Additional information specific to call:

FP7-NMP-2011-EU-Russia

Further information concerning the envisaged Russian Coordinated Projects

Publication of Russian Call for tender.

The publication of the Russian call for tender for the corresponding, coordinated Russian funded projects is expected to be published in January 2011 and can then be found on the following address:

www.zakupki.gov.ru

Start Date and Duration.

It should further be noted that the EU projects are recommended to plan with a time schedule that accommodate the fact that the Russian coordinated projects will have a duration of max 30 month, expected to start in July 2011 and run until December 2013 at the latest.

Technical Requirements / Terms of Reference for the Russian Call for Tender for the coordinated projects.

The coordinated call with Russia will lead to two coordinated projects being selected to work together, within each of the 3 sub-topics identified by the call. These will be financed by the European Union, and the Russian Ministry of Education and Science under its own rules.

In order to allow applicants to prepare the coordinated projects simultaneously , information about the envisaged Russian coordinated project call for tender and its specific technical requirements / Terms of Reference relating to each of the EU Sub-topics is provided.

This information is provided below for each of the 3 sub-topics of the EU call.

EU SUB-TOPIC 1. Theoretical analysis, design and functional virtual testing of hetero or hybrid nanostructured elements for use in smart systems, integrated systems, OLEDs, photo-voltaics or energy saving applications.

Envisaged Russian Coordinated Project Call for Tender: Specific technical requirements / ToR relating to EU Sub-topic 1:

Goal of R&D

Elaboration of a set of physic-chemical models and methods for numerical simulation of hetero or hybrid nanostructured elements for the use in smart systems, integrated systems, OLEDs, photo-voltaics or energy saving applications. Development of software system for computer simulation, design and functional testing of these materials and systems on the basis of the proposed methods. Theoretical, technological and experimental validation of these works.

Principal requirements to R&D

4.1. Destination and content of R&D deliverables

4.1.1. The developed theoretical models and software system is intended for multi-scale simulations of physic-chemical properties of hetero or hybrid nanostructured elements for the use in smart systems, integrated systems, organic light-emitting diodes, photovoltaics or other energy-saving applications.

4.1.2. The subject of application must include at least one of the items indicated in the theme of R&D (see 4.1.1). Smart materials or integrated systems should be mandatory included as a subject of an energy efficiency application.

4.1.3. The list of theoretical models for multi-scale simulation of physic-chemical properties of multi-layer hetero or hybrid nanostructured elements must include one or more of the following models as required, also taking into account the requirements for functional characteristics of R&D deliverables, as described under 4.2:

- Theoretical model for calculation of properties of excited molecules and nanoparticles (for calculation of electron and optic spectra of molecules and nanoparticles with account of interaction with the environment);
- Theoretical model for calculation of microstructure of the functional layer (for calculation of microstructure of organic and hybrid layers of multi-layer devices);
- Theoretical models for calculation of hopping between molecules/nanoparticles (for calculation of probability of charge transfer between molecules/nanoparticles);
- Theoretical model for calculation of transport and kinetic coefficients of charge carriers in disordered organic and hybrid functional layers (including those for disordered polymer and inorganic layers);

- Theoretical model for calculation of charge carrier distribution and excitation in multi-layer heterostructures (for determination of distribution of recombination activity and efficiency of charge separation);
- Theoretical model for calculation of light propagation in optically active multi-layer nanostructured systems (including calculation of the efficiency of light adsorption and emission);

4.1.4. The developmental prototype of software system must include:

4.1.4.1. Modules for calculation of physic-chemical properties of hetero or hybrid nanostructured elements and multi-layer devices based on these elements implementing at least the models listed under bullet 4.1.3.

4.1.4.2. Hierarchically structured database for properties of systems under consideration and simulation results.

4.1.4.3. Sets of test data for verification and comparison to experimental data.

4.1.4.4. Technical documentation for software system as a whole and for each of the functional modules, including description of the physic-chemical models which represent the basis of the software system and the modules which represent components of the software system.

4.1.5 Functional modules from software system must be united by a single platform for data transfer tasks management, data storage and visualization.

4.2. Requirements for functional characteristics of R&D deliverables

4.2.1. The developed software system and underlying physical-chemical models should provide possibility of:

- determination of electronic structure and optical properties of molecules and nanoparticles;
- determination of microstructure of functional organic and hybrid layers;
- determination of hopping rates between molecules/nanoparticles;
- determination of transport properties of charge carries and excitations in functional organic and hybrid layers;
- modelling of distribution of charge carriers and excitations in multilayered heterostructures;
- modelling of light transfer in active optical multilayered nanosystems;
- predictable modelling, based on integration of the developed models and algorithms, describing considered systems at different levels.

4.2.2. The developed software system should include:

A hierarchically-organized set of modules and methods of coupling of different levels for multiscale calculation of physical-chemical properties of nanostructured organic and hybrid elements using both available theoretical approaches described in literature, and new approaches based on original experimental and theoretical investigations.

4.2.3. Constructive requirements for the developed software system and underlying physical-chemical models.

4.2.3.1. Module for simulation of excited properties of molecules and nanoparticles should provide possibility of :

- simulation of molecules and nanoparticles with maximum number of heavy atoms in molecule no less than 100, in nanoparticle – no less than 1000;
- description of environment effect based on continuum model with specified by user dielectric permittivity and effective radius of molecule.

4.2.3.2. Module for simulation of microstructure of functional layer should provide possibility of:

- description of intermolecular interaction in the framework of empirical force fields, having parameters for basic classes of organic molecules;
- simulation of layer with maximum number of molecules/nanoparticles no less than 10000;

4.2.3.3. Module for simulation of transport and kinetic coefficients of charge carriers in disordered organic and hybrid functional layers should provide possibility of:

- simulation of layer with maximum number of molecules/nanoparticles no less than 1000;
- specification of diagonal and non-diagonal disorder in the system, and existence of space correlation of the properties.

4.2.3.4. Module for simulation of distribution of charge carriers and excitation in multilayered heterostructures should provide possibility of:

- simulation of systems with maximum number of layers in multilayered system no less than 30;
- description of diffusion and drift processes of charge carriers in self-consistent electrical fields;
- description of diffusion of excitations;
- description of interaction of charge carriers and excitations;
- specification of arbitrary electrode properties;
- specification of arbitrary geometry of multilayered system;

4.2.3.5. Module for simulation of light transfer in active optical multilayered nanosystems should provide possibility of:

- simulation of systems with maximum number of layers in multilayered system no less than 30;
- simulation of isotropic and anisotropic radiation;
- specification of arbitrary optical properties of nanolayer materials;
- specification of arbitrary geometry of multilayered system;
- specification of nanostructure of surface and interface layers: periodic patters, non-periodic particles on the surface;
- description of plasmonic resonances at metallic layers, patterns and nanoparticles;
- description of luminescent quenching at metallic electrodes
- plot 3-dimensional distributions of electromagnetic fields in nanostructures;

- simulation of optical properties of systems with characteristic scale of non-uniformities in nanostructures no less than 10 nm.

EU SUB-TOPIC 2. Theoretical analysis, design and functional virtual testing of organic matrix nanocomposites for industrial applications (including optical, electrical, and mechanical properties).

Envisaged Russian Coordinated Project Call for Tender: Specific technical requirements/ToR relating to EU Sub-topic 2:

Goal of R&D

Development of models, computational methods and algorithms for multiscale simulation of physico-chemical properties of organic matrix nanocomposites, depending on the functionalization of the material of fillers, and the development of a software system based on these methods for the computer design of these materials.

Principal requirements to R&D

4.1. Content of R&D deliverables

4.1.1. The developing of a set of theoretical models and the resulting analytical software system must be intended for the predictive simulation of the effect of functionalization of fillers in the organic matrix on the nanocomposite microstructure and on the mechanical, transport, electrical, and optical properties of these materials.

4.1.2. The list of the theoretical models for multiscale simulation of physico-chemical properties of organic matrix nanocomposites must include one or more of the following models as required, also taking into account the requirements for functional characteristics of R&D deliverables, as described under 4.2:

- Theoretical model for the calculation of the atomistic structure and binding energy of the filler–organic matrix interface;
- Theoretical models for the atomistic calculation of micromechanical properties of an equivalent continual model of the nanofiller in the organic matrix;
- Theoretical model for the atomistic calculation of the electrical properties of the filler functionalized in the organic matrix and the interface resistance between fillers;
- Theoretical model for the atomistic calculation of the heat conductivity of the filler functionalized in the organic matrix and the interface heat resistance between fillers;
- Theoretical model for the atomistic calculation of the optical properties of the filler functionalized in the organic matrix;
- Theoretical model for the atomistic calculation of the diffusion properties of small molecules in the organic matrix and in the vicinity of the dispersed filler;
- Theoretical model for the calculation of the statistical microstructure of the organic matrix nanocomposite;
- Theoretical model for the calculation of the mechanical properties of the nanocomposite material at the macrolevel;

- Theoretical model for the calculation of the electrical properties of the nanocomposite material at the macrolevel;
- Theoretical model for the calculation of the heat conductivity of the nanocomposite material at the macrolevel;
- Theoretical model for the calculation of the optical properties of the nanocomposite material at the macrolevel;
- Theoretical model for the calculation of the transport diffusion properties of the nanocomposite material at the macrolevel;

4.1.3. The prototype model of the software system must include:

4.1.3.1. Modules for the calculation of the physico-chemical properties of organic matrix nanocomposites.

4.1.3.2. A structured data base of the properties of materials and simulation results.

4.1.3.3. Sets of test data for verification and comparison with experiments.

4.1.3.4. Technical documentation for the software system as a whole and for each functional module, including a description of the physico-chemical models lying in the basis of the functioning of the software system and its constituting modules.

4.1.4. Functional modules of developing software system must be united by a single platform for data transfer, task management, data storage and visualization.

4.2. Requirements for functional characteristics of R&D deliverables

4.2.1. The developing software system and underlying physico-chemical models should provide the possibility of:

- the determination of the atomistic structure and binding energy of the filler–organic matrix interface;
- the determination of the electronic structure and optical properties of functionalized nanoparticles;
- the determination of the mechanical properties of the system of a functionalized nanoparticle and the adjacent organic matrix;
- the determination of the electrical and heat resistance of the interface between fillers in the organic matrix;
- the determination of the microstructure of the organic matrix nanocomposite based on the calculated energy parameters of the filler–organic matrix interface and the properties of the organic matrix;
- the determination of the mechanical properties of the organic matrix nanocomposite based on the calculated nanocomposite microstructure and the mechanical properties of the functionalized filler;
- the determination of the electrical properties of the organic matrix nanocomposite based on the calculated nanocomposite microstructure, electronic properties of the functionalized filler, and the interface resistance between fillers;
- the determination of the optical properties of the organic matrix nanocomposite based on the calculated nanocomposite microstructure and the optical properties of the functionalized filler;
- the determination of the heat conductivity of the organic matrix nanocomposite based on the calculated nanocomposite microstructure and the heat conductivity of the functionalized filler;

- the determination of the transport diffusion properties of the organic matrix nanocomposite based on the calculated nanocomposite microstructure and the transport properties of the organic matrix;

4.2.2. The developing software system should include:

A set of models for the calculation of the physico-chemical properties of the functionalized filler, statistical methods for the calculation of the nanocomposite microstructure, methods for the conjugation of atomistic modules with composite microstructure modules, and modules for the calculation of the physico-chemical properties of the nanocomposite at the macrolevel based on the calculated composite microstructure. The conjugation of various levels of the simulation of nanocomposite properties must be based on both the already existing theoretical concepts described in the literature and the new concepts relied on original experiments and theoretical investigations.

4.2.3. Constructive requirements for the developed software system

4.2.3.1. For the module for the calculation of the atomistic structure and binding energy of the filler–organic matrix interface:

- the number of atoms in the structure should be no less than 1000;
- inter-atomic interaction between the functionalized filler and the organic matrix must be described with the use of empirical, semi empirical, or hybrid QM/MM models;
- the structure of the polymer matrix in the vicinity of the functionalized nanoparticle must be described using simulation of the polymerization process;
- the effect of radiation fluxes on the structure of the organic matrix must be described;

4.2.3.2. For the module for the atomistic calculation of micromechanical properties of an equivalent continual model of the nanofiller in the organic matrix:

- the minimum number of atoms in the functional layer must be no less than 10000;
- the use of interaction potentials that provide a correct description of the mechanical properties of the nanofiller and the organic matrix separately, and also the interaction between the matrix and the nanofiller;

4.2.3.3. For the module for the atomistic calculation of the electrical properties of the filler functionalized in the organic matrix and the interface resistance between fillers;

- the number of atoms in the structure should be no less than 1000;
- the use of quantum-mechanical first-principles-based description of charge carrier transport in the functionalized filler;
- processes of carrier scattering by defects of the filler structure and by lattice vibrations must be taken into account

4.2.3.4. For the module for the atomistic calculation of the heat conductivity of the filler functionalized in the organic matrix and the interface heat resistance between fillers;

- the number of atoms in the structure should be no less than 10000;
- the vibrational properties of the nanofiller and the adjacent matrix must be described using empirical force field;
- anharmonic phonon interactions must be taken into account up to the fourth order perturbation theory;

4.2.3.5. For the module for the atomistic calculation of the optical properties of the filler functionalized in the organic matrix:

- the number of atoms in the structure should be no less than 100;

- the use of first-principles methods of electronic structure calculation of nanoparticles based on many-body perturbation theory;

4.2.3.6. For the module for the atomistic calculation of the diffusion properties of small molecules in the organic matrix and in the vicinity of the dispersed filler:

- the number of atoms in the structure should be no less than 10000;
- the diffusion properties of small molecules in the organic matrix must be described using empirical intermolecular potentials;

4.2.3.7. For the module for the calculation of the statistical microstructure of the organic matrix nanocomposite:

- the number of elements in the structure should be no less than 10000;
- the use of methods of dissipative dynamics for the calculation of the equilibrium nanocomposite microstructure;
- the possibility of the description of phase layering in copolymers.

4.2.3.8. For the module for the calculation of the electrical properties of the nanocomposite material at the macrolevel:

- the number of finite elements in the structure must be no less than 1000000;
- the use of the method of finite elements for the calculation of the electrical resistance of the nanocomposite with a specified microstructure
- averaging of the calculated resistance over the statistical ensemble of nanocomposite microstructures;

4.2.3.9. For the module for the calculation of the mechanical properties of the nanocomposite material at the macrolevel:

- the number of finite elements in the structure must be no less than 1000000;
- the use of the method of finite elements for the calculation of the modulus of elasticity of the nanocomposite with a specified microstructure;
- averaging of the calculated moduli of elasticity over the statistical ensemble of nanocomposite microstructures;

4.2.3.10. For the module for the calculation of the heat conductivity of the nanocomposite material at the macrolevel:

- the number of finite elements in the structure must be no less than 1000000;
- the use of the method of finite elements for the calculation of the heat conductivity of the nanocomposite with a specified microstructure
- averaging of the calculated heat conductivity over the statistical ensemble of nanocomposite microstructures;

4.2.3.11. For the module for the calculation of the optical properties of the nanocomposite material at the macrolevel:

- the number of points of finite-difference meshes must be no less than 1000000;
- the use of finite-difference methods for the calculation of radiation transmission through the nanocomposite with a specified microstructure
- averaging of the calculated optical properties over the statistical ensemble of nanocomposite microstructures;
- the possibility of taking into account the effective dielectric constant of carbon nanostructures (graphenes, single-wall and multi-wall nanotubes) entering into the composition of the nanocomposite;

- the possibility of taking into account fluorescence, luminescence, and phosphorescence inside the active layers of the nanocomposite;

4.2.3.12. For the module for the calculation of the transport diffusion properties of the nanocomposite material at the macrolevel:

- the number of finite elements in the structure must be no less than 1000000;
- the use of the method of finite elements for the calculation of diffusion in the nanocomposite with a specified microstructure
- averaging of the calculated diffusion coefficient over the statistical ensemble of nanocomposite microstructures;

EU SUB-TOPIC 3 Theoretical analysis, design and functional virtual testing of behavioural features (e.g. biocompatibility and mechanical properties) of biocompatible metallic nanomaterials.

Envisaged Russian Coordinated Project Call for Tender: Specific technical requirements/ToR relating to EU Sub-topic 3:

Goal of R&D

Development of theoretical models, which describe the processes of fabrication and behavior of biocompatible metallic nanomaterials for optimization of their structure and properties using various advanced theoretical methods: finite elements, molecular dynamics, Monte-Carlo, discrete Fourier transformation, molecular mechanics. Multi-scale modeling of the structure and its refinement under sever plastic deformation, diffusion process, as well as dynamics, thermal, mechanical and optical properties of biocompatible metallic nanomaterials. Experimental verification of created models and production of experimental samples of nanomaterials.

Principal requirements to R&D

4.1. Content of R&D deliverables must include one or more of the following models as required while observing the requirements for functional characterization of the final modeling tool, as provided under chapter 4.2:

4.1.1. Theoretical model of ion diffusion in a medium modeling of living body.

4.1.2. Theoretical model which allows describing the strength resistance and yield strength depending on the structure and composition of biocompatible metallic nanomaterials.

4.1.3. Theoretical dynamic model of formation and growth of biocompatible metallic nanomaterials with regular lattices or with irregular fractal structures.

4.1.4. Theoretical model of nanoindentation process of biomaterials and analysis of their stress and strength resistance.

4.1.5. Theoretical model which describes structure, dynamic, thermal, mechanical, and optical properties of various biocompatible metallic materials.

4.1.6. Modeling description of the processes of deformation, evolution of microstructure and dislocation structure under severe plastic deformation.

4.1.7. Theoretical model of deformation of alloys with superelasticity and shape-memory effects, calculation of the martensite reorientation degree and dependence of its lattice parameters on temperature, solid solution concentration and austenite defect structure.

4.1.8. Mechanism of localized deformation of multicomponent bioactive nanostructured films on metallic nanomaterials.

4.1.9. Experimental samples of metallic nanomaterials including materials with superelasticity and shape-memory effects for verification of theoretical models.

4.1.10. Laboratory instruction for the fabrication of experimental samples of metallic nanomaterials.

4.1.11. Programs and methods of control of the structure and properties of experimental samples.

4.1.12. Report about patents search.

4.2. Requirements to functional characteristics of R&D deliverables

4.2.1. Developing models must be suitable from describing of the processes of fabrication and behavior of biocompatible metallic nanomaterials for optimization of their structure and properties.

4.2.2. Developing models must be suitable for the description of structure, deformation processes and structure refinement under sever plastic deformation, diffusion process, as well as dynamics, thermal, mechanical and optical properties of biocompatible metallic nanomaterials.

4.2.3. Programs and methods of control of the structure and properties of experimental samples must be suitable for the verification of the results of theoretical calculations.

4.2.4. The results obtained must be suitable for applications in Russian and EC organizations.

4.3. Technical characteristics

4.3.1. Theoretical models are based on modern simulation methods: finite elements, molecular dynamics, Monte-Carlo, discrete Fourier transformation, molecular mechanics.

4.3.2. Multi-scale modeling approach for carrying out of simulation on macro-, micro-, nano- and atomic level should be used in theoretical modeling.

4.3.3. Experimental samples of biocompatible metallic nanomaterials in amount no less than 3 pieces should be produced and tested as applied to each developed model.

4.3.4. Experimental samples should be studied using the modern analytical techniques and methodics for investigation.

List and content of work

The content of work (description of main works fulfilled by head contractor and associate contractors, as well as work fulfilled using external funding)

The list and main description of work fulfilled under the contract should be presented, for instance:

1. Development of methodic/methods:

Overview of existing models about microstructured and textural transformations of metallic materials under severe plastic deformation

2. Conduction of research

- Development of theoretical model of ion diffusion in a medium modeling of living body;
- Development of theoretical model which allows to describe the strength resistance and yield strength depending on the structure and composition of biocompatible metallic nanomaterials;
- Development of model of formation and growth of biocompatible metallic nanomaterials with regular lattices or with irregular fractal structures.
- Development of theoretical model of nanoindentation process of biomaterials and analysis of their stress and strength resistance.
- Development of theoretical model which describes structure, dynamic, thermal, mechanical, and optical properties of various biocompatible metallic materials.
- Development of modeling description of the processes of deformation, evolution of microstructure and dislocation structure under severe plastic deformation.
- Development of theoretical model of deformation of alloys with superelasticity and shape-memory effects, calculation of the martensite reorientation degree and dependence of its lattice parameters on temperature, solid solution concentration and austenite defect structure.
- Study of the mechanism of localized deformation of multicomponent bioactive nanostructured films on metallic nanomaterials.

3. Fabrication of experimental samples of metallic nanomaterials including materials with superelasticity and shape-memory effects for verification of theoretical models.

4. Elaboration of laboratory instruction for the fabrication of experimental samples of metallic nanomaterials.

5. Development of programs and methods of control of the structure and properties of experimental samples.

6. Other activities, including:

- patents search;
- technical-economical estimation of market potential of the results obtained;
- development of the project of technical specification for experimental-constructional or experimental-technological works.