

# Scientific Tracks & Sessions July 23, 2018

### **Material Science 2018**



International Conference on

Materials Science and Engineering July 23-25, 2018 | Moscow, Russia



# Materials Science and Engineering

July 23-25, 2018 | Moscow, Russia

### Hybrid resonant organic-inorganic Nanostructures for Optoelectronics

#### V M Agranovich

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n hybrid resonant organic/inorganic nanostructures there is a combination of good charge transport properties of inorganic semiconductors and good light-emitting properties of organic substances(high quantum yield, colour detuning). Also it has the excitons of small radius for typical organic materials and Wannier-Mott excitons for inorganic semiconductors having large radius excitons and creating the basis for modern semiconductor industry. Organic and inorganic component can have electronic excitations with nearly equal energies and such contacting structures collect the best properties of both classes of materials in hybrid structure. Theoretically such structures have been investigated earlier. At pumping of such structures we can have the irreversible non-contact and nonradiative energy transfer from inorganic quantum well to organic emitting material. Important that in the beginning of this century such effect indeed was observed and continue to be observed for many different organic-inorganic nanostructures. In all earlier considered hybrid structure it was assumed that the energy of excitons in semicondactor layer is large in comparison with the

energy of exciton in the organic layer and pumping the energy was transfered from semiconductor to organics. In our recent papers we considered the hybrid structures where energy of exciton in organic layer is large in comparison with energy of exciton in semiconductor. The properties of hybrid structure in this case are very different and in this talk the results of a new approach arising with pumping of semiconductor thin film through overlayer is going to demonstrated.

#### **Speaker Biography**

V M Agranovich received PhD in Kiev, degree of Doctor of Science from Institute of Chemical Physics(Moscow) and in 1963 he received the Professor Diploma from VAK (Commission of Government). Between 1956 and 1969 he worked as a Head of Theoretical Laboratory of Physical- Energetical Institute in Obninsk and in 1969 he joined the newly founded Institute of Spectroscopy of the Russian Academy of Science (ISAN) as Head of the Theoretical Department. He was in this position during 40 years and now he is a Principal Investigator of ISAN. He published about 400 papers, four books and many invited chapters in contributed volumes.For about 20 years he was the regional Editor of Solid State Communications and before Perestroika he was main organizer of bilateral workshops and conferences USSR-USA, USSR-Germany.

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### Tiles roof support focus study: Bituminous plywood

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This study is intended to improve the tile roofing system from a carefully designed roof support. The use of tiles as roofing materials often leads to the use of either a wooden frame or a floor with a concrete slab. For this study, the timber framing on which a support made of bituminous plywood for laying tiles is retained. This bracket includes a plywood of width 1.22m, length 2.44m and thickness 4mm covered with a cotton fiber fabric impregnated with petroleum bitumen fluidized to 65% by kerosene. The liquefaction is carried out at a temperature in between 140 and 150°C. The permeability test is carried out successfully on samples of 40x40cm of bituminous plywood obtained after three weeks of drying. The time of observation

of the behavior of the sample is one day corresponding to the duration of a continuous rain of 24 hours. This material is therefore impermeable and can be used as an intermediate support for laying the tiles.

#### **Speaker Biography**

E Ouo-Djobo Samah has completed his Civil Engineering and Master of Technical Sciences at the age of 28 years from Leningrad Institute of Construction, USSR and Doctorate at the age of 52 years from Abomey-Calavi University, Cotonou, Bénin. He is the director general of Regional Road Maintenance Training Centre, Lomé, Togo. He has publications that have been cited several times, and some of them are indexed in well knowned and reputed Journals.

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### **Calcium phosphate-based Biomaterials**

### Sergey V Dorozhkin

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alcium phosphates (CaPO,) are of the special significance for the human beings because they represent the inorganic part of major normal (bones, teeth and antlers) and pathological (those appearing due to various diseases) calcified tissues of mammals. For example, atherosclerosis results in blood vessel blockage caused by a solid composite of cholesterol with CaPO<sub>4</sub>, while dental caries (tooth decay) and osteoporosis (a low bone mass with microarchitectural changes) mean a partial decalcification of teeth and bones, respectively, that results in replacement of a less soluble and harder biological apatite by more soluble and softer calcium hydrogen orthophosphates. Although the biological mechanisms appear to be quite different, chemically, the processes of both normal and pathological calcifications might be considered as an in vivo crystallization of CaPO4. Similarly, dental caries and osteoporosis might be considered as an in vivo dissolution of biologically formed

CaPO<sub>4</sub>. Due to the compositional similarities to the calcified tissues of mammals, CaPO<sub>4</sub> are widely used as biomaterials for bone grafting purposes. In addition, CaPO<sub>4</sub> have many other applications. Namely, natural CaPO<sub>4</sub> are the major source of phosphorus, which is used to produce agricultural fertilizers, detergents and various phosphorus-containing chemicals.

#### **Speaker Biography**

Sergey V Dorozhkin received his MSc in chemical engineering with honors in 1984 from Moscow Institute of Chemical Technology, Moscow, Russia, and his PhD in chemistry in 1992 from the Research Institute of Fertilizers, Moscow, Russia. From 1992 to 1994 he worked as a senior researcher at the same institute, and from 1994 to 1996 he worked as a biotechnologist at a Swiss-Russia joint venture. From 1996 to 2004 he held five postdoctoral positions in France, Portugal, Germany and Canada where he worked on various aspects of calcium phosphates. He has authored more than eighty research papers, about thirty reviews, twenty-five book chapters and seven monographs. All these publications have been cited over 5000 times and his publication H-index is 30.

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### Analysis in large deformation of a rigid plastic prestressed beam in ultra-high performance fiberreinforced concrete

Abelim Passoli, Emmanuel ET Olodo and Clement Ahouannou University of Abomey-Calavi, Benin

One of the major concerns in designing of prestressed beams in ultra-high performance fiber- reinforced concrete (UHPFRC) is improvement of their ductility fracture due to the nature of the materials used in their manufacture. This can induce plastic behaviours which it is necessary to take into account by designing of such structures, especially when they are of large spans. In the present work, it is proposed an analytical model in large deformation of a rigid plastic prestressed UHPFRC beam embedded at one end and having at other end rolled support. She is approached by a local uniform load and external moments to supports. The proposed non-linear model can find exact analytical solutions for the determination of the local arrows and the associated charge by the technique of Lagrange multiplier which allows finding the stationary points of differentiable function of one or several variables under constraints. The results of this work can be useful in designing and calculation of long span prestressed structures with plastic rigid behavior.

#### **Speaker Biography**

Abelim Passoli is a PhD student in Engineering Sciences (DOCs3s4-SPI) at the University of Abomey-Calavi, Cotonou, Benin. He is a graduate of the National Conservatory of Arts and Crafts (Cnam) of Paris in France and of Higher National School of Technology (ENSUT) in Dakar, Senegal. As a Construction and Planning Engineer, he has held several senior positions in the public and private sector with more than 26 years of experience in the field of transport and public works and the management of various phases of road infrastructure, urban infrastructure, rural equipment project studies and public contracts. As a Specialist in transport economics, since 2004 he has been involved in the technical and economic studies of infrastructure projects in Togo and in the sub-region through the SITRASS network in the expertise and valuation of companies' real estate assets.

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# Scientific Tracks & Sessions July 24, 2018

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### Construction of a dynamic finite element model for vibration analysis of reticulate systems

Abelim Passoli, Emmanuel E T Olodo and Villevo Adanhounme University of Abomey-Calavi, Benin

In the present work a model of dynamic finite element for vibration analysis of reticulate systems is proposed. It is proposed a method of construction of dynamic stiffness matrices and inertia matrices for the cases of bending, traction and torsion in free and forced vibrations. From exact analytical solutions of vibration equations it is established that the dynamic shape functions allows obtaining the coefficients of dynamic stiffness matrices and inertia matrices. These coefficients depend on frequency of free vibrations of the system. This dynamic finite element model allows obtaining an exact solution for reticulate systems in classical approach of the dynamic analysis of structures.

#### **Speaker Biography**

Abelim Passoli is a PhD student in Engineering Sciences (DOCs3s4-SPI) at the University of Abomey-Calavi, Cotonou, Benin. He is a graduate of the National Conservatory of Arts and Crafts (Cnam) of Paris in France and of Higher National School of Technology (ENSUT) in Dakar, Senegal. As a Construction and Planning Engineer, he has held several senior positions in the public and private sector with more than 26 years of experience in the field of transport and public works and the management of various phases of road infrastructure, urban infrastructure, rural equipment project studies and public contracts. As a Specialist in transport economics, since 2004 he has been involved in the technical and economic studies of infrastructure projects in Togo and in the sub-region through the SITRASS network in the expertise and valuation of companies' real estate assets.

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# Materials Science and Engineering

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### Hard matter-soft matter interface: Molecular dynamics

#### Alexey A Tsukanov and Sergey G Psakhie

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ecent outcomes of nanotechnology allow for the K development of multifunctional hierarchical nanoparticles and their application in numerous fields, including biomedicine. The use of hierarchicaly composed nanoparticles, possessing both the biological action and contrast physical properties, permits a combination of medical therapy and diagnostics into one procedure. Such an approach forms the basis for "theranostics" (therapy plus diagnostics), which is a rapidly growing direction in modern medicine, especially in oncology. As a rule, multifunctional nanoparticles with ahierarchical structure comprise an inorganic carrier and a soft bioactive part. The formation mechanism and the stability of such nanohybrids are determined by the effects within the soft matter-hard matter interface. Moreover, the interaction of nanoparticles with the cell membrane and the cellular uptake mechanism are the result of interaction effects within the hard matter-soft matter interface (HSI). Thus, the behavior of the subsystems at the HSI can determine the behavior of the whole system. Such heterogeneous interfaces are important and complex objects for study. The use of the so-called in silico approach provides a significant contribution to the comprehensive investigations of the soft matter systems and the phenomena within the HSI.

The presentation is devoted to the use of numerical molecular

models to study the interaction between biological nanoobjects and low-dimensional metal hydroxide nanostructures, which lay the basis for the development of multifunctional hierarchical nanoparticles for biomedical applications. The report consists of two parts, including an introductory review on soft matter systems, nanoceramics, hierarchical nanoparticles, and hybrid systems with the HSI. The second part is a discussion of the computer simulation outcomes obtained by our scientific group for organic-inorganic heterogeneous systems with the HSI using unbiased and steered molecular dynamics.

The work was financially supported by the Ministry of Education and Science of the Russian Federation (Agreement No. 14.604.21.0156, project identifier RFMEFI60417X0156).

### **Speaker Biography**

Alexey A Tsukanov graduated from of the Physics Faculty (Dept. of Computer Methods of Physics) of Lomonosov Moscow State University (MSU) in 2007. In 2006-2007 he participated in international project at the International Material Institute for New Functionality in Glass, Lehigh (PA, USA). He completed his PhD at the MSU and IPE RAS in 2010. After that he had a five-year long experience in the oil&gas industry. In 2014-2016 he continued his researches as postdoc at the Skolkovo Institute of Science and Technology (Skoltech), Skolkovo, Russia. Since 2016 Alexey Tsukanov is scientific researcher at the Institute of Strength Physics and Materials Science (ISPMS) SB RAS, Tomsk, Russia. He has over 40 publications that are cited about 200 times. He serves as an editorial board member of ABioDeM journal.

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### X-ray Fluorescence analysis at total reflection in conditions of planar waveguide resonators application

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ne of the most task of material diagnostics is the element analysis of thin fluorescence analysis executed in conditions of total external reflection of X-ray exciting beam on the studied surface-TXRF analytical method is the best experimental technique for the task solution.. TXRF is characterized by very attractive detection limits owing to low magnitude of the background deposit and exemption from matrix effect. X-ray fluorescence yield intensity in the method is proportional to element concentration in the excited layer. It's thickness is nearly 3-5 nm. In the result, the critical parameter of TXRF spectrometry is the exciting beam radiation density. Modern X-ray nanophotonics has suitable device called planar X-ray waveguide-resonator (PXWR), which can form X-ray nanosize beams with nanosize width and enhanced radiaiton density. In comparison with X-ray beams formed by slit-cut devices the PXWR is able to increase the radiation density in the beam on 3-4 orders. In the result, X-ray waveguide-resonance devices

are used as the exciting beam for TXRF spectrometry allows to decrease contamination detection limits on 1.5-2 order in comparison with measurements executed by slit-cut systems application. Report discusses different TXRF measurement schemes built on base of X-ray beam waveguide-resonators with different design. It has shown the way for TXRF spectrometry development on base of these devices. There are presented TXRF experimental data obtained for the real solid objects and dry residues of different solutions.

### **Speaker Biography**

Vladimir Egorov was born in Moscow in 1947 year. In 1971, he completed his graduation in Moscow Engineering and Physical Institute with the specialization of Material science. In 1981 he defended a doctoral thesis in the specialization of Solid state physics. Currently, he is working as a senior scientist in laboratory of X-ray crystallo-optics of Institute of Microelectronics Problems of Russian Academy of Science.He is an expert in ion beam analysis of material, X-ray study of materials and in specific field of X-ray nanophotonics based on waveguide-resonance propagation phenomenon.

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### NFFA-Europe: Enhancing European competitiveness in Nanoscience research and innovation

Ennio Capria European Synchrotron, France

 $N^{\mbox{\scriptsize FFA-Europe}}$  is an European open-access resource for experimental & theoretical nanoscience that carries out comprehensive projects for multidisciplinary research at the nanoscale ranging from synthesis to nanocharacterization, to theory and numerical simulation. Advanced infrastructures specialized on growth, nano-lithography, nano-characterization, theory and simulation and fine-analysis with Synchrotron, FEL and Neutron radiation sources are integrated into a multisite combination to develop frontier research on methods for reproducible nanoscience research thus enabling European and international researchers from diverse disciplines to carry out advanced proposals impacting on science and innovation. NFFA-Europe coordinates access to infrastructures on different aspects of nanoscience research that are not currently available at single specialized sites without duplicating specific scopes. Internationally peer-reviewed approved user projects have access to the best suited instruments, competences and technical support for performing research, including access to analytical large scale facilities, theory and simulation and highperformance computing facilities. Access is offered free of charge to European users. Two researchers per user group are entitled

to receive partial financial contribution towards the travel and subsistence costs incurred. The user access scheme includes at least two "installations" and is coordinated via a single entry point portal that activates an advanced user-infrastructure dialogue to build up a personalized access programme with an increasing return on science and innovation production. NFFA-Europe's own research activity addresses key bottlenecks of nanoscience research: i.e. nanostructure traceability, protocol reproducibility, in-operando nano-manipulation and analysis, open data.

#### **Speaker Biography**

Ennio Capria is actually Deputy Head of Business Development (Experiment Division) of the European Synchrotron (ESRF). He gained his PhD in Applied Physics at Cranfield University (UK). He then undertook a series of academic and industrial positions in different sectors of Nanotechnology. In his research career he has worked on the development of Nanobiosensors and on Nanocomposites for various applications. In 2011 he joined Elettra where he worked on manufacturing of optoelectronic devices and particularly their characterisation with synchrotron light. Finally, from September 2013 he joined ESRF as the IRT NanoElec Industrial Liaison Engineer, dedicated to the domain of micro-electronics. He has a strong background in the application of a wide range of synchrotron techniques to industrial and applied R&D problems

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