers together with metal salts are reduction-oxidation pairs. Within the framework of Hartree-Fock theory with the minimal basis 3-21 G, the energies of molecules and molecular fragments are calculated. In this energy model, the equilibrium atomic geometry of the fragments and the interaction energy of the reaction centers are determined.

The modeling results are realized in the experiments starting with mixing melts or solutions of the 3d metal chlorides (Cr, Mn, Fe, Co, Ni, Cu) with aromatic hydrocarbons or polyvinyl alcohol solution.

Heating of the reaction masses up to 400C is carried out in a step-like manner. The control over the processes is performed using spectral, microscopic and chemical methods. Nanoproducts are studied with the use of X-ray photoelectron spectroscopy, transmission electron and scanning electron microscopy, diffractometry and the method of electron microdiffraction. Depending on the conditions of the process, giant fullerenes and tubulenes inclusive of metals and metal-containing compounds are formed.

Synthesis of Multi Wall Carbon Nanotube (WCNT) over thin films of SiO₂-Fe₂O₃ deposited by Combustion Chemical Vapor Deposition

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Carbon nanotubes (CNT) constitute a new class of materials discovered in 1991 by Sumio Iijima that present unusual mechanical, electrical and thermal properties. CNT synthesis directly over metallic or ceramic substrates is of great interest in the electronic industry for the development of circuits or displays. Many ceramic catalysts have been reported for CNT growth, and a great part of them is based on the formation of a solid solution between transition metallic oxides (Fe, Ni, Co) and ceramic oxides. In this report homogeneous mixtures of Fe₂O₃ and amorphous SiO₂ were prepared through their co-deposition by Combustion Chemical Vapor Deposition (CCVD). This technique allows the deposition of thin films using low cost equipment and precursors. After that, they were kept in an atmosphere of H₂/CH₄ to promote the CNT growth. The temperatures of synthesis were varied from 950 to 1100 °C. The efficiency of the synthesis process was evaluated according to its thermal analysis, mass variation during the synthesis, purification, scanning and transmission electron micrographies. Multiwall Carbon Nanotubes were obtained with diameters of less than 15 nm.

Integrated Nanotechnology - Small Things with Big Impact on National Security

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Nanoscience and its ultimate application in new technology is generating a great deal of excitement throughout the world's scientific, engineering and financial communities. Nanoscience addresses the ability to create, image, and measure properties of materials and devices that are designed and built in the size range between individual atoms and the continuum of bulk materials. On the nanometer scale, completely new properties and functions emerge. As a result, we are seeing the potential for nanotechnology to change our lives in ways ranging from computing and communications to drug discovery and human health. While new technology has always played a key role in supporting our nation's military strength, today's new and emerging national security landscape places even greater emphasis and opportunity for nanotechnology to play an important role in areas of countering terrorism, economic vibrancy, environmental safety, and energy security. This presentation will point to some existing and developing areas where rapid advances in nanotechnology are critical to our nation's security. Ultimately, success will require a dedicated and sustained effort to advance this new field of science and a visionary approach to guide new science into the development of critical new technologies.

¹Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Nano Convergence: Real Time Legal Risks & Opportunities

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The 21st Century will be known as the era of sensors, implants, interfaces, and networks, pervasively concealed and ubiquitously deployed in knowing and unknowing environments and systems. Integrated convergence at the nanoscale is happening within biotechnology through bio- and genetic- engineering, information technology through advanced computing, and cognitive science and neuroscience. The impact and implications for benefits, as well as unintended consequences, is expected to be felt across all societal and economic sectors on a global scale. What are the short- and long-term legal challenges and opportunities? Are we prepared to deal with the perceived, known, unknown and yet undefined risks? Are infrastructures in place to cope with the ramifications of the rapid advances of research and development? Is today's societal framework ready for the Age of Convergence?

Synthesis of MWCNT over thin films of SiO₂-Fe₂O₃ deposited by Combustion Chemical Vapor Deposition

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Carbon nanotubes (CNT) constitute a new class of materials discovered in 1991 by Iijima that present unusual mechanical, electrical and thermal properties. CNT synthesis directly over metallic or ceramic substrates is of great interest for the electronic industry for the development of circuits or displays. Many ceramic catalysts have been reported for CNT growth, and great part of them is based on the formation of a solid solution between transition metallic oxides (Fe, Ni, Co) and ceramic oxides. In this report homogeneous mixtures of Fe₂O₃ and amorphous SiO₂ were prepared through their co-deposition by Combustion Chemical Vapour Deposition (CCVD). This technique allows the deposition of thin films with low cost equipment and precursors. After that, they were submitted in an atmosphere of H₂/CH₄ to promote the CNT growth. The temperatures of synthesis were varied from 950 to 1100 °C. The efficiency of the synthesis process was evaluated according to its thermal analysis, mass variation during the synthesis and purification and scanning and transmission electron micrographies. MWCNT were obtained with diameters inferior of 15 nm.

Quantum effects in signal transduction biology: perspectives for 21st century nanoelectronics

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Sizeable quantum effects in a specific biological signal transduction event have been recently discovered. Linear-scaling quantum mechanical calculations performed on the complex between the SH2 domain of a protein tyrosine kinase and a phospho-peptide indicate that upon binding the macrodipole of the protein is rotated by ~150 degrees from its initial orientation. This interesting finding suggests about the possibility of employing the SH2 domain as a molecular switch for 21st century nanoelectronics. Furthermore, additional aspects concerning both signal integration and signal amplification in biological systems are also discussed.

Technology funding opportunities at the National Cancer Institute Through the Cancer Diagnosis Program

Avraham Rasooly

National Cancer Institute, Cancer Diagnosis Program

The National Cancer Institute (NCI) is a component of the National Institutes of Health (NIH), one of eight agencies that compose the Public Health Service (PHS) in the Department of Health and Human Services (DHHS). The NCI is the Federal Government's principal agency for funding cancer research and training.

Technology development for cancer diagnosis is critical for public health. The NCI Cancer Diagnosis Program (CDP) supports research on cancer diagnosis and encourages programs that move new scientific knowledge into clinical practice. Within CDP, the Technology Development Branch (TDB) stimulates and supports research focused on the development of innovative technologies and devices leading to better tools to aid clinical decision-making.

Grant Funding at NCI: Grants funded by NCI include researcher initiated projects as well as projects received in response to specific Requests for Applications (RFA) and Program Announcements (PA). NCI funds a variety of programs from large program projects to small exploratory grants, TDB support early and later stages of technology development with relevance to cancer diagnosis. These include special programs (SBIR and STTR) for investigators employed by small businesses. In addition NCI funds career development award, equipment, meetings and courses.

Eligibility for funding: The program support broad range of research organizations including medical centers, hospitals, research institutions, businesses, government organizations and universities throughout the United States and abroad.

New NCI Request For Applications (RFA) for technology development:

- Innovative Technologies for Molecular Analysis of Cancer (CA-05-002, CA-05-006)
- Application of Emerging Technologies for Cancer Research (CA-05-003, CA-05-007)
- Developing Cancer Sample Preparation Methodologies (CA-05-004, CA-05-008)

Research areas of interest to the Technology Development Branch

Devices: Micro-technology, nano-technology, microfluidics or MEMS systems for comprehensive molecular analysis; Biosensors. Technologies for automated sample preparation, other automated, high-throughput systems and integration of technologies into diagnostic systems.

Other Research areas of interest to TDB: Genomic, Proteomic and Bioinformatics technologies relevance to cancer diagnosis.

Nanoscale Science and Technology at Oak Ridge National Laboratory

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Over the next two years, significant new capabilities for nanoscale materials synthesis, characterization, and simulation and modeling will become available at Oak Ridge National Laboratory. These capabilities will be accessible to the scientific community through the \$65M Center for Nanophase Materials Sciences (CNMS), a new Department of Energy user facility currently under construction at ORNL. The CNMS will include state-of-the-art equipment for nanoscale materials research and will be linked to the Spallation Neutron Source (the world's most powerful facility for neutron scattering), the upgraded High Flux Isotope Reactor (with a new world class cold source), the Center for Computational Science (with leadership class computing capabilities), and ORNL's broad array of materials synthesis and microcharacterization facilities. The promise of these new capabilities for nanoscale science and technology will be illustrated with results from recent ORNL research including advances in polymer architectures, nanostructured alloys, correlated electron materials, carbon-based nanostructures, interfaces with biological systems, superconductivity, magnetism, and subangstrom electron microscopy.

Transforming and Responsible Nanotechnology Research and Development

M.C. Roco

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Nanotechnology has opened an era of scientific convergence and technological integration with the promise of broad societal implications. The foundation of understanding, manufacturing and medicine is changing from the macro and micro domains to the nanoscale, where all fundamental material structures, properties and functions are defined. Research and development (R&D) provides new transforming tools at the confluence with biotechnology, information technology and cognitive sciences. It is expected that this general purpose technology will affect almost all sectors of the economy, and will cause structural changes in markets, industrial organizations and business models. This makes it all the more critical that we strike a proper balance between the promised benefits, and the necessary measures to mitigate and prepare for possible undesirable secondary effects.

The National Nanotechnology Initiative (NNI) is a long-term program announced in January 2000 that coordinates 21 departments and independent agencies with a total budget of about \$1 billion in fiscal year 2005. A report on societal implications and a material for the public were prepared at the beginning of the R&D program. As government investments worldwide approach \$4 billion per year, expectations of nanotechnology R&D results, commercialization and other potential benefits are raised, and concerns about unexpected societal implications need to be answered to the public's satisfaction. Nanotechnology has evolved into a field of broad international interest, increasing collaboration and stimulating competition.

For the next five years, new priorities are envisioned in exploratory research for nanomedicine, energy conversion, food and agriculture, realistic simulations at the nanoscale, molecular nanosystems, and improving human performance. Transitioning to technological innovation will continue for nanostructured materials, nanoelectronics, catalysts, and pharmaceuticals, development of tools. A focus will be advancement of societal goals such as education and sustainable development. After a brief overview of the long- and short-term issues of the responsible nanotechnology R&D, the presentation outlines the U.S. investment in the area of environmental, health and safety (EHS), and aspects of risk governance. Since collaboration with industry is an indispensable component of the NNI, this paper also outlines the current interaction in the areas of EHS with various industry sectors, including the electronic, chemical, and pharmaceutical sectors.

References (also on the website www.nsf.gov/nano):

- Roco, M.C., 2003. Broader Societal Issues of Nanotechnology. J. Nanoparticle Research, Vol. 5 (3-4), 181-189.
- Roco, M.C., 2004. The U.S. National Nanotechnology Initiative after 3 years (2001-2003). J. Nanoparticle Research, Vol. 6 (1), 1-10.

Pulsed Laser Heteroepitaxial Deposition of Ge Quantum Dots on Si(111): Size Control, Positioning and Wiring

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We have used $\lambda=248$ nm pulsed laser heteroepitaxial deposition techniques to produce randomly positioned but narrow Ge quantum dots size distribution on Si(111) substrates by controlling the laser fluence. Before growth it has been established by quadrupole mass spectrometry time of flight and linear time of flight that laser ablated Ge plume contains a significant portion of high energy Ge^+ ions and their population and energy increases with laser fluence. It has been observed that for Ge films grown at 600°C using laser fluences of 1.77 J/cm^2 , 2.02 J/cm^2 and 2.26 J/cm^2 the average height of dots for the faster growth rate was $7.0 \pm 3.5 \text{ nm}$, $4.4 \pm 1.8 \text{ nm}$ and $3.1 \pm 1.2 \text{ nm}$ respectively which is a progressive improvement in the size and size distribution of quantum dots. We believe that laser deposition techniques produce results due to "ion-stimulated nucleation", a physical process that occurs during film growth.

Further improvements of results were obtained using the chemical means of carbon pre-deposition in the form of C_{60} to induce the Ge dots. Under similar growth conditions, spin coating and drop casting pre-deposition of C_{60} , before Ge growth, gave the same results in Ge dot size and size distribution.

Wiring of Ge dots was done using carbon nanotubes. Nanotubes were pre-deposited in the same manner as C_{60} before Ge growth which subsequently resulted in the convenient self-assembly of dots atop the tubes at temperatures of 600°C and 650°C . Unfortunately, no great improvement was observed in the spatial positioning of the dots on the Si substrate.

In efforts to produce better addressability of dots, Si(111) substrates were fashioned into periodic arrays of self-wired submicron nanostructures using reactive ion etching through a self-assembled mask. The Si(111) surface was found not to be the preferred surface for self assembly however thermodynamically limiting growth modes were employed to force dots to assembly on top of our Si nanostructures.

We believe that our findings in these areas of growth, positioning and wiring of self-assembled semiconductor nanostructures provide new means by which quantum dot based devices can be more easily fabricated.

Electron Magnetic Resonance studies of Nanomanganite $\text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$.

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Electron Magnetic Resonance is a powerful microscopic technique to probe the complex spin dynamics, magnetic phase transitions and phase separations¹ in the rare earth manganites. Nano manganites have technological importance in addition to their rich physics. $\text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ (NSMO) nanoparticles with the grain size of about 30 nm are prepared by sol-gel method. These nanopowders are annealed at four different temperatures viz 800° C, 900° C, 1000° C and 1100° C to study the effect of particle size on magnetic, transport and electron magnetic resonance spectral parameters. The prepared samples are characterized by XRD, SEM, EDAX and TEM. The a.c susceptibility experiments have been done on all the four samples. It shows that as the particle size increases, the ferromagnetic to paramagnetic transition temperature (T_c) decreases, which is considered to be the one of the technologically important achievements as these materials (CMR) can be used for data storage applications to operate at room temperature. Another important finding of our results is that metal to insulator transition temperature also changes with the particles size as revealed by resistivity measurements. Electron Magnetic Resonance spectra of the nano powders are recorded from room temperature down to 4K using an X- band ESR spectrometer. EMR spectra could be fitted using two broad-gaussian lineshapes below T_c and suggested the ferromagnetic nature of the sample. Above T_c a single Lorentzian fits the signals as expected for a paramagnetic sample. The EMR spectra of the four samples and the spectral parameters obtained by fitting appropriate line shapes are found to be different from the bulk(polycrystalline) sample data². The spectral parameters show variation with the particle size. The presence of the two signals in the ferromagnetic phase is attributed to core and shell regions of the nanoparticles³. We could estimate the shell thickness (core-shell region) from the EMR intensity data as 0.7nm-1nm which agrees well with the other measurements³. This is the first experimental (through EMR) evidence which show that Core and Shell in a nanoparticle have different magnetic nature which supports the existing theoretical models⁴.

1. Janhavi.P. Joshi et. al. JMMM, (2004), in press
2. Angappane etal, J. Appl.Phys.**93**, 8334 (2003).
3. M. Bibes etal, Appl. Phys.Lett. **82**, 929 (2003).
4. M A Lopez-Quintela etal, Nanotechnology 14(2003)212-219.

Optical Spectroscopic Studies On Nanocrystalline Y₂O₃:Eu³⁺

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The optical properties of rare earth ions trapped in inorganic oxides continue to be a research attraction in terms of both their fundamental and technological importance. Yttrium oxide doped with Eu³⁺ is one of the main red-emission phosphors. The effect of the peculiar structural properties of these rare-earth compounds on their electronic states is the cause of their interesting optical behaviour. In modern nanotechnology, for enhancing the brightness and resolution of the displays, it is important to develop phosphors with controlled morphology and small particle size (nanopowder). To use them in device fabrication with their full potential, one needs to understand the fundamental properties of these low dimensional systems in detail. A considerable amount of investigations on luminescence properties in bulk materials (powders of particle size in micron scale) of Y₂O₃:Eu³⁺ have been reported in the literature. But the detail electronic properties of the corresponding nanomaterial are still unknown.

We have investigated and optical properties of both bulk and nanocrystalline Europium doped Yttria, of average particle size 20 Å. The nanopowder has been synthesized by soft chemical method and characterized by X-ray diffractometry and Transmission electron microscopy. The electronic transition spectrum has been studied for the range 450 nm – 900 nm by Photoluminescence spectroscopy. We have observed antiStokes's emission, which arises due to thermally excited electrons in the material. To analyze the antiStokes's emission spectrum we have calculated the internal thermal energy of the system from the intensity ratio of Stokes and Antistokes Raman scattering. Such studies help us to get a more complete idea of the electronic energy states of Eu³⁺ in this material. By calculating the crystal field parameter from the intensity ratio of different electronic transitions, the crystal field effect in both bulk and nanopowder has been compared. In our sample the narrow electronic transition spectrum clearly suggests a crystalline surrounding in this nanopowder. Moreover, due to defect free electronic states of the nanomaterial, its quantum efficiency is nearly equal to that for corresponding bulk system. To the best of our knowledge this result is unique compared to what has been reported till date and significant for its application in using these lanthanide doped oxides as phosphors.

Topic Area : Nanomaterials

Electron Magnetic Resonance studies of Nanomanganite $\text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$.

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Electron Magnetic Resonance is a powerful microscopic technique to probe the complex spin dynamics, magnetic phase transitions and phase separations¹ in the rare earth manganites. Nano manganites have technological importance in addition to their rich physics. $\text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ (NSMO) nanoparticles with the grain size of about 30 nm are prepared by sol-gel method. These nanopowders are annealed at four different temperatures viz 800° C, 900° C, 1000° C and 1100° C to study the effect of particle size on magnetic, transport and electron magnetic resonance spectral parameters. The prepared samples are characterized by XRD, SEM, EDAX and TEM. The a.c susceptibility experiments have been done on all the four samples. It shows that as the particle size increases, the ferromagnetic to paramagnetic transition temperature (Tc) decreases, which is considered to be the one of the technologically important achievements as these materials (CMR) can be used for data storage applications to operate at room temperature. Another important finding of our results is that metal to insulator transition temperature also changes with the particles size as revealed by resistivity measurements. Electron Magnetic Resonance spectra of the nano powders are recorded from room temperature down to 4K using an X- band ESR spectrometer. EMR spectra could be fitted using two broad-gaussian lineshapes below Tc and suggested the ferromagnetic nature of the sample. Above Tc a single Lorentzian fits the signals as expected for a paramagnetic sample. The EMR spectra of the four samples and the spectral parameters obtained by fitting appropriate line shapes are found to be different from the bulk(polycrystalline) sample data². The spectral parameters show variation with the particle size. The presence of the two signals in the ferromagnetic phase is attributed to core and shell regions of the nanoparticles³. We could estimate the shell thickness (core-shell region) from the EMR intensity data as 0.7nm-1nm which agrees well with the other measurements³. This is the first experimental (through EMR) evidence which show that Core and Shell in a nanoparticle have different magnetic nature which supports the existing theoretical models⁴.

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Diamond Chain-like Nanowires

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One-dimensional structures with nanometer diameters, such as nanotubes and nanowires, have attracted extensive interest in recent years because of their unusual quantum properties and potential applications as nanoconnectors and nanoscale devices. Since the discovery of carbon nanotubes in 1991, various one-dimensional materials have been fabricated. However, until now there has been no report on the synthesis of diamond with nanometer scale one-dimensional structure. Here we report the preparation of diamond nanowires consist of chain-like diamond structure, produced by using hydrogen plasma treatment of carbon nanotubes.

The purified carbon nanotubes were dispersed onto silicon substrates and then were placed into the radio- frequency plasma-enhanced chemical vapor deposition reaction chamber. After the samples were heated to a temperature of about 1000 K, hydrogen was fed into the chamber at a gas flow rate of 50 sccm to maintain the reactant pressure at 150 Pa and plasma with a power density of 0.5 W/cm^2 was initiated simultaneously. After reaction for several hours, the specimens were cooled down in vacuum.

Fig.1a shows the TEM image of the diamond chain-like nanowires (similar to silicon chain-like nanowires) from the carbon nanotube specimen after treatment in hydrogen plasma at temperature of 1000 K for 10 hours. Instead of ordered concentric graphite sheets of MWCNTs, many nanoparticles were formed on the original carbon nanotube walls after hydrogen plasma treatment. The nanotube hollow structure is reserved to some extent, indicated by two rows of nanoparticle array formed along the carbon nanotube precursor. The ring pattern in the inset of Fig. 1a from electron diffraction confirmed the diamond structure of nanocrystallines.

The microstructure of diamond chain-like nanowires was further confirmed by HRTEM observation. Fig.1b gives a lattice image of a nanowire, in which the core-shell structure is clearly visible. The crystalline core is wrapped in an amorphous outer layer with an atomically sharp interface. The spacing between the parallel fringes of the crystalline core was measured to be about 0.21 nm, which is equal to the spacing of $\{111\}$ planes of crystalline diamond. These nanocrystals are connected by an ultrathin amorphous carbon layer. If the nanowires form a closely aligned network on a substrate, we can simply estimate that a nucleation density above $10^{11} \text{ nuclei/cm}^2$ is achievable. To the best of our knowledge, current nucleation density achieved is about $10^{10} \text{ nuclei/cm}^2$, which is one order of magnitude lower than our current nucleation density. High-density and large area diamond nucleation is the basis for growing high quality diamond films. The present method of hydrogen plasma treatment has great potentials for the preparation of high quality diamond films in a more controllable way. In addition, combining diamond negative electron affinity, high nucleation site density and nanosize effect, this kind of chain-like diamond nanowires is expected to possess more excellent properties than other nanowires for numerous important applications, especially in field emission.

Challenges and Opportunities for Materials in Nanotechnology

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Over the past 3 decades the semiconductor industry has doubled the number of transistors on integrated circuits every 2 years, following an empirical law widely known as Moore's law. The ability of the semiconductor industry to stay on Moore's law has enabled the digital revolution and now the convergence of communications and computing. However, as the size of the smallest structures decrease, this has required the introduction of many new materials and the interactions of these heterogeneous materials and processing is increasing in complexity. The increasing use of the nanomaterials and the ever-shrinking dimensions requires development of an improved understanding of material properties (electronic, thermal, mechanical, and optical) at differences scales. Due to the presence of multiple thin films and metal alloys in the nanotechnology, grains, and interfaces assume more significance than before. This paper reviews some of the challenges in materials and the opportunities for using fundamental modeling and characterization techniques to enable successful management of these heterogeneous interactions. As the industry evaluates new materials for future technologies, research is needed to develop new modeling and characterization techniques to evaluate nano-materials and materials with nano-scale dimensions and structure.

Pulmonary Oxidative Stress, Inflammation, And Fibrosis Induced By Carbon Nanotubes

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Society is currently amidst a revolutionary development of remarkable new technologies based on novel applications of nanomaterials. From drug delivery tools and microcircuitry elements to microcomputer networks and super-durable composite materials – this is just an illustration of the unprecedentedly broad range of applications and approaches using nanomaterials. One of the most interesting examples of nanomaterials are carbon nanotubes (CNT), new members of carbon allotropes similar to fullerenes and graphite. Previously, we reported that exposure of human bronchial epithelial cells to CNT induced oxidative stress, depletion of antioxidants, morphological changes, cytotoxicity, and apoptosis. In the current study, we investigated pulmonary toxicity of CNT after pharyngeal aspiration by C57BL/6 mice. We found that CNT caused dose dependent formation of granulomatous bronchointerstitial pneumonia, fibrosis (collagen accumulation), and changed pulmonary function. Administration of carbon nanotubes to C57BL/6 mice also resulted in a dose-dependent augmentation of biomarkers of inflammation quantified by bronchoalveolar lavage (BAL) cell counts, total protein, lactate dehydrogenase (LDH) and α -glutamyltranspeptidase (GGT) activities in BAL fluids and accumulation of pro-inflammatory and pro-fibrotic cytokines. Mice exposed to an equal mass of ultrafine carbon black or fine crystalline silica exhibited less PMN recruitment and cytotoxicity than mice receiving CNT. Furthermore, CNT particles elicited a persistently 10- and 25-fold higher acute inflammation in the lungs of the mice compared to SiO₂ and UFCB as plotted per surface area dose. CNT induced release of pro-inflammatory and pro-fibrotic cytokines from macrophages in vitro. Overall, our data suggest that exposure to CNT leads to pulmonary toxicity realized through synergized interactions of inflammatory response and oxidative stress culminating in the development of multifocal granulomatous pneumonia and fibrosis.

Challenges and Opportunities for Applied Nanotechnology to the Regeneration of the Central Nervous System

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The design and application of engineered nanomaterials and devices that have different functional properties and are able to interact with central nervous system (CNS) cellular elements at the nanoscale by themselves or in conjunction with other neurobiological approaches provide very novel and potentially powerful ways for achieving the functional regeneration of the CNS. As with other applied nanotechnologies to biology and medicine this emerges from the controlled ability to influence and respond to cells at their functional building block level, the level associated with the constituent protein elements that make up the functional cellular unit, including for example cell surface receptors, transmembrane proteins, ion channels, and the cell's cytoskeleton. It is foreseeable that emerging nanotechnologies will contribute towards the study of cellular and sub-cellular neurophysiology and neuropathophysiology by providing new tools and experimental approaches, or be developed to actively promote functional regeneration of CNS neurons following trauma or degenerative disorders. Despite this potential however, nanotechnologies for the CNS have been slow to develop, in part due to the unique and very difficult anatomical and physiological challenges presented by the CNS to any interventional technologies that aim to interface with it, especially at the cellular level. This talk will introduce the main scientific obstacles associated with achieving functional CNS regeneration following injury, how emerging nanotechnologies can play a role in this, and what unique challenges imposed by the CNS must be addressed. Specific approaches by our own group and those of others will be presented.

Diamond Chain-like Nanowires

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One-dimensional structures with nanometer diameters, such as nanotubes and nanowires, have attracted extensive interest in recent years because of their unusual quantum properties and potential applications as nanoconnectors and nanoscale devices. Since the discovery of carbon nanotubes in 1991, various one-dimensional materials have been fabricated. However, until now there has been no report on the synthesis of diamond with nanometer scale one-dimensional structure. Here we report the preparation of diamond nanowires consist of chain-like diamond structure, produced by using hydrogen plasma treatment of carbon nanotubes.

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Fig.1a shows the TEM image of the diamond chain-like nanowires (similar to silicon chain-like nanowires) from the carbon nanotube specimen after treatment in hydrogen plasma at temperature of 1000 K for 10 hours. Instead of ordered concentric graphite sheets of MWCNTs, many nanoparticles were formed on the original carbon nanotube walls after hydrogen plasma treatment. The nanotube hollow structure is reserved to some extent, indicated by two rows of nanoparticle array formed along the carbon nanotube precursor. The ring pattern in the inset of Fig. 1a from electron diffraction confirmed the diamond structure of nanocrystallines.

The microstructure of diamond chain-like nanowires was further confirmed by HRTEM observation. Fig.1b gives a lattice image of a nanowire, in which the core-shell structure is clearly visible. The crystalline core is wrapped in an amorphous outer layer with an atomically sharp interface. The spacing between the parallel fringes of the crystalline core was measured to be about 0.21 nm, which is equal to the spacing of { 111 } planes of crystalline diamond. These nanocrystals are connected by an ultrathin amorphous carbon layer. If the nanowires form a closely aligned network on a substrate, we can simply estimate that a nucleation density above 10¹¹ nuclei/cm² is achievable. To the best of our knowledge, current nucleation density achieved is about 10¹⁰ nuclei/cm², which is one order of magnitude lower than our current nucleation density. High-density and large area diamond nucleation is the basis for growing high quality diamond films. The present method of hydrogen plasma treatment has great potentials for the preparation of high quality diamond films in a more controllable way. In addition, combining diamond negative electron affinity, high nucleation site density and nanosize effect, this kind of chain-like diamond nanowires is expected to possess more excellent properties than other nanowires for numerous important applications, especially in field emission.

Unimag For Treating Of Pyo-Septic Processes

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In spite of numerous methods and remedies, treatment of pyo-septic processes remains problematic, that calls for an urgency of research of new effective remedies in this direction.

Offered by us "Unimag" represents stable suspension of high disperse magnetite (HDM) on water bases. HDM particles are spherical form, 10-15 nanometers in size, X-Ray contrast and magnet-sensitive.

Experimental investigations of medico-biological characteristics show that HDM is characterized by bactericidal and bacteriostatic activity, with a remarkable ability to adsorb and neutralize toxic components as an antibacterial of metabolic origin. HDM can be shown to , increase proliferating activity of mononuclear and phagocytic activity of eliminated cells, as well as stimulate the production of Interleukin -1 and other factors of grow by macrophages.

Analysis of clinical materials showed high affectivity of "Unimag" in the complex of treating and prophylactics of pyo-septic processes.

The study of the mechanism of action suggests that that HDM actively takes part in the process of fighting aggressive factors, compensating some broken functions of detoxification system of organism. The main question in this direction is the decision of the problem of local inflamed processes, as the main source of the toxic components.

Morphological investigations showed, that HDM particles adsorbs on the surface of tissue at the lesion places (Figure.1), where they could function as open doors for the penetration of aggressive factors. Located at this place HDM particles hinder the penetration of infection in the depth of tissue.

It has been demonstrated that being adsorbed at the sites of lesion HDM particles gradually move in the depth of tissue, adsorbing on erythrocytes and phagocyted by neutrophils and penetrating in bloodstream. Phagocyted by macrophages HDM particles move to lymphatic capillaries and consequently lymphatic nodes (Figure.2). HDM leaves the organism in (IN-9011025-G the liver in unchanged form.

Besides of medico-biological characteristics described above, the "Unimag" can easily be prepared in water soluble solutions. Because of large surface area due to high disperse size of magnetite particles, HDM solution can easily penetrate into tissues together, and has demonstrated successful application in treating various etiology and localized inflamed processes of soft and bone tissues.

Quantum Mechanical Investigations of Electronic Structure, Spectra, Electron Charge and Spin Density Transfer and Magnetically Features of Organic Molecules Suitable for Digital, Quantum and Biological Information Processing

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Quantum mechanically designed hardware of molecular electronics digital computers and molecular NMR and ESR quantum computers are presented. Maximal lengths of these molecular electronics digital and quantum information processing logic gates are no more than four nanometers and maximal width 2.5 nm.

There are presented several two and three variable gates of molecular electronics digital computers. The results of light induced internal molecular motions in azo-dyes molecules [1-3] have been used for the design of light driven logically controlled (OR, AND, NOR, NAND) molecular machines composed from organic photoactive electron donor dithieno[3,2-b:2',3'-d]thiophene, tetrathiofulvalene (TTF) or ferrocene molecules and electron accepting 4,5-dinitro-9-(dicyanomethylidene)-fluorene (DN9(CN)₂F), tetracyano-indane, and moving azo-benzene fragment. After detail investigations of various electron insulator bridges between electron donor and electron acceptor parts occurs that non-conjugated bridge -CH₂-CH₂- should be applied to join thiophene and DO3 molecules in order to design OR logical function that significantly improved quality in comparison with our previous designed devices [1-3]. Density functional theory (DFT) B3PW91/6-311G model calculations were performed for the geometry optimization of these molecular electronics logical gates. Applied DFT time dependent (DFT-TD/B3PW91) method and our visualization program give absorption spectra of designed molecular gates and show from which fragments electrons are hopping in various excited states. There are designed set of single supermolecule fluorescing devices containing OR and AND logic functions.

There are presented quantum mechanical investigations of hydrogen and nitrogen atom Nuclear Magnetic Resonance (NMR) values of Cu, Co, Zn, Mn and Fe biliverdin derivatives and their dimers and aza-fullerene C₄₈N₁₂ adducts using Hartree-Fock (HF) and DFT methods indicate that these modified derivatives should generate from one to seven and eleven, twelve, eighteen, nineteen Quantum Bits (Qubits). The chemical shifts are obtained as the difference of the values of the tetramethylsilane (Si(CH₃)₄) and ammonia (NH₃) molecules Gauge-Independent Atomic Orbital (GIAO) nuclear magnetic shielding tensor on the hydrogen and nitrogen atoms and that of the magnetically active molecules. There are designed several single supermolecule and supramolecular devices containing molecular electronics digital logic gates, photoactive molecular machines and elements of molecular NMR quantum computers that allowed to design several supramolecular ControlNOT NMR quantum computing gates and induced idea of molecular quantum computing life.

Implementation of the quantum information processing based on spatially localised electronic spins in stable molecular radicals are discussed. The necessary operating conditions for such molecules are formulated in self-assembled monolayer (SAM) systems: 1) a tailoring group, to be attached to a substrate; 2) a localised unpaired electron spin; 3) a noncompensated chemical bond, responsible for an unpaired spin must be strong enough. We suggest to use the neutral radical molecules with Schiff base which satisfy these conditions. Using first principles quantum chemical calculations we prove that these molecules have the stable localised electron spin, which may represent a qubit in quantum information processing. Geometry of neutral radical molecules were optimized by using DFT Unrestricted B3LYP (Becke exchange and Lee-Yang-Parr correlation functionals) model with polarization 6-311G** basis functions. The spin density analysis shown that unpaired spin of radical molecules is located in the region of not-compensated valence bond. There were performed analysis of overlap population of chemical bonds in the region of unpaired spin density that gives evaluation and comparison of stability of various neutral radical molecules. Using optimized geometry it were calculated isotropic Fermi contact couplings constants and anisotropic spin dipole couplings using special EPR-II basis set in the method of UB3LYP that shown that the largest hyperfine splittings (HFS) of Electron Spin Resonance (ESR) spectra are on atoms of above mentioned region of not-compensated valence bond. For the reasons of construction of logic gates of ESR molecular quantum computers were calculated electronic spectrum and electron charge and spin density transfer in various excited states of neutral radical molecules. Analysis of electron charge and spin density transfer in different excited states show that this

phenomenon might be used for the construction of ControlNOT logical gate for the QuBit associated with unpaired spin in the stable neutral radical molecules.

There are developing molecular electronics devices for natural and artificial living systems using exact quantum chemical *ab initio* and DFT methods [4,5]. Self-assembly of various VS/UV sensitive peptide nucleic acid fragments are investigating by DFT-TD B3LYP 6-311G** method in order to design molecular information system for programmable artificial living cell.

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Immobilisation of Gold Nanoparticles on Amine Functionalised Carbon Substrates

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The assembly of metal nanoparticles on solid surfaces is important for making electrical connections in nanodevices and for constructing sensors and new nanomaterials. Nanoparticles can also be used as easily detectable "tags" for specific functional groups on a surface. Our work seeks to assemble nanoparticles on molecularly modified carbon substrates.

Very smooth carbon films (pyrolysed photoresist film (PPF)) were prepared by spincoating photoresist onto silicon wafers and pyrolysing at 1100 °C. The resulting films are 1.5 µm thick with physical and electrical properties similar to glassy carbon but with typical RMS surface roughness of 0.2 ÷ 0.5 nm. Electrochemical oxidation was used to covalently couple primary amines to the PPF surface via a radical coupling reaction. Amine modifiers varied in length and chemical composition, and their film thickness and surface coverage were monitored using atomic force microscopy (AFM) scratching and electrochemistry, respectively.

Assembly of 13 nm, citrate-capped gold nanoparticles on the surface films relies on electrostatic attraction to the protonated amine containing modifier films. Amine and diamine molecules were compared for the immobilisation of nanoparticles. Nanoparticles did not assemble on surfaces modified with other functional groups. The nanoparticle layers can be observed by eye and were characterised using scanning electron microscopy (SEM).

Topic Area:

Micro and Nano Structuring and Assembly

Dielectric Properties of the Hybrid Board of Polytetrafluoroethylene/ Nano-scale SiO₂ Powder

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The dielectric properties (dielectric constant, dielectric loss factor) of the hybrid board of polytetrafluoroethylene(PTFE) emulsion/ nano-scale SiO₂ powder are studied. The process parameters of board fabrication including powder add-on(1-3%), rotational speed(1200-3200 rpm), temperature(30-345 κ), stage of sintering and cooling(1-16) and calendaring times(1-12) are altered. The impacts of these parameters on the dielectric properties of the hybrid board are studied.

The experimental proceeded as follows: 60% solid content PTFE emulsion was blended and mixed with nano-scale SiO₂ powder and coupling agent in a blender. During the mixing, the fabrications of PTFE were formed and impacted by the rotational speed of the blender. After mixing, the viscosity of mixed solution was increased and became to a gel (semi-solid) state. The gel was proceeded with moulding and calendaring in order to release bubble and increase surface uniformity. Then, the gel was solidified by sintering and cooling to hybrid board. The temperature and stage of sintering and cooling plays an important roll for the solidification of hybrid board.

Both dielectric constant and dielectric loss factor are decreased with addition of SiO₂ powder.. Both dielectric constant and dielectric loss factor are decreased with increased rotational speed and reach a maximal, in this study 3000 rpm, and then increased. The temperature and stage of sintering and cooling plays the most important rolls for both dielectric constant and dielectric loss factor.

Keyword ~ Polytetrafluoroethylene(PTFE), hybrid board , nano-scale SiO₂ powder, dielectric constant, dielectric loss factor

Formation of ZnS nanorod and nanoclusters by simple vacuum evaporation for solar cell applications

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ZnS is a well-known II-IV semiconductor with multi faceted applications and possessing a direct band gap of 3.66eV. Our interest on this material in the nanorods and nanoclusters form mainly lies behind its use as an n-window layer for our investigations on different window layers for CdTe and CIS based solar cells and for photocatalytic production of hydrogen from water using photocatalysts CdS/ZnS. ZnS films are deposited on to well cleaned glass substrates at a vacuum of 5×10^{-5} Torr and various parameters are determined. Structural analysis reveals the cubic nature of the films. Variation of structural parameters like grain size, dislocation density and strain with thickness has been analyzed. The composition and the surface morphology were analyzed using EDX and SEM. From the AFM analysis, formation of the discrete nanorods and nanoclusters has been identified. The band gap of the vacuum deposited ZnS films are found to vary from 3.65 to 3.78 eV. It is observed that the band gap (E_g) decreases with increase of film thickness. The variation of optical parameters like refractive index and extinction coefficient with thickness were discussed. The mechanism of conduction phenomenon in the material can be understood from the ac conductivity studies of the films in MSM(Al/ZnS/Al) structure forming a capacitor. From the ZnS thin film capacitors, the capacitance and dielectric constant have been measured over the frequency range of 20Hz to 1MHz at different temperature. From a.c conductivity measurements, σ (conductance) is calculated at different frequencies for various temperatures and it is found that the conduction mechanism is hopping. The d.c conduction studies revealed the non-ohmic type of conduction. (Log I versus Log V). From the Log I versus $F^{1/2}$ plot, the field-lowering coefficient $\hat{\alpha}$ is evaluated.

NADH Specific Signal Generation through an Electrochemically Active Biocatalytic Assembly

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A molecular assembly consisting of a redox enzyme, NADH peroxidase, a metallized double-helical peptide, and a gold nanoparticle immobilized onto a gold wire derivatized with a benzenedithiol compound, initiated and conducted redox signals in the presence of H_2O_2 and NADH. The current generated by the binding of NADH, the electron donor, was transduced through the molecular assembly with apparently little loss of signal to the solution. The currents measured correlate to an electron transfer rate constant on the order of 3000 s^{-1} within each assembly. This electron transfer rate is two orders of magnitude higher than the endogenous electron transfer rate from NADH to the native enzyme, 27 s^{-1} . This rate indicates that the metallized peptide is in a conformation conducive for electron transfer, and, in conjunction with the nanoparticles, form effective conduits for the electrical signals. The gold nanoparticle, acting as a relay between the metallized peptide.

Surface-plasmon related ultra-sensitive analytical methods and their bio- & nano- applications

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Surface plasmon fluorescence spectroscopy (SPFS) ^[1-3] and surface plasmon diffraction spectroscopy (SPDS) ^[4-6] are two recently developed high performance sensing techniques. For SPFS, the surface plasmon field enhancement in combination with a three-dimensionally extended surface function matrix (CM5, Biacore) ensures an atto-molar (10^{-18} M) sensitivity in detecting fluorescently labelled antibodies. ^[1] In a complementary way, SPDS offers label-free sensing with highly improved performance in comparison with the conventional surface plasmon resonance spectroscopy (SPR). The promising future of both techniques is strongly demonstrated by abundant examples in DNA assay, (clinical) immunoassay and nanoparticle analysis.R

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