European Cooperation in the field of Scientific and Technical Research
- COST -

Brussels, 24 May 2013

COST 007/13

MEMORANDUM OF UNDERSTANDING

Subject :	Memorandum of Understanding for the implementation of a European Concerted Research Action designated as COST Action CM1302: European Network on Smart Inorganic Polymers (SIPs)

Delegations will find attached the Memorandum of Understanding for COST Action CM1302 as approved by the COST Committee of Senior Officials (CSO) at its 187th meeting on 15-16 May 2013.

MEMORANDUM OF UNDERSTANDING
For the implementation of a European Concerted Research Action designated as

COST Action CM1302
"EUROPEAN NETWORK ON SMART INORGANIC POLYMERS" (SIPS)

The Parties to this Memorandum of Understanding, declaring their common intention to participate in the concerted Action referred to above and described in the technical Annex to the Memorandum, have reached the following understanding:

1. The Action will be carried out in accordance with the provisions of document COST 4154/11 “Rules and Procedures for Implementing COST Actions”, or in any new document amending or replacing it, the contents of which the Parties are fully aware of.

2. The main objective of the Action is to focus the research activities on inorganic polymers across Europe and to explore the full potential of inorganic polymers in materials science and technology with emphasis on advanced smart properties and applications.

3. 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 56 million in 2013 prices.

4. The Memorandum of Understanding will take effect on being accepted by at least five Parties.

5. The Memorandum of Understanding will remain in force for a period of 4 years, calculated from the date of the first meeting of the Management Committee, unless the duration of the Action is modified according to the provisions of Chapter IV of the document referred to in Point 1 above.

A. ABSTRACT

This Action on Smart Inorganic Polymers (SIPs) will synergise the European activities in relevant areas in order to establish widely applicable rules for the rational design of smart inorganic polymers. The combination of leading scientists with common motivation but diverse expertise (main group/transition metal chemistry, polymer synthesis, characterisation, processing, applications, and theory) in concert with industrial partners will act as a nucleus for translational efforts towards the design and application of novel inorganic polymers (e.g., polyphosphazenes, polyamino- or phosphinoboranes, polysilanes, metallopolymers, nanoparticle-based hybrids). The network will coordinate and concentrate scattered existing national programmes and informal collaborations, which will be kick-started by including new complementary skills. SIPs will intensify the European exchange of knowledge and technologies and provide a forum for recent developments and innovative aspects. By implementing a sorely missed annual European conference on inorganic polymers, SIPs will increase its visibility in related communities. This will allow the systematic expansion of SIPs by inclusion of additional interested parties with desirable expertise and resources to boost the developments in this area.
Keywords: Inorganic polymers (Si, B, P, metallopolymers); advanced applications (e.g., opto-electronics, flame retardants, energy storage devices, plastics); functional materials; inorganic nanomaterials; advanced catalysts; Smart Inorganic Polymers (SIPs); European Conference on Smart Inorganic Polymers (EuSIP)

B. BACKGROUND

B.1 General background

Environmentally friendly, cost-efficient multifunctional materials are indispensable for modern society. Polymers are one of the major areas of molecular and materials science with uses as plastics, thermosets, elastomers, fibres, films and structural materials. Worldwide, about 250 million tons of polymers are produced per year, with increasing tendency. Applications range from electronics, adhesives, lubricants and structural components for cars, aircrafts, buildings and medical applications to more mundane uses in children’s toys, clothing and food packaging.
So far most commercial polymers are petroleum-based organic materials (polysiloxanes being a notable exception). The production of such polymers has been shifted more and more to Asia, a trend which still continues. Importantly, during the last two decades, polymers with backbone

elements other than carbon are increasingly being applied in high-end technologies where materials with a combination of specific properties are required. The discovery of new synthetic approaches to metallopolymers is in part responsible for these rapid developments. The drastically increased range of available monomeric building blocks in the synthetic toolbox of inorganic chemistry (compared to carbon chemistry) can be expected to allow for fine-tuning of custom-tailored properties. The diverse nature of the chemical requirements mandates the coordination of existing and future single-investigator-driven research projects throughout the European Research Area in order to fully harness the extraordinary electronic properties of novel bonding modes of heavier main group and transition metal elements in novel smart inorganic polymers.

Even now inorganic polymers offer attractive physical properties like low glass-transition temperatures and flexibility over a wide temperature range with no need for plasticizers as in petroleum-based polymers. Moreover, their biodegradability is mostly superior to that of carbon-based polymers and their recyclability is also significantly higher. In the longer term, inorganic polymers could even make a sustainable contribution to the imperative replacement of hydrocarbon/oil-based feedstocks by more abundant sources. Furthermore, the combination of polymers based on two or more different monomeric building blocks in block copolymers is an area of increasing interest. For instance, by merging the advantages of organic and inorganic polymers, the features of both areas can be ideally combined to achieve a new level of quality in polymer chemistry. Strong interaction of experimental with theoretical groups is essential to further develop structure–property relationships in these innovative materials and to improve the design for specific applications. This Action therefore represents more than the simple sum of all benefits: our collaborative efforts will establish a modular set of inorganic monomers with unprecedented electronic, redox, photo-emissive, magnetic, pre-ceramic, self-healing, catalytic and other “smart” properties that can be implemented into polymers as blocks or single units. The compatibility and interplay of monomeric units that stem from various areas of cutting-edge inorganic chemistry will be established. The feedback of the generated structure–property relationships into the improvement and de novo design of complementary monomers will efficiently boost the development in this area. A number of internationally leading European research groups work in this area, although the community is highly fragmented. The traditional boundaries predominantly based on the Periodic Table of the Elements have to be considered obsolete in a more and more function-guided world of chemistry. This Action (Smart Inorganic Polymers) will help overcome these boundaries and guide national efforts towards an efficient and targeted development and investigation of new inorganic polymers. In order to establish widely applicable rules for the rational design of smart inorganic polymers it is mandatory to unify the skills and talents of leading experimental and theoretical groups covering related interdisciplinary areas in chemistry, physics, biochemistry, medicine, materials science and engineering. SIPs will boost these developments by promoting collaborations and continuous exchange of results and ideas on a pan-European level and will thus strengthen the leading position of the European community in the field.

B.2 Current state of knowledge

Research in functional materials science is one of the top priority strategic areas of development in science and technology. Due to the tremendous variability of the backbone, inorganic polymers exhibit a broad spectrum of properties (often superior to their organic counterparts) that make them suitable for many *advanced applications*, e.g. as oils, greases, rubbers, polishes, coatings and insulating materials (e.g., polysiloxanes), ceramic precursors, electronics (polysilanes), water repellents, non-flammable fibres, foams, fuel pipes and metal ion conductors in batteries (polyphosphazenes). Some inorganic polymers exhibit low to very low flammability and can be used as flame retardants in thermoplastics and in thermosets, e.g.. polyphosphates.
The preparation of *functional building blocks* is typically the first step for the rational design of inorganic polymers. *Strained inorganic ring systems* are suitable monomeric precursors for polymers, but to date only a limited number has been employed in ring-opening polymerisation (ROP) e.g., using oxaphosphiranes (C/P/O), and some theoretical calculations have been carried out for these strained ring systems, the reason being the lack of interaction between molecular, polymer and theoretical chemists.
Saturated *polysilanes*, in contrast to alkanes, are appealing alternatives to π-conjugated conductors due to extensive sigma conjugation. Potential applications include UV photoresists, photoconductors, non-linear optics and radical initiators.
Saturated silicon clusters in the polysilane chain increase s-conjugative effects. Unsaturated clusters show pronounced electronic anisotropies and offer the potential for further functionalisation. Other *inorganic alkanes* have been used as suitable monomers (especially of group 13/15 compounds) for dehydro-polymerisation reactions.
Heteroalkene π-bonded building blocks were introduced for π-conjugated polymers in which substitution of the carbon atom in molecularly defined oligoacetylenes by phosphorus or silicon results in large variations in the electronic properties.
So-called *heteropolyacetylenes*, such as polymers based on a conjugated P=P backbones, (*polyphosphazenes*), were reported as early as 1896 by Stokes and described as “inorganic rubber”. Polyphosphazenes are ideal multi-tool polymers, as their properties (hydrophobicity, hydrophilicity,

crystallinity) are easily tuneable post-polymerisation; polymers with ligands and cross-linkable groups (reversible, photo- and thermally induced) are thus readily accessible.
Block copolymers (BCPs) have been extensively studied, but to date virtually all studies concentrated on organic materials and their self-assembly. The recent *hybrid block copolymers* based on inorganic or/and organometallic blocks show fascinating nanostructures with new properties e.g. templates for nanopatterning surfaces and nanostructuring silicon gates in flash-memory devices, hollow vesicles with tunable permeation for drug delivery.
Research in *π-conjugated* organic *molecular materials* is currently a rich and proliferating area in view of their cost-efficient applications in optoelectronics, electronics and devices. Heavier main group elements (e.g., Si, P, S, Se, Te) have previously been incorporated into electroactive organic polymers mainly as *peripheral* structure-guiding motifs *outside the effective conjugation path*. Molecular siloles, for instance, exhibit aggregation-induced photoluminescence, which has been exploited for the detection of explosives.
The strategy of incorporating reactive heteroatoms *into the conjugated chain* afforded heteroatom-incorporated analogues, especially with nitrogen (e.g., pyrrole and carbazole) and sulfur (e.g., thiophene) heterocycles. Organic solar cells with high power conversion efficiencies are accessible on this basis.
Polymers containing transition metal centres in the main chain, *metallopolymers*, combine the processing advantages of polymers with the functionality of metal centres. Poly(ferrocenylsilanes) that exhibit a controlled response to a redox stimulus are of interest, e.g., in photonic crystal devices. Coordination polymers (CPs) which are composed of metal ions (or clusters) connected by linear organic linkers have potential applications as gas sensors. An exciting way to expand their potential is to prepare complex CPs with new structural motifs, e.g., by improving self-assembly through π-stacking of their basic molecular components in a rational “one-pot, multi-components” approach.
Microfluidic synthesis allows continuous production of microgels with precise control over their size and size distribution, shape, composition and morphology. Microfluidic fabrication is eminently suited for creating non-equilibrium, kinetically trapped hydrogel particle shapes. While microfluidic techniques have been recently used to prepare microgel particles, preparation of nanogel redox stimulus responsive polymer particles by fluidics has not been documented. The nanofluidic fabrication of cross-linked porous nanoparticles would offer tremendous potential in controlled release and as micro- or nanoreactors.
The joining of forces of internationally leading scientists (with diverse expertise on novel molecular building blocks, inorganic polymers and theory) with industrial partners will allow the development

of the modular concept of this Action Smart Inorganic Polymers. The design and preparation of custom-built inorganic materials such as inorganic copolymers and block-copolymers will bring European competitiveness in this area to new levels.
The community of leading scientists working in the area of suitable building blocks for and preparation and application of inorganic polymers is highly fragmented in Europe. Thus, a COST Action is the most appropriate tool to combine the expertise and knowledge for the tasks at hand: the rational synthesis of smart inorganic polymers.

B.3 Reasons for the Action

Exciting discoveries in the past decades point toward tremendous potential of inorganic polymers for broad applicability in diverse fields. Inorganic polymers provide greater consumer safety owing to improved properties and environmental compatibility (no need for plasticizers, intrinsically flame-retardant properties of polymers), technological and economic advancement of the European Research Area (solid polymer electrolytes for consumer electronics based on polymers with a low glass-transition temperature)), molecular electronics with non-metal elements as improvement and replacement for metal-based conductors and electronic circuits. Furthermore, inorganic polymers are an innovative approach for sustainability by switching from petroleum-based polymers to element-based polymers and lessen the burden on scarce non-renewable resources or even provide alternatives to them.
Despite the intensive research and novel developments in the field of inorganic polymers there is currently no coordinated exchange mechanism for funded collaboration, training, knowledge transfer, networking and dissemination. Inorganic polymers as an emerging field are currently hardly visible, being mostly an annex to other polymer/material communities. The COST Action SIPs is a scientific and technological network that specifically aims to coordinate and focus existing national programmes in the field of Smart Inorganic Polymers, which is to this day a predominantly single-investigator research area in Europe. While organic polymer chemistry has naturally arisen from the historical development of synthetic methods in preparative organic chemistry, modern society cannot afford to leave the paradigmatic new developments in inorganic chemistry of the last few decades unguided. Numerous new building blocks have been disclosed (heavier element–element double bonds, low-valent species, (anti-)aromatic entities, etc.) that await incorporation into smart polymers so that their full potential of electronic anisotropy will be brought to bear. By definition many of the molecular compounds of heavier elements exhibit semiconducting properties and are consequently predisposed to contribute to various areas such as energy transformation and

storage or information technologies.
No single group can meet these challenges by itself. By joining forces in the Action, experts with support from industry have the opportunity to contribute to state-of-the-art science in a robust research environment, of relevance to the international community. The relative fragmentation of the inorganic community requires a coordinated effort to bring together the experts of their various fields in order to produce bespoke solutions for the problems of modern society. The Action will take maximum advantage of the enormous experience in inorganic polymers that exists in the central and eastern European countries by establishing a Smart Inorganic Polymers network (SIPs). It will foster an efficient collaboration between the leading groups in Europe to ensure optimal awareness of the current developments. This will shorten the time span between the synthesis of building blocks, polymers preparation and processing and identification of their smart properties, and consequently will increase scientific and technological advancement as compared to bilateral and informal collaborations.
Currently, there are several major international conferences on relevant aspects of the Action (International Symposium on Functional π-Electron Systems (conjugated polymers), the International Symposium on Organosilicon Chemistry (polysilanes/polysiloxanes), the International Symposium on Inorganic Ring Systems and the International Workshop on Silicon-based Polymers), but these generally focus on well-established inorganic polymer systems or on molecular inorganic chemistry, while innovative inorganic polymers are hardly covered. The Action will implement an annual conference, the European Conference on Smart Inorganic Polymers (EuSIP), addressing the major research areas from fundamental to applied sciences.

B.4 Complementarity with other research programmes

SIPs will aim at consistency, complementarity and the absence of duplication between activities under the Action and other relevant current and planned European research projects. Transparency will be practiced in order to achieve the objectives of complementarity and consistency, and emphasis will put on synergetic approaches.
The current COST Action MP1202 (“Rational design of hybrid organic-inorganic interfaces: the next step towards advanced functional materials”) studies organic-inorganic interfaces, in combination with a previously supported Action (COST Action D35: “From molecules to molecular devices: Control of electronic, photonic, magnetic and spintronic behaviour”), and COST Action D36 (ended 2011) looked at “Molecular structure-performance relationships at the surface of functional materials”, demonstrating the importance of joint European initiatives towards inorganic-

organic hybrid materials with superior functionalities.

The COST Action CM0802 (European Phosphorus Sciences Network, due to end in April 2013) aims at understanding the structure–reactivity correlations to explain distinctive reactivities and properties of novel phosphorus-based compounds. Its emphasis was markedly different but also partially covered multifunctional phosphorus-based materials as one of the topics with focus on materials science and nanoscience.

The COST Action SIPs focuses solely on inorganic polymers and their potential. SIPs will adjust the focus to functionality and properties that can only be achieved by using the entire toolbox of available p- and d-block elements and beyond.

There are two projects focused on flame-retardant materials in Europe:

- COST MP1105 ‘Flaretex’ (Sustainable flame retardancy for textiles and related materials based on nanoparticles substituting conventional chemicals)
- FP-7 DEROCA (Development of safer and more ecofriendly flame retardant materials based on CNT co-additives for Commodity Applications)

Furthermore, it is anticipated that related consortia will emerge within the EU Framework Programme for Research and Innovation Horizon 2020, stimulated by the success of the transnational networking achieved in this Action.

C. OBJECTIVES AND BENEFITS

C.1 Aim

The aim of the Action is to focus the research activities on inorganic polymers across Europe and to explore the full potential of inorganic polymers in materials science and technology with emphasis on advanced smart properties. The scientific programme consists of highly interdisciplinary research in inorganic polymer chemistry for the design, synthesis, characterisation and performance of functional inorganic polymers. Considerable focus will be placed on morphology and tuning the structure–property/performance correlations. The scientific results of the Action will combine state-of-the-art monomer and polymer design with recent advances in polymer processing and applications.

C.2 Objectives

This COST Action will establish mechanisms for professional networking between leading scientists in the inorganic polymer community and systematically disseminate latest developments.

The expected research outcomes include innovative results in inorganic polymer design and the development of novel ideas and joint research projects within SIPs.

Secondary objectives:

- development of advanced materials with defined properties,
- actively promote inorganic polymer sciences in Europe by organising workshops, training schools, exchange of young researchers and inviting speakers from industrial companies, such as REPSOL, BASF, GE Lightning, Magpie Polymers, Evonik, DSM Ahead BV, Henkel, Dow Corning etc., universities and other research institutions,
- training of young and early-stage researchers in polymer sciences, thus ensuring continuity
- promote exchange of information and expertise within the network and between academia and industry participants, thus fostering further collaborations and joint research applications
- dissemination of the outcomes to a wider public and joint publication of results in high-impact journals
- dissemination of results during EuSIP to allow stakeholders and other interested parties to meet in person to exchange and identify present and future industrial requirements and devise new research strategies. Naturally, appropriate attention to intellectual property (IP) protection will be given.

C.3 How networking within the Action will yield the objectives?

The envisaged group of participants collectively possesses all the necessary skills and expertise to fully harness the potential of inorganic polymers. Internationally renowned research groups with distinctive scientific reputation in synthetic design and polymer processing will be involved in three Working Groups. Each research group is expected to participate in the Action with an average of at least four researchers, i.e., experienced scientists and young and early-stage researchers. Several senior scientists will participate with their research teams in more than one Working Group, to encourage focused research interactions spanning the different research topics of the three Working Groups' activities. Excellent experimental and technical facilities as well as scientific expertise are available at the participating institutions to achieve the research objectives within SIPs. The Action enables researchers to acquire both training in novel emerging techniques and know-how in polymer sciences (i.e., specific synthetic, characterisation and high-level processing methods). These resources will be made available to all groups of SIPs enabling transfer of techniques and applications and sharing best-practice procedures.

Close communication between the Working Groups and the Management Committee (MC) will be ensured by regular meetings and electronic means. The Action will foster and encourage the dissemination of specific expertise throughout the partnership. This goal will be achieved by setting up a specifically devoted Short-Term Scientific Missions (STSMs) by which young researchers from partner laboratories will be exposed to specific expertise available in other laboratories of the network.

The success of this Action is based on unifying the efforts of groups with vital expertise in the development of appropriate new inorganic building blocks with those specialised in polymer synthesis, characterisation and applications, whereby involvement of theoretical groups for predicting structure–property relationships is of importance. Their mutual interactions will allow highly innovative synthetic approaches to be devised, new materials to be characterised and applications to be implemented.

C.4 Potential impact of the Action

SIPs will promote synergism through cooperation beyond existing limits between scientists from different COST countries and thus increase European competitiveness in the development of innovative technologies. The main aims of the Action are scientific and technological progress.

The participating scientists have a substantial interest in novel inorganic polymers as tools for state-of-the-art solutions. Some have vital expertise in the development of appropriate new inorganic building blocks, while others have unique know-how in polymer synthesis, characterisation and applications, or in predicting structure–property relationships. Their mutual interactions in a concerted effort will allow highly innovative synthetic approaches to be devised, new materials to be characterised and applications to be implemented.

The COST Action will stimulate the sharing of expertise between research groups, paving the way for new products with special focus on smart materials. Access to and knowledge about new functional materials is very important for the competitiveness of the manufacturing industry and for the sustainable development of society. SIPs will therefore also encourage and open new opportunities for cooperation with many of Europe’s leading companies specialised in polymer technology participating in this Action. With the involvement of industrial partners, smooth technology transfer will be assured. Furthermore, strong links of the participating groups to the industrial sector will ensure a significant economic impact. An annual conference, the European Conference on Smart Inorganic Polymers (EuSIP), will be implemented and dedicated to dissemination of results. This will allow stakeholders and other interested parties to meet, exchange and devise new research strategies. This will strengthen the European position in highly competitive markets such as solar cells, OLEDs, nanoelectronics, information storage, drug-delivery systems, ceramics, etc.

C.5 Target groups/end users

Polymers are one of the major areas of molecular and materials science and constitute a significant part of the world around us. Applications range from adhesives, lubricants and structural components for cars and aircrafts to more mundane uses such as in children's toys underlining their importance for nearly every aspect of daily life.
The Action will assemble in a highly motivated consortium some of the most outstanding European expertise in inorganic polymer sciences and contribute to reinforcing and strengthening the European standing in a strategic scientific and technological area.
Target groups to be addressed will be:
- the research community in the field and the wider scientific community: academics will be provided with substantially increased access to current state-of-the-art knowledge, novel tools and techniques.
- industry: active industrial participation will be facilitated by contacts to major companies (REPSOL, BASF, GE Lightning, Magpie Polymers, Evonik, DSM Ahead BV, Henkel, Dow Corning). The SIPs meetings will offer an excellent platform for discussions and dissemination.
- the non-scientific community, general public, and policy makers: end users will benefit from the expected outcomes in the area of materials science investigated and developed by the members of the Action.

D. SCIENTIFIC PROGRAMME

D.1 Scientific focus

The focus of SIPs is the development of advanced materials. The scientific programme consists of the design, synthesis, characterisation and application of functional polymers predicted by structure–property relationships. The interplay between theory and experimental work in predicting structure–property relationships will facilitate the creation of materials with defined electronic, redox, photo-emissive, magnetic, pre-ceramic, self-healing, catalytic and other "smart" properties. This will include inorganic polymers with main group element backbones other than carbon, with a strong bias — but not exclusively — towards B-, Si- and P-containing polymers as well as metallopolymers. The implementation of novel bonding modes that are currently only observed in molecules or oligomers into polymeric systems will generate attractive bulk properties.

D.2 Scientific work plan - methods and means

Three interactive Working Groups (WG) will focus on the design and synthesis of novel functional building blocks (WG1), the formation of smart inorganic polymers (WG2) and advanced applications (WG3). Theoreticians and experts on advanced analytical methods will be included in each WG. Accordingly, SIPs will help answer important questions of an applied nature, but still includes fundamental frontier research at the cutting edge.

WG1: Novel functional building blocks *(reactive inorganic and organometallic tailor-made building blocks will be developed for the synthesis of novel inorganic polymers)*

WG1 will focus on the design, development and optimisation of suitable inorganic building blocks. New synthetic approaches are vital to overcome existing limitations regarding monomer availability, and unconventional new building blocks are urgently needed to achieve unique properties, compositions and controlled architectures of polymers. The extremely diverse nature of potential functional building blocks in inorganic chemistry — be it existing or predicted structural motifs — requires the coordination of numerous individual research groups from a broad area of expertise: (1) Strained inorganic ring systems (e.g., oxaphosphiranes, azaphosphiridines, diphosphetanes, etc.) are promising precursors for ring-opening polymerisation reactions but are also of interest due to their unusual properties even in the case of the carbon systems (bent bonds, Walsh-type orbitals). (2) Heterocycles (e.g., silole, phosphole, metallacycles and related) are excellent building blocks for conjugated polymers, since they display electronic properties markedly different from those of highly aromatic thiophene and pyrrole rings. In addition, their functional properties can be tuned by simple chemical modifications. (3) Multiple-bonded systems of heavier main group elements (e.g., heteroalkenes and heteroalkynes of groups 13–16 and mixed group 13/15) are conformationally much more flexible than in the case of carbon and additionally are characterised by a more narrow HOMO–LUMO gap, which can reasonably be expected to translate into small band gaps in related materials. (4) Transition metal based building blocks (as heterocycles, multiple-bonded systems or functionalised complexes) will allow the processing advantages of polymers to be combined with the functionality provided by the presence of metal centres. (5) Saturated element clusters can act as electron reservoirs and induce severe anisotropy into extended π-conjugated systems. (6) Unsaturated (metalloid) clusters show unique electronic anisotropies and in addition can be readily functionalised while maintaining the conductive properties of cluster building blocks.

These molecular building blocks will be characterised by state-of-the-art methods such as 1D and

2D multinuclear NMR (heteronuclei, multidimensional, solid state) and vibrational spectroscopy, UV/Vis spectroscopy, X-ray crystallography, EPR spectroscopy and mass spectrometry, CD spectroscopy (optical properties, NLO effects), fundamental theoretical investigations on electron transport properties of conjugated building blocks that might reveal potential applications (i.e. rectification), break junction setup, STEM conductance measurements on single molecules and polymer building blocks.

Including inorganic structural motifs with site-specific responses into polymeric systems not only requires straightforward preparative procedures but also needs a basic understanding of the underlying mechanisms of the inorganic building blocks in order to tune the polymer properties accordingly. Therefore, the chemical and physical properties of these building blocks will also be studied by cyclovoltammetry to explore their redox properties and to obtain experimental data which relate calculated HOMO–LUMO energies with real charge-transfer processes in condensed phase including relaxation and solvation. Some fundamental physical properties, such as the thermal behaviour (thermogravimetric Analysis (TGA), differential scanning calorimetry (DSC)), vapour pressure and viscosity, need to be explored to allow the rational development of polymerisation protocols which are expected to differ quite substantially from those of hydrocarbon-based polymers. Moreover, the functional-group tolerance needs to be modelled theoretically and explored synthetically, since the balance of competing reaction pathways may be tipped by subtle reactivity changes.

WG2: Smart inorganic polymers *(synthetic approaches to polymers with defined and optimised properties)*

In WG2, state-of-the-art polymer design will be combined with recent advances in polymer processing as developed in well-established fields such as polysiloxanes. Thus, controlled and "living" polymerisation routes to different classes of inorganic polymers will be developed.

New tailor-made inorganic, organic and organometallic building blocks (prepared in WG1) will be used as molecular precursors for the synthesis of novel inorganic polymers. Synthetic approaches to polymers with defined electronic, optical or magnetic properties will include (1) ring-opening polymerisation of small strained hetero- and metallacycles or catalytic dehydrocoupling of suitable element–hydrogen precursors (for polyaminoboranes, polyphosphinoboranes, polyferrocenylsilanes, etc.), (2) the generation of element-centred radicals as photo-initiators for polymer synthesis (radical polymerisation), (3) electropolymerisation of monomers based on heterocycles, (4) catalyst-free (co-)polymerisation of highly reactive heavier π-bonded systems, (5) self-assembly of suitable building blocks into new nanometric structures (e.g. π-conjugated polymers), (6) using coordination-driven supramolecular chemistry processes involving the metal–ligand coordination bond as reversible interaction to form extended supramolecular polymers, (7) synthesis of (chiral) block copolymers (e.g., polyphosphazenes) and the generation of chiral micelles by self-assembly. Research will also involve crystallisation-driven self-assembly of block copolymers, which provides a new route to well-defined supramolecular structures.

The resulting polymers will be characterised by a wide range of methods, such as gel permeation chromatography (GPC) for molecular weight determination and distribution, differential thermal analysis (DTA) for thermal properties, elemental analysis (for composition and impurities), NMR spectroscopy (for determination of number-average molecular weight M_n via end-group analysis or tacticity), diffusion-ordered spectroscopy (DOSY), dynamic light scattering (DLS) and small-angle X-ray scattering (SAXS) (for size, structure and shape determinations), structure determinations of self-assembled systems by X-ray and neutron diffraction, impedance spectroscopy of solutions, solids, films, etc. giving a better understanding of dielectric and electric properties of materials. In fact molecular weights determined by GPC are usually based on polystyrene standards, which is an intrinsic challenge to using this technique for other polymers. The special value of this method is, however, its insight into the modal distribution of soluble polymers. Other methods that will be employed for similar purposes are vapour-pressure osmometry, light scattering techniques etc. For insoluble materials, heteronuclear solid-state MAS (magic angle spinning) NMR will be helpful to identify building units and to quantify structural elements in the polymer backbone. Moreover, sophisticated mass spectrometric methods employing soft ionisation techniques (e.g. field desorption mass spectrometry (FD-MS)) may be used for the determination of molecular weights up to 100.000 Dalton).

Considerable focus will be placed on morphology and tuning of structure–property and performance correlations (in collaboration with theoreticians and WG3). This is especially important for understanding and modelling the specific properties of the prepared smart inorganic polymers, e.g. polyamino- or polyphosphinoboranes, poly(ferrocenyl-based) derivatives, π-conjugated materials, block copolymers, chiral polymers, metallopolymers etc..

WG3: Advanced applications *(smart properties and applications of inorganic polymers will be the focus of this area)*

Organic polymers have contributed very positively to improving the life quality of mankind, and can be considered the polymers of the 20th century. However, the technological challenges of the 21st century require an even higher degree of sophistication. Smart inorganic polymers will be a key to meeting these scientific challenges. Smart polymers are designed to exhibit certain functions prompted by external stimuli. In close collaboration with the industrial partners involved in the Action, members of WG3 will investigate future applications of the smart inorganic materials prepared in WG2, which include (1) nanoscalar electronic and optoelectronic devices, (2) stimuli-responsive polymers, (3) polymer-based catalysts and sensors, (4) tuneable flame-retardant polymers and fire protection, (5) redox-active photonic crystals, (6) (semi)conducting nanowires, heterojunctions and nanolithographic templates.

The mutual interaction between theoretical calculations and experimental results will be an extremely fruitful combination in understanding physical and chemical phenomena, which in turn can be used to develop new materials. The combination of two methodologies (calculation of oligomeric materials to understand the properties of polymers; the periodic box model) provides a better understanding and possibilities to predict new materials with new properties. Furthermore, MM and QM/MM methods for a detailed understanding of polymer properties will be developed and expanded.

Classical procedures for polymer processing will be explored as well as sophisticated techniques like electrospinning for the production of smart inorganic polymer fibres. Highly sophisticated methods will be employed for studying the properties of the obtained smart inorganic polymers (e.g. photophysical properties: fluorescence (time-resolved), chiroptical properties, NLO, UV/Vis spectroscopy, magnetic and dipolar time-resolved spectroscopy, time-resolved optical and IR spectroscopy, white light emitters; electrical properties: (photo-)conductivity, hole mobility, band structures; cyclovoltammetry: redox properties, thermal and photonic responses, magnetic and dipolar interactions, etc.; cyclic voltammetry: redox properties, electron reservoirs, charge accumulation; processability of polymers: spin coating, printing, casting; surface properties: scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDX); stability: photo- and chemical stability under working conditions) which are typically not available in a single group but necessitate collaborations in a larger network of experts from academia and industry.

E. ORGANISATION

E.1 Coordination and organisation

Much of the communication within the Action will be undertaken by electronic means (e-mail, web-based audiovisual media and the Action’s website). Decisions will be taken during the MC meetings or by e-mail per e-vote.

Management Committee (MC)

The MC will be appointed to manage, supervise and coordinate the Action. The MC will include up to two representatives from each signatory country. The Action Chair and Vice-Chair of the Action as well as the Grant Holder will be elected during the first MC meeting.

The MC will meet at least once a year during EuSIP. The MC will (1) manage and coordinate the activities of the Action, (2) plan the budget and allocate the funds, (3) set up and maintain a website of the Action, (4) coordinate the dissemination of results, (5) plan and prepare annual and final reports to the CMST Domain Committee and to the COST Office, (6) coordinate the admission of new Working Group members, and (8) establish criteria for assessing STSM applications in line with the scientific objectives of the Action. Furthermore, the MC will ensure communication of results, activities, events and achievements to the scientific and external stakeholders, as well as to the general public.

Steering Group (SG)

The SG will include the Action Chair, Vice-Chair, Working Groups Leaders, STSM Coordinator, Dissemination Manager and Equal Opportunities Manager. The members of the SG will be elected during the first MC meeting.

SG meetings will take place once a year usually in combination with the MC meeting to reduce expenses within the Action’s budget or, if necessary, at another time. The SG will (1) manage and coordinate the activities of the individual WGs, (2) plan the scientific programme of the Training Schools and EuSIP in agreement with the Local Organiser, (3) plan, prepare and report the scientific results of the WGs to the MC, (4) assist the MC in preparing the annual and final reports, (5) manage together with the MC the applications of new Working Group members, (6) manage the STSMs requests and completion, (7) prepare promotion and educational material for conferences and meetings. A Dissemination Manager will be in charge of maintaining the website and dissemination of important results. Furthermore, an Equal Opportunities Manager will make sure that all requirements for gender balance and involvement of early-stage researchers will be respected.

Short-Term Scientific Missions (STSMs)

Exchanges of young researchers between participating groups of SIPs will be actively promoted by STSMs to take full advantage of complementary expertise. Such regular exchanges will optimally exploit the diverse expertise available throughout SIPs. The STSM coordinator will oversee the appropriate allotment of STSMs based on gender, age, proposed work plan and scientific experience. The criteria for the assessment of the applications will be established by the MC, and any bias on grounds of gender, age, religion and nationality will be avoided. STSMs will take place throughout the whole year and will facilitate contacts within and among Working Groups and allow up-to-date scientific exchange of information.

European Conference on Smart Inorganic Polymers (EuSIP)

An annual "European Conference on Smart Inorganic Polymers" (EuSIP) will be organised in one of the participating COST countries with venues changing every year (200–250 participants; young/senior scientists: 3/1) including invited speakers from stakeholders interested in this Action (REPSOL, BASF, GE Lightning, Magpie Polymers, Evonik, DSM Ahead BV, Henkel, Dow Corning etc.).

SIPs Training Schools

Three Training Schools will be organised particularly for early-stage researchers within the network; the MC will decide on their scientific focus. The Training Schools will take place in one of the participating institutions in conjunction with EuSIP, so that lectures and practical discussions will enable the transfer of knowledge and experience between the participants and promote the comprehensive training of early-stage researchers.

E.2 Working Groups

Three Working Groups (WG) will be established for this Action. Each WG will be chaired by a Working Group Leader and a Vice-Leader appointed by the MC during the first MC meeting. They will be responsible for the coordination, communication, organisation, supervision and reporting within their WGs. The WG structure and admission of new Working Group members will be decided by the MC. The selection of new members in the WGs will be made with consideration of the expertise in WG activity and to ensure an optimal composition with respect to complementary skills, existing collaborations, career stages, gender balance and industrial membership. This will assure high-quality networking and focussed scientific progress.

The Working Group Meetings will take place mainly in combination with MC meetings to reduce expenses within the Action's budget or, if necessary, at another time. These meetings will represent the main platform for the WGs to coordinate their activities, to foster new collaborations and strengthen old ones, and to exchange information, thus promoting concerted research activities. The progress of the scientific activities will be monitored by means of annual reports provided by the WG Leaders.

E.3 Liaison and interaction with other research programmes

This COST Action will particularly interact with running COST Actions (MP1202, MP1105), previous successful Actions (D35, D36, CM0802) and further programmes (FP-7 DEROCA), and will thereby enable informational exchange. Scientific training of young researchers will be funded nationally by the participating institutions within the framework of national and international research training programmes or graduate schools. The participation of members of SIPs as guest lecturers in these training programmes or workshops related to the Action will be also encouraged to promote research dissemination.

E.4 Gender balance and involvement of early-stage researchers

This COST Action will respect an appropriate gender balance in all its activities and the Management Committee will place this as a standard item on all its MC agendas. The Action will also be committed to considerably involve early-stage researchers. This item will also be placed as a standard item on all MC agendas.

This COST Action will be committed to achieving appropriate gender balance with a high level of female participation and considerable involvement of early-stage researchers (ESRs). Therefore, the MC will appoint an Equal Opportunities Manager to ensure that these goals will be achieved and to avoid any bias on the ground of gender, nationality or religion. While maintaining focus on good attitudes for scientific work, the Action will also address problems that are specific for females' careers and general career problems that may affect women more than men. The Action will strive to involve more female researchers as well as early-stage researchers. The Action will actively encourage other female researchers to join and participate in the WGs once the network has been established. Furthermore, they will offer comprehensive career advice for young females and encourage them to take leadership responsibility or apply for vacant positions.

ESRs will be motivated to join the network and continue in this very applicable field of inorganic polymers. Within the Action, they will be encouraged to apply for STSMs and participate in the SIPs Training Schools to increase enthusiasm among young scientists and to stimulate movement into this field. Furthermore, the Action will prompt ESRs to pursue a science career, especially in chemistry and areas related to SIPs and will therefore also facilitate active participation of female and early-stage researchers with talks at conferences and meetings. The SIPs internet platform will be linked to several search engines providing job opportunities for young researchers and thus become an excellent tool to attract PhD students to the groups of the Action.

F. TIMETABLE

A four-year duration of the Action is foreseen according to the Timetable and taking into consideration the existing cooperation between the participating research groups and the desirable development of new cooperations.

Year	Activity	Work progress
1	1st MC meeting of SIPs	1st SIPs annual report
	1st EuSIP	
	MC/SG/WG meetings in combination with 1st EuSIP	
	STSMs of the Working Groups' ESRs	
2	MC/SG/WG meetings in combination with 2nd EuSIP	2nd SIPs annual report; (joint) publications in high-impact journals, joint applications, established collaborations
	STSMs of the Working Groups' ESRs	
	2nd EuSIP	
	1st SIPs Training School in combination with 2nd EuSIP	
3	MC/SG/WG meetings in combination with 3rd EuSIP	3rd SIPs annual report; (joint) publications in high-impact journals, publication of a special high-impact journal issue on SIPs, joint applications to binational programmes and EU calls, established collaborations
	STSMs of the Working Groups' ESRs	
	3rd EuSIP	
	2nd SIPs Training School in combination with 3rd EuSIP	
4	MC/SG/WG meetings in combination with 4th EuSIP	4th SIPs annual report; (joint) publications in high-impact journals, publication of a book with articles on SIPs, preparation of an educational movie on SIPs for youTube, joint

		applications to national programmes and EU calls, established collaborations, strong links with industry, joint patents; final report; Final Action Publication
	STSMs of the Working Groups' ESRs	
	4th EuSIP	
	3rd SIPs Training School in combination with 4th EuSIP	
	Final Action Conference in combination with final MC/SG/WG meetings	

G. ECONOMIC DIMENSION

The following COST countries have actively participated in the preparation of the Action or otherwise indicated their interest: AT, CH, CZ, DE, ES, FR, HU, IT, NL, NO, RO, SE, SI, UK. On the basis of national estimates, the economic dimension of the activities to be carried out under the Action has been estimated at 56 Million € for the total duration of the Action. This estimate is valid under the assumption that all of the countries mentioned above but no other countries will participate in the Action. Any departure from this will change the total economic dimension accordingly.

H. DISSEMINATION PLAN

H.1 Who?

This Action is aimed at disseminating its research results to the *active international research community* in the field. Thus, the dissemination of the activities of SIPs is aimed at promoting and extending the network to attract further experts in materials science and at promoting robust relationships with the many *industrial partners* that are active in Europe in the topics addressed by the three WGs structuring this Action as potential users or developers of the results of the Action. In addition, SIPs aims to train *early-stage researchers* in a strategic research area of European chemical industry, attracting and encouraging young researchers to pursue research in the field. The *broader scientific community*, such as research institutes, universities, industrial laboratories and research frameworks will be addressed, thereby promoting inorganic polymer chemistry and its

related applications to facilitate interdisciplinary research activities.
Policy makers and the *public community* will be informed about the Action network to increase interest and awareness in the field. Suitable COST-related activities will specifically be addressed to mass media to illustrate the research breakthroughs and the multiform benefits made available by SIPs research activities to European citizens.

H.2 What?

Within the active research community the results of this Action will be disseminated by established scientific communication channels, such as *publications in scientific journals, chapters and books, brochures and posters, web sites, oral and poster presentations* at conferences, and seminars at universities, research institutions, and industrial partners. Publication of the scientific results in leading, mostly European scientific journals will be targeted, such as Angewandte Chemie, Chemistry – A European Journal, ChemBioChem, ChemSusChem, ChemPhysChem, ChemMedChem, Chemical Communications, Dalton Transactions, European Journal of Inorganic Chemistry, Journal of Molecular Catalysis, etc. The potential groups involved in the Action have a well-established track record as regular contributors to the most prestigious international journals and conferences in this area.
A major focus of the Action will be the *technology transfer* of the most important results to industrial partners participating or interested in the Action. Research results suitable for industrial applications will be discussed with European industrial partners within the framework of seminars or collaboration meetings. Appropriate attention to intellectual property (IP) protection of the scientific results and technology advancements will be given.
Review articles as well as the *annual scientific reports* will be made available by electronic means to the scientific and industrial community at large with potential interest in this field. Additionally, the *final scientific report* will be printed and distributed widely to scientists and researchers of both academia and public companies with interest in the scientific achievements in the inorganic polymeric materials of the COST Action.
The annual *conference EuSIP* will gather the scientific community and enable exchange of knowledge and extensive discussions between the participants of all Working Groups and more. Industrial partners will be encouraged to contribute with their own research. Conference proceedings will be published and made available to the broader scientific public and to interested industries. One or two non-European outstanding scientists will be invited to deliver plenary lectures at the conference. The involvement of non-European leading scientists with state-of-the-art

research in inorganic polymers, especially from the USA and Asia, will be beneficial to compare and contrast the most important research achievements of the WGs of SIPs.

In addition, scientific exchanges will include S*hort-Term Scientific Missions (STSMs)* of young researchers at participating institutions. The STSMs will be organised for young researchers to become familiar with novel techniques and modern working practice to enlarge their scientific know-how by high-level specific training. STSMs will take place throughout the whole grant period to facilitate contacts within and among Working Groups and to allow up-to-date scientific exchange of information. Such exchanges will increase the participation of young and early-stage researchers in the network and will enable an optimum scientific outcome.

The *training schools* of SIPs will promote knowledge of the field and the dissemination of research activities of the Action to a wider scientific community by attracting young participants of the Action.

A *website* of the Action will provide a platform for recent developments, novelties and innovative aspects and will increase awareness of the network to attract further collaborating groups and both SME and multinational companies dealing with inorganic polymeric materials.

A *Final Action Publication* will address a larger public, other than just the scientific community involved or from outside the network. The purpose of the final publication will be to show the importance of the COST Action and the state-of-the-art research work and achievements in the area of inorganic polymers in a non-technical and non-specialised language also to the non-scientific community (including school children), non-experts or policy makers who are not familiar with the area at all. Whenever possible, promotional activities to inform the non-scientific public through *articles* in *non-technical journals* and *newspapers*, *press releases*, *stands at science fairs* and *flyers* will be pursued to foster public awareness.

H.3 How?

At the beginning of the Action, the MC will set up together with the Dissemination Manager a work plan for the dissemination of results. This work plan will be continuously updated during the MC meetings every year.

The website of the Action will provide information on the expertise of all participants as well as any new technological and scientific breakthrough. The SIPs web platform will not only provide scientific background information and disseminate results, but will also be a powerful instrument for organisation and management of the Action, announcing activities such as the EuSIP, the training schools, STSMs and open positions for early-stage and experienced researchers available in the network laboratories. Furthermore, all partners' research websites will become an excellent tool to promote and attract awareness to the Action. The Action will be further advertised also outside Europe by making use of the worldwide collaborations of the involved groups.

Joint publications involving researchers from more than one group participating in the Action will be particularly encouraged. All presentations at meetings and conferences, scientific publications and articles in non-specialised newspapers and participations in public events such as scientific fairs within the Action SIPs will acknowledge COST support. The network partners have well-established track records as regular contributors to the most prestigious international journals and conferences in the Action's area, as well as in acquiring patents.

Transfer of knowledge is a key element of the COST Action. Involvement of industrial partners in SIPs will ensure technology transfer and internships offering hands-on experience. Excellent collaborations with industrial partners already exist; additional European companies will be contacted and informed about the Action and if possible involved in the WGs' activities. Attracting additional support from industrial and third-party sponsors will further promote the Action and also ensure continuity.

The final SIPs conference will be organised to round up the Action and disseminate scientific highlights to the scientific community. Interested parties and potential users, including representatives from industry and related scientific fields, will be invited.