M-ERA.NET Call 2014: Funded projects

Call topic	Acronym	Full Title	Nr. Partner	Funding organisations
Integrated Computational Materials Engineering	COR_ID	Design of corrosion resistant coatings targeted for versatile applications	4	MISZ (Slovenia), ANR (France), NKFIH/OTKA (Hungary)
Integrated Computational Materials Engineering	MODIGLIANI	Modelling Photoswitchable Organic-Graphene Hybrids	4	FNRS (Belgium), ANR (France), DFG (Germany)
Integrated Computational Materials Engineering	MICROPORES-HIP	Modeling of annihilation of micropores in single-crystal nickel-base superalloys during hot isostatic pressing	4	DFG (Germany), ANR (France)
Integrated Computational Materials Engineering	ChAMPion	Simulation-assisted Design and Characterization of Abrasive Magnetic Suspensions for High Precision Finishing	3	DFG (Germany), MINECO (Spain)
Integrated Computational Materials Engineering	STOMMMAC	STOchastic Multi-scale Modeling Methodologies for the Assessment of failure performance of Composite materials	6	DGo6 (Belgium), FNR (Luxembourg), FFG TP (Austria), Innobasque (Spain)
Integrated Computational Materials Engineering	nanohype	Nanoparticle Hybrid Materials Using Plasmonic-Enhanced Upconversion FRET for Multiplexed Sensing and Optical Barcoding	5	ANR (France), DFG (Germany), MINECO (Spain)
New Surfaces and Coating	PlasmaTex	Novel type of antibacterial coatings on textile materials and plastics with controllable release of antibacterial agent	7	MIZS (Slovenia), IWT (Belgium), FCT (Portugal), UEFISCDI (Romania)
New Surfaces and Coating	NOVTINALBEST	Novel nanostructured tin based alloys for electronic applications and as electrode materials for Li ion batteries using ionic liquid analogues	3	UEFISCDI (Romania), FCT (Portugal)
New Surfaces and Coating	CARBCOATPRO	Stimuli responsive layered double hydroxide/CARBon nanotube based COATings with multi-level corrosion PROtection	4	RCN (Norway), FCT (Portugal), Innobasque (Spain)
New Surfaces and Coating	C4HEALTH	Transparent Carbon-based electrodes for in-vitro and in-vivo biomedical and life sciences applications	4	PTKA (Germany), FNR (Luxembourg)
Composite Technology	**bioVALVE**	Nonthrombogenic metal-polymer composites with adaptable micro and macro flexibility for next generation heart valves in artificial heart devices	6	FFG TP (Austria), NCBIR (Poland), Taiwan (no funding)
Composite Technology	**ACHiLiS**	Development of a cycle-stable high capacity Li2S-Si Battery	5	PtJ (Germany), MOST TW (Taiwan)

Materials for low carbon energy technologies	**SOLHET**	High-performance tandem heterojunction solar cells for specific applications	5	RCN (Norway), UEFISCDI (Romania)
Materials for low carbon energy technologies	**NEXMAG**	New Exchange-Coupled Manganese-Based Magnetic Materials	3	MINECO (Spain), RCN (Norway), UEFISCDI (Romania)
Materials for low carbon energy technologies	**NANOFOAM**	Fabrication and functionalization of nanostructured metallic foams for energy storage applications	3	FCT (Portugal), MINECO (Spain), UEFISCDI (Romania)
Materials for low carbon energy technologies	**WaterSafe**	Sustainable autonomous system for nitrites/nitrates and heavy metals monitoring of natural water sources	6	UEFISCDI (Romania), NKFIH/OTKA (Hungary)
Materials for Health	**NeutroTag**	Automated neutrophils isolation and tagging for diagnosis and therapy of infections	3	FFG TP (Austria), Tübitak (Turkey)
Materials for Health	**HierarchiTech**	Hierarchical Ionic-doped Nanocomposite Scaffolds for Osteochondral Tissue Engineering	3	FCT (Portugal), MINECO (Spain)
Functional Materials focusing on Sensors	**PhotoNanoP**	High photoconductive oxide films functionalized with GeSi nanoparticles for environmental applications	5	UEFISCDI (Romania), RANNIS (Iceland)
Functional Materials focusing on Sensors	**MOFsENS**	Synthesis of metal-organic frameworks as optical gas sensors	4	FCT (Portugal), MINECO (Spain)
Functional Materials focusing on Sensors	MYND	MetrologY at the Nanoscale with Diamonds	3	LAS (Latvia), RCL (Lithuania)

COR_ID

The COR_ID project under Topic 1: ICME addresses design and development of new targeted materials involving: modeling, simulation, experimental validation and multiscaling. The principle objective is to design and engineer new coatings with targeted properties of increased corrosion resistance, specific hydrophobic properties, prolonged service life-time and reduced ecological impact. Current state-of-the-art coatings do not satisfy completely engineering demands of having high corrosion protection and additional properties. The specific innovation is to design multifunctional compounds which would simultaneously act as high-quality corrosion protective and hydrophobic surface. It could be used to protect less corrosion resistant Al alloys and even secondary Al alloys. Industry driven needs will be solved using ICME approach and produce economical material benefiting with increased market competitiveness.

MODIGLIANI

MODIGLIANI aims at implementing an integrated computational materials engineering approach to the design of highly performing multifunctional nanocomposites, the multiscale characterization of their chemical and physical properties, and ultimately the modelling of their device characteristics. As model systems to challenge the computational approach we have chosen hybrid assemblies of graphene and self-assembled monolayers (SAM) of photochromic molecules for light-responsive field effect transistors. The strategy relies on the use of photochromic SAMs for decorating the metallic electrodes or gate dielectrics of the devices. We will develop a multi-faceted modelling platform that accounts for all relevant elementay processes in the response of the phototransistors upon light-induced switching of the photochromic molecules. The theoretical schemes will be validated against experiment and integrated as modules in a multiscale modelling environment for use in academia and industry.

MICROPORES-HIP

High-pressure turbine blades are critical components of aircraft engines. They are cast as single-crystals of nickel-base superalloys. A negative side effect are casting micropores initiating fatigue failure. The pores can be removed by hot isostatic pressing (HIP), however this technological process, performed at temperature close to solidus, can damage a costly blade by recrystallization and incipient melting. The objective of our project is to develop a computational HIP model for the simulation of micropore annihilation, enabling to optimize the HIP parameters. The target property is blade material without pores with fatigue life increased by many times. Pore annihilation in single-crystals at an ultrahigh homologous temperature of about 0.97 is a complex multiscale physical process. Therefore the computational HIP model will be composed of several physical and phenomenological models considering phenomena from the atomic level up to the continuum level.

ChAMPion

A common problem in microsystems engineering is the manufacturing of parts with surfaces of optical quality. In many microsystem applications, a nanometric surface roughness is crucial for the performance of the device. Novel manufacturing techniques as e.g. rapid prototyping, can produce a variety of complex geometries, however, with very poor surface quality. To enable the manufacturing of complex geometries with high precision surfaces, a novel finishing technique including customdesigned suspensions is developed. The high quality finishing will be achieved by tailored nano-abrasive magnetorheological fluids, controllable by forces of externally induced magnetic fields. The parameters for the design of the suspensions will be derived by a combined numerical and experimental approach in accordance with the desired nano-finishing quality. The project will provide a sound basis for future ICME approaches employing tailor-made suspensions in microsystem applications.

STOMMMAC

Although composite materials offer many advantages, such as high strength-to-weight ratio, enhanced potentials for material and structure design, and many others, their potential is not realized in practice because their properties after manufacturing suffer from scatter, leading to over-designed structures. The aim of the project is to develop an original stochastic modeling methodology, based on mean-field homogenization, able to predict the probabilistic distribution of the composite material and structure responses by taking into account constituent material and microstructural uncertainties. Such a tool can then be used to tailor the manufacturing and design process in order to ensure that the expected macro-scale performance is achieved, thus minimizing material/structural oversizing. The project will focus on two types of composite materials, namely short (SFRP) and continuous (CFRP) fiber composite polymers, as well as two performance indicators: static and fatigue failure.

Nanohype

The nanohype project will combine computational modeling, synthesis, and experimental validation to design novel metalshelled upconverting nanoparticles (UCNPs) with 1) a 50-fold enhanced photoluminescence (PL) quantum yield compared to conventional UCNPs; 2) tunable PL lifetimes between 100 ns and 600 µs; 3) tunable PL colors by multiplexed Förster Resonance Energy Transfer (FRET) to quantum dots (QDs) or dyes; and 4) colloidal stability in aqueous solutions. The multidisciplinary nanohype consortium will create new synergies and improved predictive power by modeling multifunctional photoluminescent nanomaterials (PNMs) for targeted material design and engineering. Direct validation of modeling results by experimental demonstration will be a benchmark for future PNM designs and a necessary and highly relevant step for the future integration of such PNMs in industrial production and innovative applications.

PlasmaTex

In the PlasmaTex project a new class of antibacterial coatings for medical textiles and plastics will be developed. The proposed approach is to use a layered coating with a layer containing Ag nanoparticles and an additional barrier layer for controlled release of the antibacterial agent. The coatings are deposited by atmospheric pressure plasma, a versatile technique that allows producing uniform high quality coatings on almost any material. The research issues that will be addressed in the project include the detailed physical chemistry of the plasma-assisted deposition process and the release mechanism of the antibacterial agent through the barrier layer. Advanced plasma, surface and microbiological diagnostics will be deployed to establish a relationship between process parameters and coating performance. The gained knowledge will be applied to define a scalable coating methodology that yields nanocomposite coatings with superior antibacterial efficiencies.

NOVTINALBEST

NOVTINALBEST aims to develop novel scientific and technological routes to reach high performance nanostructured and whiskers resistant Sn binary and ternary alloys with applications in electronic industries especially for advanced packaging technology and as nanostructured anodes for Li ion batteries, from environmentally friendly ionic liquids analogues (ILAs). The influence of graphene addition during electrodeposition to stop whiskers growth, to reinforce Sn alloys lead-free solders and to improve the nanostructured Sn based alloy anode performance will be also addressed. The use of ILAs will allow introducing safer and more efficient production processes with predicted impact both in environmental issues and in SME revenues for the implementation of a more efficient process and the production of novel high performance nanostructured materials. Many industries will greatly benefit from the scientific and technical output of the project.

CARBCOATPRO

The increasing needs for high-performance chromate-free coatings demand development of new systems with active corrosion protection. The CARBCOATPRO project aims at developing innovative multi-level protective “smart”coatings loaded with multifunctional additives with enhanced “self-healing” active protection properties, to improve long-term performance of metallic substrates. The key technology in focus is based on functionalization of layered double hydroxide (LDH)/carbon nanotube (CNT) additives that will be incorporated into polyhedral oligomeric silsesquioxane (POSS) based coatings. The expected impacts are: 1) improved products with respect to current existing technologies with acceptable costs; 2) reduced usage of hazardous materials; and 3) sustainability of developed technology throughout the entire products life cycle. The environmentally-green products will bring significant economic benefits to the industries without harmful impacts on both the environment and the society.

C4Health

A new type of microelectrode array (MEA) compatible with multiwell plate technology will be developed. Transparent carbonbased biostable electrodes with low electrical impedance, will enable combined measurements of electrophysiology and optogenetic applications. To this end Plasma Electronic GmbH develops a novel plasma deposition tool for cost effective high volume production of carbon electrodes for these multi well substrates. Unique thin carbon/carbon nano tube hybrid coatings allow optical transparency as well as good electrical specifications of the new micro electrodes. NMI Natural and Medical Sciences Institute will produce these new MEAs in its own clean room facility. Luxembourg Institute of Science and Technology will use characterization tools primarily based on correlative Helium-Ion Microscopy-SIMS to assess biocompatibility and biostability. MCS GmbH will apply these MEAs for high throughput substance screening with their newly developed multiwellsystems.

bioVALVE

The project goal is minimizing life-threatening thrombo-emboli formation in pulsatile heart assist devices by a new biomimetic heart valve design based on metal-polymer composites. Heart prostheses support patients with late-stage heart diseases towards recovery or as a bridge to transplantation. In future, they will assist gene therapy to treat myocardial infarction. Besides of deficient blood flow (stagnant zones), state-of-the-art systems with mechanical valves generate platelet activating shear due to a narrow disc-ring gap. The novel composite and valve design solve these pressing medical needs: Injection moulding of polyurethane with a fragile titanium mesh insert combines biologically optimal micro-scale flexibility with macro-stiffness for mechanical function. Added transnational value is joining knowhow in

(1) heart valve design for optimal blood flow,

(2) haemo-biofunctional coatings,

(3) insert injection moulding, and

(4) testing, finally on the artificial patient model.

ACHiLiS

State-of-the-art Li-S battery has safety concerns since it uses elemental lithium as anode that leads to the formation of lithium dendrites during cycling. A solution to this safety problem is to use a high capacity anode material other than elemental lithium, while replacing sulfur in the cathode with its lithiated counterpart, Li_2S. Electrolytes are also significant concerns in Li-S battery because of the shuttling effect arising from the dissolution of polysulfides in the liquid electrolyte. In the presented project, all parts of the battery: cathode, anode, and electrolyte are in focus of research to develop a new and improved battery system. The research will be supported by computational simulation, and an industrial partner will integrate and construct all components for actual applications. Finally the new battery will be also recycled to show a good life cycle.

SOLHET

The SOLHET project aims at increasing the conversion efficiency of Si solar cells beyond their traditional limitations by developing high-performance Si-based tandem heterojunction solar cells (STHSC) using low-cost, abundant, and non-toxic oxide materials. STHSCs can have a huge impact on the PV field with economic and environmental benefits. The SOLHET project objectives include: A) Research on materials for STHSC focused on low cost thin film metal oxides that have tunable properties targeting i) efficient absorber layers and ii) highly conductive and chemically stable transparent layers. B) Develop modelling and simulation tools for design optimization of STHSC. C) Fabrication of STHSC with conversion efficiency above 30%. D) Demonstration and promotion of high-performance PV module (PVM) made from STHSC. E) Patenting the innovative results of PVMs at European / national level. F) Innovation excellence of the academic and research institutions from Norway and Romania.

NEXMAG

Magnetic materials are important in the production, transmission and use of electrical energy. An increased use of low carbon technologies is necessary to ensure a high living standard. Permanent magnets (PMs), used in a multitude of technological applications, play a very important role in these efforts. However, these PMs contain critical raw materials [rare-earths (REs)] as fundamental constituents and EU does not own the natural resources.
NEXMAG project considers as main objective the development of nanocomposite Manganese-based materials that will result in $(BH)_{max}$=4.5-15 MGOe through an efficient coupling between two complementary phases:

(a) Magnetically hard phases (large anisotropy): MnAl; MnBi.
(b) Magnetically soft phases (high saturation magnetisation): metals (Fe, FeCo).
These new magnets -constituted by non-critical elements- will allow substitution of RE-PMs in many technological applications therefore contributing to solve the EU dependency of REs.

NANOFOAM

The project aims at fabricating highly porous nanostructured Ni-based metallic foams for application as redox electrodes in asymmetric supercapacitors and as catalytic surfaces for hydrogen production. The innovative approach is that the nanofoams can be functionalized and tailored to optimise their electrochemical response and enhance their efficiency when used as electrodes for energy storage devices (redox asymmetric supercapacitors) and for electrochemical production of hydrogen via water electrolysis and borohydride hydrolysis. Thus, this original approach brings a multi-target material that will allow leveraging of commonalities and synergies between the envisaged applications, accelerating the development of innovative materials for energy storage.

The project outcomes can produce disruptive knowledge towards the implementation of the European Materials roadmap enabling low carbon energy technologies.

WaterSafe

The project sets to develop a new energy autonomous system based on (photo)electrochemical sensors for detection of different ionic species in natural water sources and ultra-thin solar cells (UTSC). It focuses on three directions: high efficiency, new materials in solar energy harvesting and fabrication of small UTSC and the power stabilizing device able to supply the needed voltage to the sensors and electronic module; new microsensors for detection of nitrites/nitrates and heavy metals in water; low cost autonomous energy system integration and fabrication.

The harvester will include a UTSC, a dedicated storage and a power stabilizing device. SnO2, TiO2, ZnO materials will be optimised for sensors and (TiO2, ZnO, CuxS) or (CZTS, CuxS, TiO2) for the solar cells. Bacterial flagellar filaments will be investigated and engineered as sensitive biolayer for heavy metal detection. The project will provide a technology demonstrator and water monitoring system prototype.

NeutroTag

Neutrophils are phagocytic cells that are unmatched in speed and accuracy to approach an inflammation. NeutroTag will develop and improve a material based micro-nano device for isolating and tagging neutrophils from whole blood in clinical relevant volumes and timeframes. Pre-clinical proof of concept will be applied in the field of in vivo medical imaging using contrast agent materials and for in vivo advanced cell therapies (photo-thermal therapy). Our automated processing device and filter combination will push the throughput up to 50 ml whole blood / hour and reach a retention of 95 % of leukocytes and a removal of 99.95 % of red blood cells and platelets. Current available methods can retain 50 - 60 % of leukocytes, which are contaminated with ~100x more red blood cells and ~1000x more platelets. NeutroTag will provide the first automated technology in the market that can enrich leukocytes from whole blood and prepare injection ready cell suspension for clinicians.

HierarchiTech

Nanocomposite scaffolds hierarchically structured composed of biopolymers and calcium-phosphate cements incorporating bioactive ions for osteochondral (OC) tissue engineering will be major innovation of HierarchiTech. Ionic-dopants will play vital roles in biomechanics and stimulating the stem cells niche towards osteo- and chondro-genesis/angiogenesis. These ions can act as a contrast agent for medical imaging (e.g. X-ray), thus possibly the clinician monitors the regeneration process. Cell cultures, human adipose stem cells (clinical grade) and bioactive agents combined with the scaffolds will be developed and pre-clinically validated. The expected results will develop advanced biomaterials, technologies and therapies for health and a carrier for cells/drug delivery that target specific disease or injury in OC field, with potential to be successfully translated into clinical practice, thus enhancing the competitiveness of the EU Health industry and promote socio-economical cohesion.

PhotoNanoP

A new solution for obtaining a new advanced material (SiO_2, TiO_2 films functionalized with Ge_xSi_{1-x} nanoparticles) with targeted photoconductive (PHC) properties in VIS-NIR is proposed. This material is able to spectrally discriminate between dry, wet and icy asphalt, for reducing traffic accidents. The proposed approach and material are innovative, and technological and scientific results are original, leading to 1 patent application, 3 ISI and 4 conference papers. The project creates the frame for increasing EU cooperation, developing a pan-EU partnership between 2 research institutes, a university and 2 SMEs. Each partner will gain an advanced position in own activity field becoming more visible at EU and international level. All partners will have economic benefits by winning competitive advance in photodetector market and scientific benefits. The new material is versatile as PHC properties can be tuned leading to other environmental, biomedical, food and optosecurity applications.

MOFsENS

The main objective of this project is the synthesis of gas sensitive metal-organic frameworks (MOFs) and the development of optical sensors based on thin films of these materials. The main innovation in the proposed MOF is centered on the use of new fluorescent organic bridging ligands, exploiting both the emission sensing properties of the fluorophore and the excellent sorbing capabilities of the MOF structure. We will focus on the development of a gas sensing device with enhanced selectivity and sensitivity, for monitoring of harmful gases and chemical vapors, in order to protect human health and the environment.
Despite of the intensive research in the field of MOF materials, there are only a few examples exploiting their use as optical gas sensors. On the other hand, these studies appear outside of Europe. Thus, an EU network program as M-ERA.NET is the appropriate tool to combine the expertise and knowledge to develop the present proposal.
MYND The Magnetometry on the Nanoscale with Diamonds (MyND) project seeks to improve sensors based on nitrogen vacancy (NV) defect centres in diamonds by through new theoretical insights and by the application of novel techniques to magnetic field imaging. These insights will be subsequently applied to generating new knowledge about oxygen sensing and the behaviour of singlet oxygen in SiO_2 matrices as well as to opening up a new window on research about the fluid- and magneto-dynamics of self-directed magnetic microdevices. The result of the project will be new scientific understanding of NV centre physics that will improve sensing, in particular of magnetic fields, but also of temperature and pressure. The knowledge gained has the potential to open new technologies (e.g., novel oxygen sensors) and improve other technological fields (e.g., manufacture of magnetic nanoparticles and development of selfpropelled microdevices).