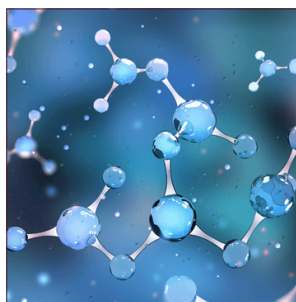
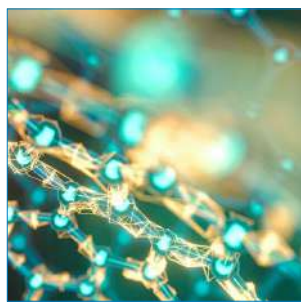
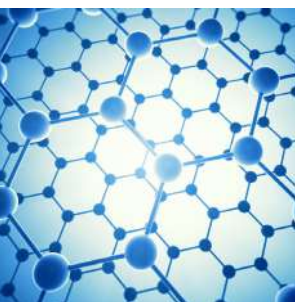
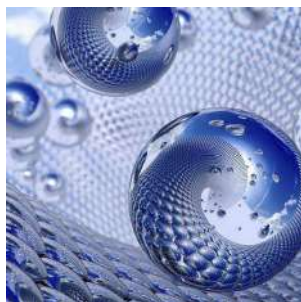

Accepted Abstracts

Nanomaterials Congress 2022



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First principles study of the 2D Mo(S1-XTeX)₂ TMD alloy: in bulk; Adsorbed on an Al-terminated Sapphire; Between Layers of Graphene; on Graphite; and on GaN

Benjamin Burton

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First principles based computational studies were performed for dichalcogenide alloys, mostly Mo(S,Te)₂, in bulk, adsorbed on Al-terminated sapphire, on graphite, and on GaN, and sandwiched between two layers of graphene. In bulk, predicted phase relations for Mo(S,Te)₂ and W(S,Te)₂ are dominated by phase separation, but when the Mo(S,Te)₂

alloy is in contact with sapphire, graphite, graphene, or GaN predicted phase relations are dominated by S:Te-ordering. The results of First Principles Phase Diagram (FPPD) calculations, binding energy calculations, and predicted band-gap variations, as functions of bulk composition, will be presented.

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Energy Efficient Designs: Cleaner and Greener Energy Technologies, Sustainable Development and Environment

Abdeen Mustafa Omer

Energy Research Institute (ERI), UK

The move towards a de-carbonised world, driven partly by climate science and partly by the business opportunities it offers, will need the promotion of environmentally friendly alternatives, if an acceptable stabilisation level of atmospheric carbon dioxide is to be achieved. This requires the harnessing and use of natural resources that produce no air pollution or greenhouse gases and provides comfortable coexistence of human, livestock, and plants. This article presents a comprehensive review of energy sources, and the development of sustainable technologies to explore

these energy sources. It also includes potential renewable energy technologies, efficient energy systems, energy savings techniques and other mitigation measures necessary to reduce climate changes. This article presents a comprehensive review of energy sources, the development of sustainable technologies to explore these energy sources. It also includes potential renewable energy technologies, energy efficiency systems, energy savings techniques and other mitigation measures necessary to reduce climate change. The article concludes with the technical status of the GSHP technologies.

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Pharmacokinetics-Pharmacodynamics Model for Nanomedicine Targeted Drug Delivery

Teddy Lazebnik

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Nanomedicines are the next generation of medicines based on pharmaceutical nanoparticles (NPs). Nanomedicines are used for medical purposes such as diagnosis, monitoring, medical treatment, etc. For better clinical results, they are designed to modify the pharmacokinetics (PK) and pharmacodynamics (PD) of their associated drugs. We present a new graph-based model for PK-PD of NPs-based drugs. The model is based on a population of NPs performing a directed walk on a graph describing the blood vessels and organs, taking into consideration the interactions between the NPs and themselves and with the environment. We define

a mechanism to perform different prediction (forward) queries on the proposed model by using analyzed two in vivo experiments with eight different NPs, done on mice. The accuracy and robustness of the proposed model were obtained by comparing the biodistribution of two types of particles (one type consists of six particles distinct from each other by their outer shell, shape, and size in five organs. The second type contains two particles that differ from each other by their core material) in five organs 24 hours after the injection. We obtain a fitting of 0.862 ± 0.01 and 0.659 ± 0.12 (mean \pm SEM), respectively, between the in vivo values and the in-silico results.

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Combined Impact of Neutron Field and Hydrogen on RPV Steel Embrittlement

Evgenii Krasikov

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As the service life of an operating nuclear power plant (NPP) increases, the potential misunderstanding of the degradation of aging components must receive more attention. Integrity assurance analysis contributes to the effective maintenance of adequate plant safety margins. In essence, the reactor pressure vessel (RPV) is the key structural component of the NPP that determines the lifetime of nuclear power plants. Environmentally induced cracking in the stainless steel corrosion-preventing cladding of RPV's has been recognized to be one of the technical problems in the maintenance of light-water reactors. Therefore, in the case of cladding failure, the problem arises of hydrogen (as a corrosion product) embrittlement of irradiated RPV steel because of exposure to the coolant. The effects of neutron fluence and irradiation temperature on steel/hydrogen interactions (adsorption,

desorption, diffusion, mechanical properties at different loading velocities, post-irradiation annealing) were studied. Experiments clearly reveal that the higher the neutron fluence and the lower the irradiation temperature, the more hydrogen-radiation defects occur, with corresponding effects on the RPV steel mechanical properties. Hydrogen accumulation analyses and thermal desorption investigations were performed to prove the evidence of hydrogen trapping at irradiation defects. Extremely high susceptibility to hydrogen embrittlement was observed with specimens which had been irradiated at relatively low temperature. However, the susceptibility decreases with increasing irradiation temperature. To evaluate methods for the RPV's residual lifetime evaluation and prediction, more work should be done on the irradiated metal-hydrogen interaction in order to monitor more reliably the status of RPV materials.

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The convergence of technologies, generates convergence in the regulations

Guillermo Valdes Mesa

Havana University Center Biomaterial, Cuba

The convergence of nanotechnologies generates synergies among different technologies to say, nanotechnologies, neurotechnology, computers and biotechnology, these technologies must converge. Stricter regulations, the application of medical devices in nanotechnologies should lead us to a link between the technical committee TC 210 and ISO technical committee 229 link that does not exist in our work in this moment in this do an analysis of the management of risk from an optical NC-ISO 14971. Studying the global trend in this respect as imported for manufacturers medical Devices worldwide. The convergences of technologies are a consequence of atomic precision, where the boundary between the biotic and abiotic must blur the interaction. The interaction between nanotechnologies, biotechnology and informatics and communications (NBI) generates a synergy of unusual consequences of all is known that the industry of semiconductor is the one of greater precision

that is atomic, the new medical devices that will be applied in the teranocis will dose Physical principles that will be governed under the laws of quantum mechanics but there are two problems that have not been solved even though they are one the non-existence of quantum biology and the transition from quantum to classical mechanics. On the other hand, the redefinition of the international system of units based on the universal constants that will be implemented by 2019 has a deficiency that is the second that redefines implies redefinition of the meter the chain of traceability proposed for nanometrology presents a serious difficulty when putting the microcopy of atomic force microscope of effect tunnel situation that is changing the verification of the Wiedemann-Franz law at atomic level yields a result where the phononic component is taken into account, a result that launches STM to the cusp of the chain of traceability above inclusive of interferometry.

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Developing nanostructured Ti Alloys for innovative implantable medical devices

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Recent years have witnessed much progress in medical device manufacturing and the needs of the medical industry urges modern nanomaterials science to develop novel approaches for improving the properties of existing biomaterials. One of the ways to enhance the material properties is their nanostructuring by using severe plastic deformation (SPD) techniques. For medical devices, such properties include increased strength and fatigue life, and this determines nanostructured Ti and Ti alloys to be an excellent choice for the engineering of implants with improved design for orthopedics and dentistry. Various reported studies conducted in this field enable the fabrication of medical devices with enhanced functionality. We review recent development in the field of nanostructured Ti-based materials and provide examples of the use of ultra-fine grained Ti alloys in medicine. Our studies have proven that nano structuring of titanium materials by means of severe plastic deformation (SPD)

techniques achieving grain refinement, increase of dislocation density, dissolution and formation of secondary phase precipitations allows for considerable improvement of the strength and fatigue properties. The advantages of nano structuring were demonstrated for CP Ti, Ti alloys including new β -Ti alloys as well as the NiTi alloy with shape memory effect. The approaches to computer design of a number of miniaturized medical implants made from high-strength nanomaterials have been suggested. Study includes the examples of manufacturing and tests of selected advanced medical devices for traumatology and surgery from Ti nanobiomaterials. Taking into account the results of recent studies on surface modification, including chemical etching of nanometals and deposition of bioactive coatings, it is assumed that the developments of Ti-based nanomaterials opens new possibilities for advanced medical implants and devices with improved design and functionality.

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