Brussels, 30 October 2015

COST 039/15

DECISION

Subject: **Memorandum of Understanding for the implementation of the COST Action "Multi-Functional Nano-Carbon Composite Materials Network" (MultiComp) CA15107**

The COST Member Countries and/or the COST Cooperating State will find attached the Memorandum of Understanding for the COST Action Multi-Functional Nano-Carbon Composite Materials Network approved by the Committee of Senior Officials through written procedure on 30 October 2015.

MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

COST Action CA15107
MULTI-FUNCTIONAL NANO-CARBON COMPOSITE MATERIALS NETWORK (MultiComp)

The COST Member Countries and/or the COST Cooperating State, accepting the present Memorandum of Understanding (MoU) wish to undertake joint activities of mutual interest and declare their common intention to participate in the COST Action (the Action), referred to above and described in the Technical Annex of this MoU.

The Action will be carried out in accordance with the set of COST Implementation Rules approved by the Committee of Senior Officials (CSO), or any new document amending or replacing them:

a. "Rules for Participation in and Implementation of COST Activities" (COST 132/14);
b. "COST Action Proposal Submission, Evaluation, Selection and Approval" (COST 133/14);
c. "COST Action Management, Monitoring and Final Assessment" (COST 134/14);
d. "COST International Cooperation and Specific Organisations Participation" (COST 135/14).

The main aim and objective of the Action is to develop lighter, stronger materials which are needed for a variety of applications such as transport, energy storage/conversion and bone/tooth replacement. MultiComp COST Action is designed to bring together theorists, experimentalists, technologists and industrialists in the field of nanocarbon materials technology to overcome the current high costs through optimized synthesis techniques. This will be achieved through the specific objectives detailed in the Technical Annex.

The economic dimension of the activities carried out under the Action has been estimated, on the basis of information available during the planning of the Action, at EUR 64 million in 2015.

The MoU will enter into force once at least five (5) COST Member Countries and/or COST Cooperating State have accepted it, and the corresponding Management Committee Members have been appointed, as described in the CSO Decision COST 134/14.

The COST Action will start from the date of the first Management Committee meeting and shall be implemented for a period of four (4) years, unless an extension is approved by the CSO following the procedure described in the CSO Decision COST 134/14.

COST is supported by the EU Framework Programme Horizon 2020

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TECHNICAL ANNEX

OVERVIEW

Summary

MultiComp is a COST Action designed to bring together theorists, experimentalists and industrialists in the field of nano-carbon materials technology. Although carbon nanotubes, graphene and Few-Layer Graphene (FLG) have been used to improve the properties of composite materials, two main problems remain to be solved before these composite materials can realize their full potential: (1) adequate dispersion of the nano-carbon reinforcement material, and (2) strong enough interfacial bonding between the nano-carbon reinforcement elements and the composite matrix. In addition to making modified MWNTs such as branched-MWNTs, the Action will explore other possibilities of strengthening composites by integrating FLG (using existing as well as unpublished methods); theoretical modelling of these nano-carbons and composites; due consideration and evaluation of the Health, Safety and Environmental implications; making and testing composites e.g. mechanical and electrical/thermal, HRTEM of interphases, voltage-contrast SEM of percolation networks, sensing and photocatalytic properties; development of new composite materials with Electronic and Multi-Functional properties. This Action will provide an ideal platform, especially via STSM exchanges, for permanent established researchers, post-doctoral workers and ECIs to enhance their research-related skills as well as their innovation and enterprise skills in this international network involving both academic and business enterprises.

Areas of Expertise Relevant for the Action	Keywords
● Materials engineering: Characterization methods of materials for material engineering applications ● Chemical sciences: Characterization methods of materials (theoretical aspects) ● Nano-technology: Nano-materials and nano-structures ● Mechanical engineering: Sustainable engineering ● Materials engineering: Structural properties of materials	● Multi-Functional materials ● Nano-carbon composite materials ● High-Performance Materials ● Atom-Economy

Specific Objectives

To achieve the main objective described in this MoU, the following specific objectives shall be accomplished:

Research Coordination

● 1. Low-cost manufacturing process to make sufficient quantities of the nano-carbons in order to bring high-performance materials to the marketplace. Implementation will include 3D Printing using NRCM-Composites designed by the Action.

● 2. Better understanding of stress, charge and heat transfer at the nano-carbon-matrix interface such that the development of applications can be targeted via coordinated modelling and experiments.

● 3. Chemical derivatisation of nanocarbon materials including Carbon Nanotubes (CNTs) and Few Layer Graphene (FLG) in order to control electrical conductivity and optical properties of the composite materials.

● 4. Exploration of alternatives to nanocarbon-polymer composites such as inorganic and/or ceramic composites by improving the understanding and control of surface/interfaces.

● 5. Production of multifunctional nanocarbon-composites and hybrid-composites for targeted applications.

Capacity Building

● 1. Develop national task forces of stake-holders.
● 2. Establish a network to share know-how and technology in order to produce lighter, stronger materials.
● 3. Draw-up a nanocarbon/composite type based characterization protocol.
● 4. Start a hub-and-spoke strategy for training and dissemination.
● 5. Make lighter, stronger, stiffer and tougher materials using nano-carbon/composites.
● 6. Evaluate the physical and technological properties of the composite materials.
● 7. Develop and refine the methods to evaluate the dispersion and interfacial bonding of the Nanoscale Reinforcing Component Materials (NRCMs) in the composite matrix.
● 8. Identify areas of multiple functionalities such as usage in Solar Cell, Li-ion batteries, sensors and thermoelectric harvester linked supercapacitors.

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DESCRIPTION OF THE COST ACTION

1. S&T EXCELLENCE

1.1. Challenge

1.1.1. Description of the Challenge (Main Aim)

The demand for carbon-composite materials has doubled in the last five years and is predicted to rise by the same amount by 2020. The four main sectors driving the growth of polymer composites have been automotive, aeronautic, construction and wind energy. All these sectors are looking to improve fuel efficiency and so the demand for high-strength lightweight materials is increasing.

MultiComp is a COST Action designed to bring together theorists, experimentalists, technologists and industrialists in the field of nanocarbon materials technology. Lighter, stronger materials are needed for a variety of applications such as transport, energy storage/conversion and bone/tooth replacement. However, a major limitation on the application of the unique properties of nanocarbon materials has been their high cost and lack of availability. In the early 1990s theoretical and experimental investigations of the pull-out of synthetic fibres with branched structures found that the strength and fracture toughness of a composite reinforced by this type of fibre were greater than that of composites reinforced with plain fibres. Historically, an early technological example of this was the use of branched plant fibres (straw) in mud to make stronger bricks. Since their discovery much work has been done on Single-Walled Carbon Nanotubes (SWNTs), Double- Walled Carbon Nanotubes (DWNTs) and Multi-Walled Carbon Nanotubes (MWNTs) as reinforcement for composites with reasonable success and commercial applications include sports equipment and car panels. Some work has also been done on branched CNTs with a view to electronic and materials technology applications. However, the methods used so far, such as using alumina as templates or pyrolysis of metallocenes, or by nanowelding of overlapping isolated nanotubes using high intensity electron beams, are complicated processes. So far Graphene Oxide (GO) has been mainly used to make composites, rather than Few-Layer Graphene (FLG) which is potentially stronger as it is less defective. Toxicological and environmental studies of the nano-carbon materials and composites with respect to possible health hazards will be carried out. Public acceptance of nanomaterials and nanotechnology will be encouraged by publicity and poling. Training, workshops and conferences will be held, and to promote technology transfer from universities and research institutes to companies. The proposed network brings together the expertise of academic and industrial groups to address the idea of incorporating nano-carbon materials into composite materials using simple processes.

Although there has been a large amount of research into property improvements of nanocomposite materials by universities, research institutions and industry this relatively new area of materials science and technology is still in the development stage with great potential for future growth. In order to realize this potential in Europe, there is a need for World Class research and intense networking to form a critical mass of expertise. The COST Action will link groups with knowledge of synthesis and characterisation of Nanoscale Reinforcing Component Materials (NRCMs) with groups that have experience of fabrication of composites (such as polymers and ceramics) and their characterisation. This will make a considerable contribution to the coordination of interdisciplinary research efforts across Europe which is required in order to facilitate the fast exchange of information between different areas of expertise and application.

1.1.2. Relevance and timeliness

COST offers by far the most appropriate framework for this Action, as it aims to bring together the existing expertise from different national initiatives in the larger EU-region to study the potential of NRCMs for new and multi-functional materials. The Action will most importantly provide a platform to combine existing knowledge and to identify common issues and problems in order to develop new lighter, stronger materials. The Action will lay the foundation for future collaborations and enable interested teams to go forward to apply for joint research projects under the scope of Horizon 2020. The Action will also seek to maximise participation in International Cooperation programmes – in particular the various Bilateral Agreements which exist between some of the Action's Countries.

1.2. Specific Objectives

1.2.1. Research Coordination Objectives

The proposed network initially brings together the expertise of 37 groups to address the idea of incorporating nanocarbon materials into composite materials using simple processes. Without the proposed cooperation this cannot be achieved. Therefore, this initial group will attract additional European research groups to fully explore the potential of nanocarbon composite materials in a wide variety of engineering and technological areas.

Recognised goals which this Action will address in this area are:-

1. Low-cost manufacturing process to make sufficient quantities of the nano-carbons in order to bring high-performance materials to the marketplace;

2. Better understanding of stress, charge and heat transfer at the nano-carbon-matrix interface such that the development of applications can be targeted via coordinated modelling and experiments;

3. Chemical derivatisation of nanocarbon materials including CNTs and FLG in order to control electrical conductivity and optical properties of the composite materials;

4. Exploration of alternatives to nanocarbon-polymer composites such as inorganic and/or ceramic composites by improving the understanding and control of surface/interfaces.

5. Production of multifunctional nanocarbon-composites and hybrid-composites for targeted applications.

1.2.2. Capacity-building Objectives

MultiComp will be built upon an integrated experimental and theoretical approach aimed at the understanding of the chemical and physical properties of nanocarbon-composites. This will open up new exciting opportunities of growth for SMEs and "spin-offs". The complexity of this effort requires a multi-technique effort: development of novel and integrated approaches for synthesis, manipulation, characterisation and engineering of nanocarbon-multifunctional composites that will promote and implement new perspectives for science and technology. The Action will link together European scientists with critical expertise in the fabrication and characterization of nanocarbon composite materials. During the Action, the fundamental science and technology of these materials will be studied in detail and suitable theoretical models will be developed. This cumulative effort will help to improve basic understanding and also control the properties of the multifunctional composites. At the beginning, MultiComp has the potential to address several economic and scientific needs and by the end of the Action this potential will be assessed. It is envisaged that it

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will be able to provide European researchers reliably with the know-how to fabricate and test nano-carbon composites tailored to specific applications:-

1. Develop national task forces of stake-holders.

2. Establish a network to share know-how and technology in order to produce lighter, stronger materials.

3. Draw-up a nanocarbon/composite type based characterization protocol.

4. Start a hub-and-spoke strategy for training and dissemination.

5. Make lighter, stronger, stiffer and tougher materials using nano-carbon/composites.

6. Evaluate the physical and technological properties of the composite materials.

7. Develop and refine the methods to evaluate the dispersion and interfacial bonding of the nanocarbons in the composite matrix.

8. Identify areas of multiple functionalities such as usage in Solar Cell, Li-ion batteries, sensors and thermoelectric harvester linked supercapacitors.

1.3. Progress beyond the state-of-the-art and Innovation Potential

1.3.1. Description of the state-of-the-art

Since the discovery of fullerenes nearly thirty years ago, there has been increasing research into the area of nano-carbon materials boosted first by the discovery of carbon nanotubes and more recently graphene. The unique mechanical properties of carbon nanotubes, as well as their low density and enormous aspect ratio (and hence surface area) make them an ideal candidate to act as reinforcement for polymer composites. Their electrical and thermal conductivity makes them further attractive for conductive polymer applications. The preference of single over multiwalled CNTs as reinforcement for polymer composite applications is still somewhat controversial. It has been proposed that only the outermost layer of multiwalled CNTs is loaded during tensile loading, since the relatively weak (van der Waals) bonding between the concentric layers causes slippage of the inner layers, reducing its load bearing capacity. This slippage, however, seems to provide an extraordinary elastic deformation capability to the multiwalled CNTs when loaded in compression. In addition to being more demanding and expensive to synthesize, single-walled CNTs are more prone to form bundles, which may hinder their superior mechanical performance with respect to the multiwalled ones. In general, two main issues are widely recognized as being critical for the development of mechanically efficient nanocomposites:

(1) Adequate dispersion of the nano-reinforcement filler within the matrix, and

(2) Strong interfacial bonding between the reinforcement element and matrix.

1.3.2. Progress beyond the state-of-the-art

These problems can be addressed by utilizing branched-MWNTs and also FLG as it is known (from theory and simulation experiments) that branched fibres greatly enhance interfacial bonding. The key innovation of this Action is the development and exploration of new nanocarbon composite utilizing the properties of branched-MWNTS and also the properties of few-layer graphene (FLG) by:-

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1. The establishment of better means to disperse the nanocarbon filler materials. As the property of the whole matrix is crucially dependent on good dispersion to maximise reinforced surface area which affects the neighbouring materials and therefore, the properties of the entire matrix.
2. Combined theory and experiments aimed at the realization of properties/materials by design. Multifunctional materials based on nanocarbon composites are expected to have big impacts in various fields of technology - two examples are the automotive and aircraft industries where energy costs can be reduced both in manufacture and operation. The Action can achieve this goal by bringing together scientists from different research fields and representatives from various innovative technology sectors.

1.3.3. Innovation in tackling the challenge

MultiComp will be built upon an integrated experimental and theoretical approach aimed at the understanding of the chemical and physical properties of nanocarbon composites. This will open up new exciting opportunities of growth for SMEs and "spin-offs". The complexity of this effort requires a multi-technique effort: development of novel and integrated approaches for synthesis, manipulation, characterisation and engineering of nanocarbon-multifunctional composites that will promote and implement new perspectives for science and technology. The Action will link together European scientists with critical expertise in the fabrication and characterization of nanocarbon composite materials. During the Action, the fundamental science and technology of these materials will be studied in detail and suitable theoretical models will be developed. This cumulative effort will help to improve basic understanding and also control the properties of the multi-functional composites. MultiComp has the potential to address several economic and scientific needs and by the end of the Action this potential will be assessed. It is envisaged that it will be able to provide European researchers reliably with the know-how to fabricate and test nanocarbon-composites tailored to specific applications.

Description of the MultiComp tasks tackling the challenge:

Task 1: Dissemination of knowledge and practical skills for making and characterizing branched-MWNTs/composite materials.

Task 2: Development of robust methodology to make modified-MWNTs and FLG.

Task 3: Development of robust methodologies to produce Nano-Composites.

Task 4: Advancing characterisation methodologies through the studies of these systems.

Task 5: Establishment of theory-based explanations of observed properties of the materials.

Task 6: Defining the means to maximise Atom-Economy in the production of the new materials.

1.4. Added value of networking

1.4.1. In relation to the Challenge

MultiComp brings together pre-existing informal specialist networks. Each of these informal networks focuses on areas of interest to MultiComp, which will provide an overarching framework within which they can work together towards development of new understanding and applications of nanocarbon composites. The national and European research projects currently underway deal with the development of well-defined topics. One major task of MultiComp is the coordination and further integration of the achievements of those R&D projects for the generation of a broad knowledge-base for the entire field of nanotechnology. Without this collaboration European research in this field will

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fall behind that in the USA and Asian countries where massive coordinated R&D programmes are currently being deployed.

1.4.2. In relation to existing efforts at European and/or international level

Past and current EU funded work in the area of Carbon Nanotube/Carbon Nanofibre composites include:-

FP7 - Carbon Nano Tube Fibres COMPOSITES – (CNTF COMPOSITES), Project Reference

251477, 2010-2014;

FP7 - Nano-Optical mechanical Systems (NOMS). Theory and modelling of optical actuation in nanocomposites through in-situ electron microscopy studies - NMP 228916, 2009-2012;

FP7 – Nanostructured polymer-matrix composites (POCO). NMP-2007-2.1-1, Grant agreement no. CP-IP 213939-1, 2008-2012;

All are EU funded research which have either ended or will end soon. However, there remains the need to understand why the properties of CNT-composites, like thermal conductivity and mechanical strength, stiffness and toughness remain far lower than the properties of individual CNTs.

MultiComp is complementary to Graphene Flagship's Roadmap on Characterization - "In relation to Spectroscopic characterization roadmap identifies spectroscopy and Raman as interesting methods to investigate on graphene but also identifies its limitations. Further improvement of the above-mentioned optical characterization techniques and development of new approaches are critically important for in-situ monitoring. Outside the visible-range and Infra-Red (IR) optical spectroscopy, detailed studies of defects in graphene can be addressed using scanning transmission electron microscopy (STEM), energy loss spectroscopy (EELS), low-angle X-ray spectroscopy, and resonant inelastic X-ray scattering (RIXS). Since there are several routes towards viable mass production, the suitable energy/wavelength range for the standardized spectroscopic characterization toolkit is not known yet, thus spectroscopic studies of graphene need to be carried out over a broad energy range, from microwaves and far IR to UV and X-ray"

MultiComp is innovative in that the Action aims to model, develop and explore new Nano-Carbon Composites by utilizing the properties of branched-MWNTS and also the properties of Few-layer Graphene (FLG). The COST Action will link groups with knowledge of theory, synthesis and characterization of Nanoscale Reinforcing Component Materials (NRCMs) with groups that have experience of fabrication of composites (such as polymers and ceramics). This will make a considerable contribution to the coordination of interdisciplinary research efforts across Europe which is required in order to facilitate the fast exchange of information between different areas of expertise and application.

2. IMPACT

2.1. Expected Impact

2.1.1. Short-term and long-term scientific, technological, and/or socioeconomic impacts

Some 70% of all technical innovations hinge directly or indirectly on the properties of the materials they use. Materials innovation can be used in practically all technology sectors and branches of industry. Materials innovation has the potential to reduce environmental pollution, save energy, conserve resources, and generally improve the quality of our life.

The major scientific impacts are the increased understanding of the interfacial interplay of modified-MWNTS and FLG reinforcements with the matrix. The main societal impacts reside in the prospect of producing lighter, stronger materials for transport (automotive, aeronautics) plus potential applications in as sensors and in energy conversion including wind-turbine blades, Solar Energy, Li-Ion Batteries. In nano-carbon networks the junction resistance is the dominant limiting factor. However, FLG and/or a network of branched CNTs will significantly reduce network resistance. Therefore, in addition to the composite applications, the electrical properties of networks made of nano-carbons would have major benefits to Solar Cell and Li-Ion battery design, development and production as well as sensors and as photocatalysts.
This Action will provide an ideal platform for permanent established researchers, post-doctoral workers and ECIs to enhance their research-related skills as well as their innovation and enterprise skills in this international network involving both academic and business enterprises.

2.2. Measures to Maximise Impact

2.2.1. Plan for involving the most relevant stakeholders

The establishment of a MultiComp network for NanoCarbon Composites will produce significant benefits to the participating countries as representatives from the most relevant stakeholders are involved such as Industrial Groups, European Platforms, Lobbies etc. Specific plans include:-

1. Dissemination by holding Technology Transfer Workshops to Clusters representing SMEs in relevant Stakeholder Groups e.g. Plastipolis in France:

2. Establish links to European Technology Platforms e.g. Nanofutures, EUMat;

3. Strengthen collaborative links with the European Virtual Institute on Knowledge-Based Multifunctional Materials (KMM-VIN AISBL);

4. Provide Press Releases on Major Advances – also aimed at the Newsletters of Clusters, Platforms and Associations with relevant Stakeholders.

2.2.2. Dissemination and/or Exploitation Plan

1. Establishment of a MultiComp network

2. Dissemination of knowledge and practical skills for making and characterizing branched-MWNTs/composite materials.

3. Dissemination of results via STSM (all WGs); Publications; Summer Schools, and Presentations at International Meetings.

4. Development of robust methodology to make modified-MWNTs and FLG.

5. Development of robust methodologies to produce Nano-Composites.

6. Advancing characterization methodologies through the studies of these systems.

7. Establishment of theory-based explanations of observed properties of the materials.

8. Defining the means to maximize Atom-Economy in the production of the new materials.

2.3. Potential for Innovation versus Risk Level

2.3.1. Potential for scientific, technological and/or socioeconomic innovation breakthroughs

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There are still two main problems facing MWNT/composite materials:-

(1) adequate dispersion of the nanotube-reinforcement material filler within the composite matrix, and
(2) strong enough interfacial bonding between the nanotube-reinforcement elements and the composite matrix.

The MultiComp network aims to find solutions to these problems. In addition to modifying MWNTs the Action will explore other possibilities of strengthening composites by integrating FLG (using existing as well as unpublished processes) or even find novel scaffolds through combinations of MWNTs and graphene. This will be explored via theoretical modelling of these nano-carbons and composites, making and testing composites (mechanical and electrical/thermal), characterization (e.g. HRTEM of junctions, SEM of percolation networks) and testing properties such as photocatalysis and sensing in the actions outline below:-

1. Develop simple methods to make nanocarbons using inexpensive materials.

2. Develop suitable theoretical models to analyse the properties of nano-carbons as well as their inclusion in the composite matrix. This will necessitate a multi-dimensional and multi-scale approach ranging from molecular dynamics simulations to ab initio calculations.

3. Develop new methods and processes to make nanocarbon composite materials.

4. Develop effective methods to test nanocarbon composite materials such as methodologies based on indirect but bulk characterization e.g. phase behaviour that reflect the aspect ratio of the particles, rheology, light scattering, etc., as well as direct methods such as TEM and Voltage- Contrast SEM (VC-SEM) of Percolation Networks to assess the reproducibility of different synthetic routes and about different varieties of nanocarbon composite materials. Atomic models based on experimental data can then be used in theoretical investigations in order to make assessments and predictions about mechanical strength and conductivity of nanocarbons.

5. Evaluate the possibilities for Solar Cells, Li-Ion Battery, Sensor, Photocatalysts, thermoelectric harvesters and supercapacitors.

6. Explore the possibilities for recycling the composite materials to achieve maximum Atom-Economy.

3. IMPLEMENTATION

3.1. Description of the Work Plan

3.1.1. Description of Working Groups

The work plan is organized in five complementary working groups, each devoted to a progressive development of synthesis, characterization, integration and modelling aspects, dissemination and communication:

WG1: Synthesis and Fabrication

WG2: Theory and Modelling

WG3: Characterization, Health, Safety and Environment (HSE)

WG4: Engineering and Technological Applications

WG5: Outreach and Dissemination

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WG1: Synthesis and Fabrication

Synthesis of branched-MWNT materials and few layer graphene (FLG) materials – these materials will be the nanoscale reinforcing component (NSCRs). This will provide large amounts of starting material for producing composites.

Design of composites with polymers, ceramics and other matrix materials and the nano-scale reinforcing components (NSRCs)

Introduction of branched-MWNTs and FLG into various polymers, commercial as well as research grade, either via dispersion directly in the polymer or via pre-dispersion will be investigated. Liquid crystal polymers and polymerisable low-molar mass liquid crystals will be also studied as possible hosts. Samples for further characterization will be prepared by different fabrication technologies, such as e.g. electrospinning, fibre spinning, vapour deposition, and in-situ injection moulding.

Various methods for thin film deposition (spin coating, dip coating, etc.) of the nanocarbon composite material will be investigated. Nanostructured films suitable for glass and flexible substrates will be prepared by various chemical methods in order to be incorporated as e.g. the transparent conducting electrode in organic optoelectronic devices. Particular attention will be paid to the correlation of the theoretical and real performance of the films in comparison with the commercial available indium tin oxide (ITO) films in terms of sheet conductivity and optical transparency.

Furthermore, the nanostructures will be dispersed in highly conductive thiophene derivates, such as PEDOT/PSS and evaluated. Different methods for FLG alignment within the polymer network will be examined: flow alignment, unidirectional mechanical and/or thermal treatment, application of external electric/magnetic field, photo-polymerisation with linearly polarized light (LPP), use of liquid crystalline polymers, etc. Lyotropic liquid crystalline suspensions will be prepared from the TMCH particles, similar to those which have been made using well-dispersed MWNTs at high concentration, and which can be further processed into fibres with excellent mechanical properties due to the spontaneous alignment of the nanotubes.

Deliverables: Short Term Scientific Missions (STSM) of scientists active in WG1 to groups active in WG3 will be stimulated to exchange knowledge on material preparation and manipulation procedures and to establish valuable interlinks between chemists, physicists and material scientists. Mapping of competences in the Synthesis and Fabrication of Nanoscale Reinforcing Components (NSCRs). Samples of NSCRs will be produced and supplied to WG3 for Characterization and Health, Safety and Environmental assessment. The NSCRs will also be supplied to WG4 for prototyping in Engineering and Technological applications. Joint publications – Technical Report on the synthesis and characterization of NSCRs; Introduction of the NSCR in Different Types of Composites.

WG2: Theory and Modelling

Development of basic theoretical models: Existing theoretical frameworks for MWNT-polymer composites will be taken as starting point and optimised and/or modified for the case of NSRCs-polymer composites, for instance with respect to the guest-host interaction strength in these composites, and for identifying the optimum usages of composites containing branched-MWNTs and FLG, respectively. Mechanical properties of the composites will be analysed in the frame of micromechanics (composite-) models and percolation models. Temperature, nanocarbon type and nanocarbon volume fraction and orientation order will be used as control parameters.

Modelling of structure-property relationships: Charge transport, heat transport and optical properties will be investigated in these essentially one-dimensional systems, including linear and nonlinear

effects. In connection with the question of nonlinear effects and transport properties, the possible existence of solitonic solutions will be examined. Finally, the effect of the reduced dimensionality will be investigated.

Development of new modelling tools: New approaches in implementing localised basis set DFT using novel basis set contraction approaches, alternative functionals, as well as cross-over with multi-scale modelling approaches such as DFTB and embedding will be explored with the aim of producing a rapid code whose speed scales linearly with the number of atoms. New functionality will be added to the existing code (e.g. incorporation of dispersion forces) making it better adapted to the modelling of nanoscale interfaces. In parallel with this, improved transport codes based on non-equilibrium Green's functions (NEGF) will be developed, both for effective modelling of transport properties in realistic nanomaterials (e.g. with defects, substrates, gates and/or contacts), as well as for complete STS simulations of nano-interfaces. Given the range of theoretical experience represented within Multi-Branch, there is scope for exchange of best practise, shared development of new functionality that may be useable in different codes, as well as benchmarking and 'round robin' testing of new methods using real-world test systems from the more applications- geared theoretical groups.

Deliverables: Short Term Scientific Missions (STSM) of scientists active in WG2 to groups' active in WG3 will be arranged within the Action to correlate various theoretical models with most important experimental problems and findings. Mapping of competences and advances in Theory and Modelling of NSCR-Composites. Assessment and refinement of Theory and Models in the light of prototypical results from WG3 and WG4. Carrying out common experiments which lead to joint publications.

WG3: Characterization, Health, Safety and Environment (HSE)
Structural characterization of the composites: To study the NSRCs and matrix interphase leading edge electron microscopy techniques, such as high resolution electron microscopy (HRTEM) and scanning transmission electron microscopy (STEM) will be used together with conventional techniques (TEM, AFM, etc.). These techniques will be applied also to determine the microstructure of the formed NSRCs within the composite, their dispersion in polymer matrix and interface properties between the NSRCs and polymer. Composites will be analysed by X-ray (SAXS) and neutron scattering techniques at various conditions, like temperature (cryogenic facilities), applied external electric field or stress, etc. This will provide information on volume fraction, spatial arrangement and alignment of the nanotubes in the polymer matrix. Structural properties of the composite and its alignment and anisotropy will be studied by spatially-resolved micro-Raman spectroscopy. Electron paramagnetic resonance spectroscopy (EPR) will be used to characterize radical polymerisation reaction in composites in combination with in-situ optical excitation of photo-induced polymerisation. Advanced methods, such as High Angle Annular Dark Field (HAADF) imaging and TEM imaging methods in combination with Energy Loss Spectroscopy (EELS) will be used to determine the position of dopant atoms, bonding configurations and elucidate their effect on the properties of nanocarbon composite materials.

Characterization of mechanical properties: Universal testing machine (UTM - determination of Young's and shear modulus, tensile strength, etc.), dynamical mechanical analysis (DMA) and rheometry will be used to resolve stress-strain properties and to allocate the linear and nonlinear regimes in the mechanical response of the composites. Measurements with different directions of applied force will be performed to resolve possible elastic anisotropies of the material. Time dependent stress/strain analysis will be performed to study possible non-recovery phenomena. Time resolved optical techniques with sub-picosecond resolution (e.g. optical Kerr effect) will be used to investigate fast local vibrations and slow structural dynamic processes.

Characterization of thermal properties: Temperature dependence of structural and physical properties will be studied. Various phase transitions will be determined via differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA) measurements, with particular interest in glass transition temperatures (Tg). The value of Tg is essential for the selection of materials for various applications. The effect of degree of crosslinking/ branching of the polymer on glass transition temperature will be studied. Thermal conductivity and thermal diffusivity will be measured. Time-resolved techniques (e.g. impulsive transient grating experiments) will be used to investigate acoustic/elastic properties, structural rearrangement and thermal diffusion phenomena in relation with the local nanostructure of the material.

Characterization of electrical properties: Electrical (I-V) measurements will be routinely used to investigate the evolution of a percolation network of the NSRCs within the composites as their concentration increases. Chemical analysis at the nanoscale will be carried out using STEM to explore the change in electronic properties and variation in bonding due to chemical treatment of the NSRCs. Dielectric spectroscopy will be used to determine AC current properties depending on temperature, frequency and composition. Tensoresistance will also be investigated and field emission properties will be tested. In view of applications in solar cells the composites will be sandwiched between a metal anode and a transparent ITO (Indium-Tin Oxide) cathode on glass. The associated measurements will cover: complete characterization of the solutions from which the active layer is formed, the study of the homogeneity of the photoactive composite layer (morphological and opto-electronic properties); the precise determination of the photovoltaic parameters in correlation with the open environment conditions; and the exploration of efficient sealing materials and techniques.

Characterization of optical properties: Conventional optical analysis (refractive index, birefringence, optical absorption measurements) and optical spectroscopy (Raman, IR, UV-VIS, ellipsometry, fluorescence, etc.) will be used to resolve optical properties of the nanocarbon composites. Optical holographic techniques will be employed in view of possible applications of the FLG composites in optical information processing and also for characterization of the alignment-induced local anisotropy. Electro-optic, elasto-optic and/or nonlinear optical properties will be investigated, such as frequency conversion and waveguide characterization. Hyper-Rayleigh and hyper-Raman scattering will be used for nonlinear optical (NLO) characterization. Charge transport in relation with photoluminescence will also be investigated. Nonlinear refractive index of the composites will be analysed in view of all-optical switching applications. Various studies on possible photonic applications of the composites in large-scale-integrated photonic devices will be made.

Health and Environmental Impacts: Graphene and graphene oxide (GO) are being developed for a wide variety of applications are in active development including both bulk applications, and those implying biological or environmental contact, such as drug delivery, biosensing, or water purification. Therefore, graphene/ GO, as potential hazards must be assessed, before their production and use is spread more widely. A combination of aberration corrected electron microscopy, analytical TEM and confocal microscopy techniques will be used to visualise the distribution of graphene flakes inside lung cells. Toxic endpoints and the permeability of the cells will be identified in the presence and absence of graphene/ GO flakes. The effects of graphene and GO on compression resistance of pulmonary surfactant will be quantified by examining changes in the isothermal behaviour of the monolayers after addition of nanoparticles using the Langmuir – Blodgett trough (LT). The effect of graphene on the domain structure of the monolayers will be monitored using atomic force microscopy. LT experiments will be used to select specific graphene samples for further study in contact with alveolar epithelial and macrophage cells. The influence of surface derivatisation, diameter and layer number on toxic endpoints and cellular uptake will be investigated.

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Deliverables: Short Term Scientific Missions (STSM) of scientists active in WG3 to other WGs will be stimulated within the Action to broaden and deepen the knowledge of especially ECIs with their origin from different scientific disciplines. Mapping of competences in Characterization, Health, Safety and Environmental techniques and procedures. Joint publications. Technical report on "The Public Perception of Nanotechnology Risks compared to Scientifically Validated Findings".

WG4: Engineering and Technological Applications
New nano-carbon composites: These will be developed with tailored material properties leading to improved thermal conductivity for thermal management (e.g. for heat dissipation for computer chips), improved electrical conductivity (e.g. for the use as electromagnetic-interference shielding and electrostatic dissipation), improved mechanical properties (e.g. for applications as wear protection), and improved linear and non-linear optical properties (e.g. for optical communication networks) and strong exciton dissociation at the bulk heterojunctions (organic solar cells), as well as new promising materials for large area flexible multifunctional sensors that could be integrated into the material and can be used for multiple location sensing. An example of practical motivation is for instance to consider the use of smart sensors in-situ ability to detect symptoms of potentially catastrophic events of vehicles in real time (such as over-heating of aircraft Li-Ion battery systems).

Deliverables: Short Term Scientific Missions (STSM). Testing these new composite materials in cooperation with partners from the Higher Education & Associated Organisations; Business Enterprise; Government/Intergovernmental Organisations, and Non-Governmental Organizations (NGOs) involved in this COST Action. Mapping of competences in the application of Engineering and Technology to NSCR-Composite materials. Prototyping of test-objects fabricated from NSCR-Composites – 3D printing using NSCR-composite feedstock test materials.

WG5: Outreach and Dissemination
This WG is in charge of internal and external public relations. It is responsible for developing and maintaining the web page of the action, the collection of information from the scientific WGs in order to produce dissemination material. It will present the network as a whole at international conferences (e.g. World Cancer Congress), organise public talks and establish contacts with hospitals to win over new community members, international experts and stakeholders (e.g. industry, European Society for Composite Materials, European Materials Research Society, and Horizon 2020 expert group on Nanotechnologies, Advanced Materials, Advanced Manufacturing & Processing and Technology).

Deliverables: WG5 will obtain a report from each Action event and will stay in contact with the scientific WG leaders (e.g. via the bi-monthly Core Group (CG) e-conferences, joint WG meetings) to ensure the correct public dissemination of scientific progress via Press Releases on Major Advances. WG5 will give general feedback (electronically) to the scientific WGs. Seek out new conference participation, International Funding opportunities e.g. HORIZON 2020 Open Calls, Bilateral Agreements between Countries etc. Establishment of a MultiComp Web-Site. Dissemination meetings.

Milestones:

Year 1

- 1st Quarter: 1st MC Meeting; MC set up; Work Plan is established.
- 3rd Quarter: WG meetings; Scientific Strategic meeting; Call for MultiComp Training Schools.
- 4th Quarter: MC meeting; Workshop/Topical meeting.

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Year 2

• 1st Quarter: MC meeting; Workshop/Topical meeting; Meeting/Discussion to identify the best dissemination activities.

• 3rd Quarter: WG meetings; WG Chair meeting to review the MultiComp scientific strategies.

• 4th Quarter: MC meeting; MultiComp Training School; Interim report containing summary and ideas from the workshops.

Year 3

• 1st Quarter: MC meeting; Workshop/Topical meeting.

• 3rd Quarter: WG meetings; Scientific Strategic meeting.

• 4th Quarter: MC meeting; MultiComp Training School.

Year 4

• 1st Quarter: MC meeting; Scientific Strategic meeting.

• 3rd Quarter: WG meetings; MultiComp International Conference.

• 4th Quarter: MC meeting; Final Report.

Deliverables

The Action will proceed over four years. Below is given a timetable for deliverables. Due to the nature of the COST framework of collaboration, the specific topics of work may be shifted with time in order to adjust to specific needs identified by the Action.

The first period of six month is devoted to building the WGs in line with the topics outlined earlier. The MC will ensure that the work is well focussed, that fruitful collaborations between the participants are either initiated or developed and that synergy is created between the WGs.

The MC will organise 4 Action workshops covering all research activities involved, one start-up meeting, one midterm review during the Action and one final meeting before drafting the final report. The MC will be proactive in also organising joint seminars - preferably across the WG borders- where and when relevant.

The main tasks of the Start-up meeting include finalising details of the WGs R&D focus and finalizing the timetable of the Action. The following events/activities (deliverables) will take place:-

1. 1st MC Meeting to finalize Work Plan: beginning of Year 1.

2. MultiComp web-site operational: second quarter of Year 1.

3. Formation of the WGs: first half of Year 1.

4. WGs Meetings: one meeting in the middle of each year, Year 1 - Year 4.

5. MC Meetings: one meeting in Year 1, two meetings in Year 2, two meetings in Year 3, two in Year 4.

6. Topical meetings and workshops: one meeting in the second half of each year, Year 1 - Year 4.

7. Training school for young researchers: end of Year 3.

8. Scientific exchange programme: at all times during the course of the Action.

9. Information exchange: at all times during the course of the Action.

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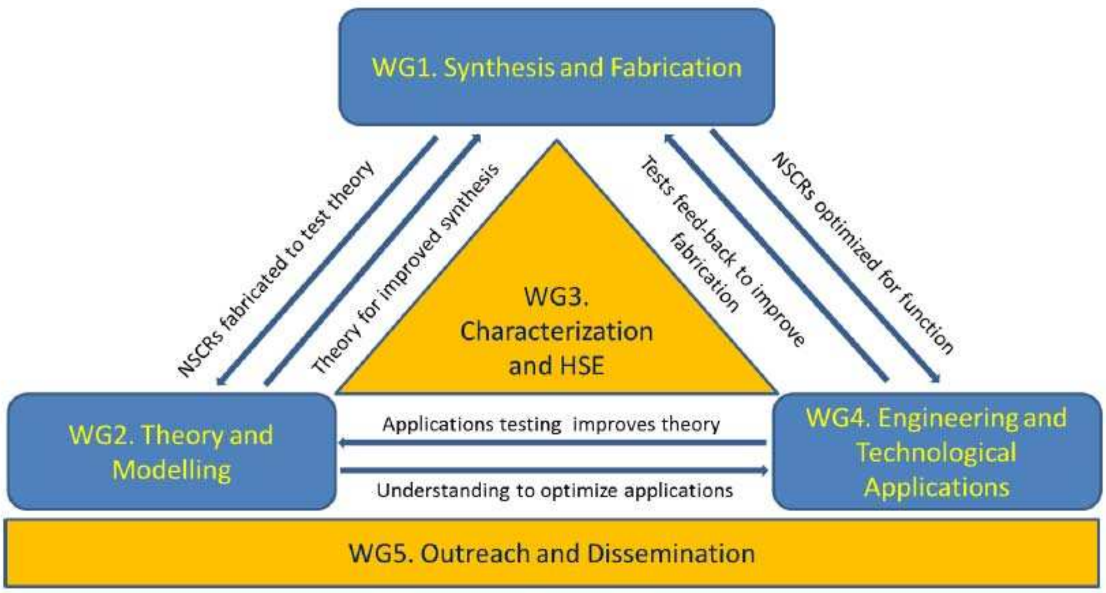
10. Reports: end of each year, Year 1 – Year 4; Mid-term evaluation: end of Year 2.
11. Final Evaluation and Report: End of Year 4
12. End of the Action: International Conference towards the end of Year 4.

3.1.2. GANTT Diagram

	Year 1				Year 2				Year 3				Year 4			
Activity	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
MC Meetings	KO		X		X		X		X			X	X			X
WGs (1-5) Meetings	X		X		X		X		X		X				X	
Workshops	X		X		X		X		X		X	X				
Conferences							X		X						X	
Training Schools					X						X					
CG e-Meetings	X	X	X X	X	X	X X	X	X X	X	X	X X	X	X	X	X	X
STSMs																
Web-site Update																
Reports - All WGs				X				X				X				X

x = Meeting; Vertical column with same colour indicates simultaneous Activity, and Horizontal row with same colour indicates continuous Activity.

3.1.3. PERT



3.1.4. Risk and Contingency Plans

Provisions for the inclusion of new participants and unforeseen activities: The tasks listed above are flexible and liable to alterations should new participants and unforeseen activities become available during the implementation.

The COST Action is flexible enough to incorporate a variety of projects ranging from fundamental research on materials properties and innovative characterization methods up to processing and specific applications of nano-carbon composites. All the projects carried out by the participating scientists and laboratories will be driven by the need to fulfil the primary objective of the COST Action to transfer the obtained scientific results into application and support their exploitation by European SMEs by overcoming the present technological barriers identified as secondary objectives in section C. This approach is securely based on the extensive knowledge already available at the participating laboratories which has been created by national and European wide projects of the past or by projects which are still underway. It will be the scientific focus of the COST Action to concentrate the joint efforts on those scientific and technical items which are identified barriers for successful applications in industry preferentially in SMEs. The open character of COST Actions is considered as particularly appropriate for the rapidly evolving field addressed here.

3.2. Management structures and procedures

The MC, chaired by the MultiComp Chair and Vice-Chair, will steer and oversee the activities, and ensure that the milestones are accomplished so that the Action is correctly implemented according to COST rules. The number of MC members is likely to increase during the course of the Action so, a Core group (CG) will be established. During the 1st MC Meeting, CG members, WG leaders, the MC Chair and MC-Vice Chair will be elected by the MC. Moreover, it will be debated about the distribution of financial means, the potential adaption of the Action strategy, WG composition and work plans to ensure successful networking. Certain administrative duties will be delegated to individual MC members, such as the coordination of gender-balance, STSM and training coordination as well as the involvement of Early Career Investigators (ECIs). Chair and Vice Chair will report to the COST Association on the Action’s progress and the financial issues, after approval by the MC. The annual MC meetings are dedicated to review the Action strategy, to approve internal and external reports and to vote about upon suggestions of the CG for new members possibly also from International Partner and Near Neighbour Countries and the assessment of financial means.

The CG, which includes all WG leaders and the persons responsible for STSM managing, ESR participation and gender policy, will review the WG composition and, emphasising hereby that scientists of different background are present in each WG, that there are enough Early Career Investigators and that the gender policy is respected. It will further propose to the MC new Action members, MC observers and external experts to be invited for the Training Schools / Action Workshops, will control the compliance of the work plan according to the milestones and deliverables foreseen, will report yearly to the MC on the achieved activities and will make recommendations to the MC about future visions of this COST Action. The CG will discuss via email ca. every two months about administrative tasks and the scientific progress. The latter shall guarantee inter alia the strong exchange of unpublished aspects of knowledge. The CG also will set up the agenda for joint WG workshops and STSMs, the latter in coordination with a STSM manager. The CG will report regularly on their bi-monthly email “meetings” to both the Chair and the Vice Chair.
The project is best carried out within the COST framework as the research in the fields required for this Action is being carried out in and financed by the proposed participants. However, the cooperative opportunities provided by COST are essential to maximize the results of this funded research, and to avoid duplication of results. The initial consortium combines all the necessary expertise to engage in this network but further partners with complementary skills are anticipated to join.

Due to beneficial importance of the collaboration between experienced researchers and Early Career Investigators (ECIs), MultiComp will promote this collaboration by placing both at the same management levels. Each WG will include a number of ECIs from the participating countries. ECIs will be especially encouraged and given the opportunity to contribute to all management levels of the Action, and present their views and results during meetings and will be given the opportunity to extend their knowledge through training schools and short-term scientific missions.

3.3. Network as a whole

The initial consortium comprises of 37 groups who expressed an interest to join this COST Action (includes 20% Business enterprise) from 16 COST countries – 25% of which are COST Inclusiveness target countries, 1 COST Cooperating State and 3 International Partner Countries (IPCs) and 1 International Organization. The initial network has 37% female partners - with the aim of 50%. There are currently 3 Early Career Investigators but this number will increase once the Action is launched. The Action is committed to respect an appropriate gender balance, with both men and women having equal opportunities in all the activities (including management, spreading excellence, research, networking and scientific integration).

The initial consortium has the critical mass, expertise and geographical distribution needed for addressing the challenge and objectives. However, it is envisaged that further groups will join the COST Action once it is in place.

The IPC institutions in the proposal all welcome collaboration possibilities and will do all that they can to support the Action. The mutual benefits deriving from their participation stem from: -
a) Advanced Electron Microscopy and Spectroscopy (HRTEM and EELS) capabilities; b) Specialist knowledge of Applied Polymer Science, especially “New Age Polymers” including light weight composites; c) Specialist knowledge of polymer and supramolecular gel based research; c)
Specialist skills in the understanding of natural phenomena and the translation of concepts from nature into the laboratory (bio-mimicry) to develop new metal complexes and inorganic materials
for a diverse variety of applications that include solar energy conversion, therapeutics and biosensors; d) Specialist skills in synthetic chemistry and chemical functionalization which are
crucial for maximising the technological applicability of nano-carbon materials. A good example is the field of Super-Capacitors (a multi-functional application of nano-carbon composite materials) where chemical functionalization determines the energy storage density of the material

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