Domain: CHEMISTRY AND MOLECULAR SCIENCES AND TECHNOLOGIES

The Domain Chemistry and Molecular Sciences and Technologies has the mission of fostering European expertise in discovering, understanding, producing and manipulating molecular species. These research activities aim to develop experimental, theoretical and analytical tools to enhance the development of chemical transformations, reactivity and function. The CMST aims to apply such knowledge and innovation to industrial processes and production. The following examples are illustrative of actual research within this Domain, although it is not restricted to these activities alone.

Chemistry for life: a multidisciplinary collaboration between chemists, biologists, clinicians and agronomists in the design and development of new products for pharmacy, medicine, public health, and agriculture, including a more efficient and safe food production.

Manipulating molecular matter: learn how to handle, synthesise and manipulate matter at the molecular level, understand and control its reactivity and function, develop new catalysts to control the shape, size and properties of the product molecules; move from single molecule chemistry to supra- and macromolecular chemistry, producing smart materials tailored for specific applications.

Energy production: shifting from oil, natural gas and coal consumption to more efficient ways of using combustible fuels and investigate technologies based on renewable resources, in particular sunlight.

Caring for the planet: continuous improvement of the standards of living by reducing the environmental impact of technology in order to establish a sustainable growth, develop clean technology for innovative production, ensure increasingly accurate means for quality control, mastering ground remediation, hazard control, preserving and maintaining cultural heritage.

Space understanding and exploitation: rationalising processes occurring under extreme conditions in space and interstellar media, understanding processes occurring around spacecrafts, exploiting resources of stars and planets.

New ideas and initiatives are welcome as well as those with high interdisciplinary elements and close links and overlaps with other domains.

Action D34: Molecular Targeting and Drug Design in Neurological and Bacterial Diseases

Entry into force : 20/01/2005
End of Action : 23/06/2010

The **main objective** of the Action is to build on existing knowledge at the chemistry/biology interface, in order to develop new target oriented molecules and classes of molecules with therapeutic applications in the area of bacterial and

neurological diseases. Molecular targeting covers drug design, both on the basis of mechanistic studies and of structural studies of the molecules.

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Action D35: From Molecules to Molecular Devices: Control of Electronic, Photonic, Magnetic and Spintronic Behaviour

Entry into force : 21/01/2005
End of Action : 06/01/2011

The **main objective** of the Action is to increase the knowledge and understanding of molecular electronic, photonic, magnetic and spintronic behaviour and to design new active chemical systems and processes that could find use in molecular devices. The collaborative research will be centred around the following three general areas:

1. Design and synthesis of molecular building blocks and their organisation into molecular systems with new photonic, electronic, magnetic and spintronic behaviour.
2. Search for and investigations of photonic, electronic, magnetic and spintronic properties and processes ranging from a singlemolecule level to understanding of environmental effects, molecular cooperativity and build-up of organised molecular nano- and micro-size systems. Physical, mechanistic, time- and space- dependent studies will proceed from a fundamental level to property-evaluation for possible device applications.
3. Methodology development: quantum-chemical methods to simulate environmental effects and dynamical processes, time and space- resolved methods, laser control in condensed phase, property-evaluation procedures.

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Action D36: Molecular structure-performance relationships at the surface of functional materials

Entry into force : 14/10/2005
End of Action : 23/02/2011

The **main objective** of the Action is to increase the fundamental knowledge and understanding of the chemistry occurring at surfaces and interfaces and the factors that tune it. An interdisciplinary, combined effort is the approach. A fundamental approach is advocated, even for industrially oriented research projects. This requires precisely defined problems at all levels and an interdisciplinary approach i.e. synthesis and activation of the materials; measurement of the surface properties; understanding surface properties at the atomic, molecular or cluster level and theoretical understanding of these properties in relation to chemical composition and the structure of the surface. As a consequence, the secondary objective is to gain advanced knowledge for modelling/predicting of the structure/composition reactivity/surface properties relationships of the materials, by means of characterisation of the bulk and surface properties under real operation conditions and for preparing materials with tuneable properties.

More information can be obtained by contacting the Chair of the Action:

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Action D37: Grid Computing in Chemistry: GRIDCHEM

Entry into force : 31/05/2006
End of Action : 05/07/2010

The **main objective** of the Action is to facilitate the creation and use of distributed computing infrastructures ('Grids') in chemistry with the goal of bringing computer modeling and simulation in chemistry to new frontiers in complexity and to a new regime of time-to-solution.

More information can be obtained by contacting the Chair of the Action:

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Action D38: Metal-Based Systems for Molecular Imaging Applications

Entry into force : 15/05/2006
End of Action : 24/08/2011

Statement on the incidence of Nephrogenic Systemic Fibrosis: Given the prevalence of nephrogenic systemic fibrosis in patients who have been administered either Omniscan or Optimark, the fact that such patients were often proven to be acidotic or renally insufficient and that for some of these patients gadolinium retention in the body has been unequivocally established, the condition may be linked to the known relative kinetic instability of these 'Gd-DTPA-diamide' complexes to acid promoted dissociation, leading to retention of Gd in the skeleton, liver and /or kidney.
The COST Chemistry D38 Action group supports Regulatory Agencies statements recommending that Omniscan and Optimark should not be given to patients with severe renal impairment. Preferred contrast agents are those which are more kinetically inert with respect to any pathway leading to premature gadolinium dissociation, e.g. the macrocyclic based agents Dotarem, Prohance and Gadobutrol. No cases of NSF have currently been traced to the use of the latter contrast agents.

More information can be obtained by contacting the Chair of the Action:

Professor Silvio AIME

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Action D39: Metallo-Drug Design and Action

Entry into force : 31/05/2006
End of Action : 18/07/2011

The **main objective** of the Action is to increase knowledge and understanding of the design and mechanisms of action of metallo-drugs, and to use this enhanced knowledge in combination with modern genomic research to develop new classes of metallo-drugs with truly novel mechanisms of action and novel spectra of biomedical activity.

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Action D40: Innovative Catalysis: New Processes and Selectivities

Entry into force : 06/10/2006
End of Action : 05/11/2011

Action Web Site: http://www.nottingham.ac.uk/~pczsw/D40/site/index.html

The **main objective** of the Action is to allow the containment of new innovative C-H, C-O, C-C and C-Heteroatom bond forming processes, using metal-ligand approaches for the synthesis of organic compounds of biological, pharmacological and organic nanotechnological utility.

More information can be obtained by contacting the Chair of the Action:

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Action D41: Inorganic oxides: surfaces and interfaces

Entry into force : 20/09/2006
End of Action : 24/09/2010

Action Web Site: http://www.cost-d41.unimib.it/

The **main objective** of the Action is to increase our knowledge and understanding of the properties of oxide surfaces and interfaces at an atomistic level and to develop means of predicting and controlling their structures and functions at the nanometer scale.

More information can be obtained by contacting the Chair of the Action:

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Action D42: Chemical Interactions between Cultural Artefacts and Indoor Environment (EnviArt)

Entry into force : 20/09/2006
End of Action : 01/10/2010

The Action **aims** at exploring chemical interactions between cultural artifacts and typical indoor environmental conditions through field studies and laboratory experiments and to translate the results into preventive conservation practice.

More information can be obtained by contacting the Chair of the Action:

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Action D43: Colloid and Interface Chemistry for Nanotechnology

Entry into force : 04/10/2006
End of Action : 09/11/2011

Action Web Site: http://costd43.unige.ch

The **main objective** of the Action is to fabricate functional nanostructured materials and nanoscale devices for analytical, biomedical and life science applications.

More information can be obtained by contacting the Chair of the Action:

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Action CM0601: Electron Controlled Chemical Lithography (ECCL)

Entry into force : 28/03/2007
End of Action : 14/05/2011

Objective: The ability to understand, manipulate and control chemical reactions at the molecular level is one of the great challenges of modern research. Since chemical processes are dominant in most areas of science and technology, the ability to control their pathways provides exciting new opportunities that may be exploited by both the research and technological communities. Such 'single molecule engineering' requires selective bond cleavage in target molecules to allow subsequent management of the local site chemistry. In electron beam experiments it is well established that low energy electrons offer this selectivity with high efficiency, a selectivity that is controllable by simply 'tuning' the electron energy. Recently, low energy electrons derived from the tip of a scanning tunnelling microscope have also been used to control bond rupture and subsequent linkage of individual molecules to the substrate. This Action aims at an interdisciplinary European programme to combine state-of-the-art in electron induced chemistry and surface science with these recent advances in scanning tunnel microscopy to pioneer a new field of 'Electron Controlled Chemical Lithography', with the prospect of designer synthesis down to the nanoscale and electron controlled manipulation of surface properties with spatial resolution ranging from the millimetre down to the nanometre scale.

Keywords: Electron controlled chemistry, molecular engineering, low energy electron interactions, scanning tunnel microscopy, inelastic electron tunnelling spectroscopy.

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Action CM0602: Inhibitors of angiogenesis: design, synthesis and biological exploitation (ANGIOKEM)

Entry into force : 18/04/2007
End of Action : 06/06/2011

Excessive or insufficient angiogenesis (new blood vessel formation) is connected with many human diseases, cancer included. For effective disease intervention, interdisciplinary approach in the research is necessary. This COST Action focuses on networking of interdisciplinary oriented chemistry and biology researchers who are actively involved in rationale designing and development of small organic compounds with anti-angiogenic properties. Exchanges of information and presentations of experiences and skills from chemical and biological research will be performed for effective introduction, exploitation and improvement of modern methods for development of new angiogenic inhibitors. Meetings, short-term scientific missions, workshops, training schools and conference will ensure the expansion of effective cooperation in the development of new drug candidates.
Keywords: Inhibition of neovascularisation; lead compounds and drug design; treatment of cancer and other diseases; in silico predictions; multivalency in organic synthesis and biology.

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Action CM0603: Free Radicals in Chemical Biology (CHEMBIORADICAL)

Entry into force : 28/02/2007
End of Action : 14/06/2011

The **main objective** of the Action is to promote a chemical biology approach for the investigation of free radical pathways. Chemical reactivity and molecular libraries are the start of a multidisciplinary research context ‘from small molecules to large systems’, culminating in the biological complexity. The Action aims at improving communication and exchange among neighbouring scientific fields, such as chemistry with several domains of life sciences, specifically addressing the real barrier consisting of specialist language and tools. Four working groups address the formation, reactivity and fate of

free radicals involving bio-molecules, such as unsaturated lipids, aromatic-, cyclic- and sulphur-containing amino acid residues, sugar and base moieties of nucleic acids. Tasks concern the role of free radicals in normal cell metabolism and in damages, defining structural and functional modifications, in the framework of physiologically and pathologically related processes relevant to human quality of life and health. The Action also promotes the training of young researchers in multi-faceted research tasks. The Action is expected to involve research groups with funds amounting approximately to 31 million EUR.

Keywords: Radical-based biological processes and mechanisms, biomarkers, radical functioning and damage, modification of unsaturated lipids, degradation or modification of peptides/proteins and nucleosides/DNA.

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