EUROPEAN SCIENCE FOUNDATION
SETTING SCIENCE AGENDAS FOR EUROPE

EUROCORES Programme
European Collaborative Research

Chemical Control at the Nanoscale (EuroNANOCHEM)

DRAFT Call for Outline Proposals

What is EUROCORES?

The ESF European Collaborative Research (EUROCORES) Programmes offer a flexible framework for researchers from Europe to work on questions which are best addressed in larger scale collaborative research programmes. The EUROCORES Programmes allow excellent researchers from different participating countries to collaborate in research projects 'at the bench'. They also allow, when appropriate, colleagues from non-European countries, for example the US, to participate. The Programmes encourage and foresee networking and collaboration of researchers to achieve synthesis of scientific results across the programme, to link to related programmes, and to disseminate results.
EUROCORES Programmes allow national research funding organisations in Europe and beyond to support top class research in and across all scientific areas, by matching the needs articulated by the scientific community with their strategic priorities.
Funding decisions on the projects and the research funding remain with the national research funding organisations, based on international peer review operated by ESF. ESF also provides support for networking the researchers and for the scientific synthesis of research results and their dissemination[(1)]. This way, the EUROCORES Scheme complements the EC Framework Programme and other collaborative funding schemes at European level.

For further information see:
http://www.esf.org/eurocores

[(1)] Currently supported through a contract with the European Commission under the Sixth Framework Programme (EC Contract no. ERAS-CT-2003-980409).

Chemical Control at the Nanoscale (EuroNANOCHEM)

Following agreement with funding organisations in # countries, the European Science Foundation is launching a Call for Outline Proposals for Collaborative Research Projects (CRPs) to be undertaken within the EUROCORES Programme EuroNANOCHEM. EuroNANOCHEM will run for 3-4 years and it includes national research funding, as well as support for networking and dissemination activities provided by the ESF[1].The Programme aims to support high quality multidisciplinary research.
Outline Proposals are to be submitted by **9th May 2008**. It is expected that Full Proposals will be invited by 30th June 2008 with 15th September 2008 as expected deadline for submission.
A Programme-specific website can be consulted for the latest updates at **http://www.esf.org/euronanochem**

Background and objectives

The ability to control chemical reactions has been a longstanding goal of chemical physics. Current methods used to control chemical pathways and hence the synthesis of many materials are based on thermodynamics with both the rate and products of a chemical reaction controlled largely by the temperature of the media in which the chemistry occurs. In order to develop chemistry on the micro/nanoscale it is necessary to develop new methodologies that allow chemical control of individual molecules in the gas phase, in clusters and on associated substrates. Such 'single molecule engineering' requires both selective bond cleavage to control local site chemistry and the development of techniques that permit the chemistry to be manipulated spatially on the nanoscale and allow novel molecular architectures to be developed. Recent research has revealed that it is possible to control the excitation and dissociation of molecules using both light (generated from ultrafast lasers) and electrons (e.g. low energy beams or free electrons in a plasma) which, when coupled with the spatial resolution gained from scanning tunnel microscopes, may provide a route for developing such nanoscale chemical control. Such research is expected to underpin several new technologies in the 21st century, for example the development of *nanolithography* - one of the first commercial examples of nanotechnology - in which chemical structures may be designed and constructed from single molecules on a surface. Furthermore, molecular site selectivity induced by both electrons and photons has been found to play a key role in radiation damage of biomolecular systems opening possibilities to develop new methods of radiotherapy. Electron and photon induced chemistry may also explain the dynamics of molecular synthesis in interstellar medium and plays a key role in heterogeneous chemistry in the terrestrial atmosphere. EuroNANOCHEM is a four year programme through which we wish to develop a pioneering research programme that brings together and coordinates the cross-disciplinary skills of three major research communities in Europe (femtosecond chemistry, electron driven processing; scanning tunnelling microscopy) to develop a new field of *nanoscale chemical control.*

Scientific goals

The primary focus of EuroNANOCHEM is to develop methodologies that will provide complete control of chemical pathways with high selectivity. The first method uses laser pulses with a duration of a few femtoseconds/picoseconds, the timescale on which the atoms in a molecule move, to manipulate molecular wavepackets and control dissociation pathways. The second method uses very low energy electrons to dissociate the molecular target at well defined reaction sites while the third methodology uses scanning tunneling microscopes to manipulate single molecules absorbed on surfaces. Together these three techniques offer the unique ability to select and 'tune' chemical pathways to provide unprecedented control over chemical reactions. To date Europe's research efforts in chemical control remains fragmentary and Europe currently lacks an infrastructure to bring together and coordinate the research skills of these three research communities (femtosecond chemistry; electron driven processing; scanning tunnel microscopy) with the cross-disciplinary skills needed for the development of such research. EuroNANOCHEM seeks not only to support pioneering research of the highest quality but will provide the mechanisms by which such interdisciplinary collaboration may be fostered. Therefore EuroNANOCHEM will support both Collaborative Research Projects (CRPs) and necessary networking activities such as mobility grants, short term visiting fellowships, conferences and training workshops.

Research topics

The research programme is conveniently divided into three core themes but the programme specifically aims at integrating these themed areas. Therefore projects that combine two or more of the themes outlined below are particularly welcome. It should also be stated explicitly that theoretical projects that stand alone from experiments are equally valid (it being possible to infer from discussion below that theory is primarily to used to support experiment research). Projects that provide a link with industrial partners to develop the commercial exploitation of this research are also strongly encouraged.

Theme 1. Chemical Control using photons.
Theme 2. Chemical Control using electrons.
Theme 3. Chemical Control at the nanoscale.
Each theme will be discussed in turn and specific objectives defined for each.

Chemical Control using photons – *Scientific context.*

Since the invention of the laser the practicality of using light to actively manipulate and control chemical reactions has been widely pursued. By tuning the monochromatic energy of the laser light to the specific vibrational energy of a specific chemical bond, energy leading to selective bond dissociation. However such selectivity is often lost because of rapid intramolecular energy redistribution within the molecule, requiring the energy to be placed into the bond on timescales of a few femtoseconds (the timescale on which the atoms move within the chemical bond). Modern chemical control techniques have been proposed which exploit the optical phase of coherent laser light, entitled "coherent control". Such techniques employ quantum mechanical interference between the pathways leading to products of a chemical reaction. More recently, chemical control has been achieved employing optical phase manipulation and shaping of intense ultrafast (femtosecond) laser fields, leading to the selective breaking of chemical bonds.

Such techniques are not confined to the gas phase -- it is equally practical to develop such chemistry in the condensed phase, where new catalytic reactions on surfaces may be induced, and the methodology has also been successfully demonstrated in the liquid phase. The latter with great significance for exploring biochemical processes for example exploration of therapeutic techniques for the human retina and the development of new specialised pharmaceuticals (with distinct chirality).

Key Objectives of theme 1:

In this programme we wish to support research to develop ultrafast femtosecond chemistry for selective bond cleavage by:
(a) developing automated optimization of branching ratios of gas phase photodissociation reactions
(b) developing the technique of femtosecond polarization pulse shaping to vary intensity, momentary frequency, and light polarization as functions of time within a single femtosecond laser pulse to study the interaction of functional groups with surfaces of materials such as semiconductors, molecular self-assembled monolayers or nanoparticles;
c) supporting research on light induced chemical reactions
particularly relevant for nanotechnology (e.g. molecular switching)
(d) extending present studies into the liquid phase to explore more biologically relevant chemical processes, and
(e) complementing these experiments by theoretical studies.

Chemical Control using electrons – *Scientific context.*

The opportunity of using electron induced dissociation of molecules as a tool for chemical control has been recognised for several years and is widely adopted by the low temperature RF plasma community to prepare reactive species for surface processing. Traditionally such processes are using high energy electrons. However, one of the most exciting advances of recent molecular physics has been the discovery of the ability of low energy electrons to initiate and effectively drive selective bond cleavage in molecular systems efficiently due to the Dissociative Electron Attachment process (DEA). DEA is a resonant process occurring only over a narrow (1 eV) energy range) and in contrast to direct electron impact, where an excess energy of several eV (e.g. 4 to 5 eV) is required to fragment a molecule, DEA can dissociate a molecule at very low, thermal (meV) energies with very large cross-sections. Furthermore DEA is bond selective, each resonance often having a preferred dissociation channel. Once DEA has released reactive fragments they are free to initiate chemical reactions. Low energy dissociative electron attachment (DEA) therefore combines remarkable selectivity with very high efficiency hence providing a new route for chemical control of any reaction since the production /yield of chemical reactants may be 'tuned' by varying the electron energy.

DEA may occur within a cluster or aggregate or on a surface in a mixed multilayer. Such specific chemical reactions can also be used to bind *specific functional groups* to the surface of a solid material in a controlled way providing a tool for functionalization of the surface for further surface chemistry with relevance to biochips relying on the immobilization of proteins or nucleotides or of nanoparticle patterned surfaces.

Key Objectives of theme 2:

In this programme we wish to

(a) study intermolecular reactions leading to controlled coupling of a reactive fragment to another material by identifying the products of electron-induced reactions in the gas phase, within clusters and in molecular films; reactions initiated by e-beam will be compared with electrochemical initiated reactions;

(b) study the attachment of functional groups to surfaces of materials such as metals, semiconductors or molecular self-assembled monolayers; the surfaces of semiconductors could also be modified by e-beam;

(c) extending the present studies from individual building blocks (e.g. aminoacids, DNA bases) to larger biological macromolecules and their complexes including the study of the effect of salvation,

(d) explore the potential of these reactions for chemical lithography and e-beam techniques, and

(e) to guide these experiments by theoretical studies, i.e. to predict which of different possible intermolecular reactions is energetically the most likely.

Chemical Control at the nanoscale – *Scientific context.*

New capabilities of atomic-scale imaging, analysis and manipulation are revolutionizing the scientific approach in the material and life sciences. In particular the technique of Scanning Tunnelling Microscopy (STM) has deepened our understanding of material surfaces by providing us, for the first time, with atomic resolution spatial images. For many years STM lacked chemical specificity, requiring complementary spectroscopic tools to identify the chemical species being imaged, however, recently STM–IETS (STM Inelastic Electron Tunnelling Spectroscopy) has been developed to *measure the vibrational spectrum of a single molecule,* allowing STMs to be used as a tool for chemical analysis of single molecules.

Our ability to fashion structures and control chemical processes at the fundamental level using electronic excitations requires a combination of the Scanning Tunneling Microscopy with an understanding of the dynamics of electron-molecule interactions. Electronic excitation of the adsorbed molecule by using inelastic tunnelling of electrons from the STM tip appears to be an appropriate method for controlling, with nanoscale precision, molecular reactions. Using inelastic tunnelling effects, individual bonds in molecules or bonds between a molecule and the substrate can be broken in order to induce selective dissociation or desorption of the molecule. Such "molecular surgery" introduces the prospect of *designer synthesis on the nanoscale.*

Key Objectives of theme 3 :

In this programme we will support:

a) STM experiments on molecules adsorbed on surfaces with the aim of fabricating complex molecular architectures of any desired shape and size on the surface. This will involve STM tip manipulations of the molecule and substrate along with STM imaging and single molecule vibrational spectroscopy.

b) Electron Stimulated Desorption (ESD) and High Resolution Electron Energy Loss Spectroscopy (HREELS) experiments to identify the ion resonances and the electronic transitions involved in the excitation mechanisms as well as the final products of the molecular reactions.

c) Development of a comprehensive simulation of the coupled surface and STM tip

system to model excitation and bond breaking or other reactions of single molecules by STM-IET.

d) Molecular dynamical calculations to unravel details of atomic and molecular manipulation at surfaces, leading to lateral motion, bond making or breaking, and desorption of the adsorbates.

Guidelines for applications

(Outline and Full Proposals)

Collaborative Research Project (CRP) proposals from individual scientists or research groups eligible for funding by the organisations participating in the Programme will be accepted for consideration in the EUROCORES Programme EuroNANOCHEM.
Scientists or groups not applying for or not eligible to apply for funding from these organisations (including applicants from industry), can be associated with a proposal where their added scientific value is demonstrated. Their participation as Associate Partners in a project must be fully self-supporting and will not be financially supported by the participating funding organisations.

Proposals are only eligible, if they fulfil the following **criteria**:

- Proposals must involve, as a minimum, three eligible Principal Investigators (PIs) from **three different countries.**
- A maximum of 50 % of the Individual Projects (IPs) in a Collaborative Research Project (CRP) can come from one country.
- Proposals must involve more PIs than Associated Partners

Applications should normally be for three years although applications for shorter or longer time periods may be considered depending on the rules of the participating funding organisations. Taking into account the selection and approval processes, the successful projects are expected to begin their activities in **March 2009**.

Online submission of applications

Outline and Full Proposals will be submitted online. Applicants should follow the proposal structure as indicated in the application template for outline proposals available on the Programme website at: **http://www.esf.org/euronanochem**

On this Programme website, links to information on national funding eligibility and requirements as well as to a EUROCORES Glossary and Frequently Asked Questions (FAQs) are available.

Prior to submitting Outline Proposals, all applicants <u>have to</u> contact their national funding organisations in order to verify eligibility and to ensure compliance with their relevant organisations' granting rules and regulations (see contact persons listed on page 8).
At the time of online submission of the Outline Proposals, the Project Leader is asked to confirm this on behalf of all the participants in the CRP.

Outline Proposals

Outline Proposals are invited by 9th May 2008.
Outline Proposals will be examined by the participating funding organisations for formal eligibility. Therefore, it is crucial that all applicants contact their national funding organisation prior to submitting their proposals.
In compliance with the rules and regulations of the participating national funding organisations, the requested funds under the EUROCORES Programme EuroNANOCHEM can include salaries for scientific and technical staff, equipment as well as travel costs and consumables within the project, specifying the amount requested from each Funding Organisation. National policies may also require the proposal to contain additional specific information. Applicants should be aware that the participating funding organisations can make significant adjustments to the requested funds in order to bring these in line with their rules and regulations.

Applications will be assessed according to a set of criteria in a two-stage procedure, as to ensure a thorough selection of scientifically excellent proposals. At the outline stage, the Review
Panel will select proposals with potential for scientific excellence, by applying the following criteria:

- Relevance to the Call for Proposals
- Novelty and originality
- European added value (scientific)
- Qualification of the applicants

An Outline Proposal submitted must comprise:

- A short description of the CRP (max. 1200 words, including objectives, milestones, methodologies (for example experiments and fieldwork);
    - Short description of how (and why) the partners contributing to the CRP will work together;

- Short CVs of Project Leader (PL), all PIs and Associate Partners (max. one page each, including five most relevant publications);
- Estimated budget (consistent with the rules of relevant national funding organisation) tabulated according to a provided template.

Associated Partners (APs) are also considered part of a CRP and will be assessed as such at both the Outline and Full Proposal stage.

It will be assumed that arrangements for the handling of IPR (Intellectual Property Rights) will be in place within projects, following the applicable national legislation and national funding organisation rules. Applicants are strongly urged to have such arrangements in place, covering all research groups (including any associated groups) before the start of the projects. It is expected that the results obtained by the projects supported under this EUROCORES Programme will be placed in the public domain.

It is also expected that all relevant clearance of other national or international committees (for example ethics) has been obtained before funding is granted. It is the responsibility of applicants to clarify any such matters (if applicable) with their national contact points.

Full Proposals

Full Proposals will be invited following the recommendations of the Review Panel. The deadline for full proposals will be announced later, but is expected to be around 15th September 2008.

Please note that only applicants who submitted an Outline Proposal can submit a Full Proposal.

For the Full Collaborative Research Project (CRP) proposals, the most important selection criterion is "Scientific quality". Other criteria include interdisciplinarity (according to the scope of the call), qualification of applicants, level of integration and collaboration, feasibility and appropriateness of methodologies, European added value and relation to other projects (risk of double-funding and track record for collaboration).

The Full Proposals will be assessed by at least three independent external expert referees who are selected by the ESF from a pool of scientists suggested by the participating funding organisations and the Review Panel. A list of all referee names used for the international peer review will be published once the selection process is complete.

After receiving all referee reports, they will be made available (anonymous) to the applicants for their information and for commenting (optional). The Review Panel will rank all Full Proposals based on the assessment of the Full Proposal, the anonymous referee reports and the applicant's responses to these.
The Review Panel will create a ranked list consisting of the best Full Proposals and will subsequently make recommendations to the Management Committee for the funding of these proposals. The actual granting of the funds to the Individual projects on the ranked list will depend on the total amount of funds available in each country by the participating Funding Organisations. The use of funds in a project will be subject to the rules and regulations of each participating Funding Organisation as well as to the national laws of those countries.

Full proposals must include a well-argued scientific case (both for the collaboration envisaged and for the individual contributions), a list of participants, a detailed tabulated budget and other supporting information. A single, common scientific case must be made throughout the proposal to demonstrate an aim for scientific synergy and integration of multinational expertise. In addition, the amount requested from each national funding organisation has to be clearly and separately specified. Detailed instructions on requirements and how to complete the application forms will be made available once Full Proposals are being invited.

The **Project Leader** will be the main CRP proposal contact point for ESF for the duration of the project. He/she will be responsible for representing the Collaborative Research Project, for its participation in programme activities, and for any reporting requirements placed on the project as a whole.

All **Principal Investigators** will be responsible for dealing with the requirements attached to the contributions of their own funding organisation.

Programme Structure and Management

Programme Structure

The overall responsibility for the governance of the programme lies with a *Management Committee*, whose membership is formed by one representative from each participating funding organisation (usually a senior science manager) together with an ESF representative.

Proposal assessment and selection are the responsibility of an international, independent *Review Panel*. The members of this panel are leading scientists, appointed by ESF following suggestions from participating Funding Organisations. The membership of the Review Panel will be available on the Programme website for information. The Review Panel is also expected to monitor the overall scientific progress of the programme.

The Scientific Committee which is formed by the Project Leaders of all funded CRPs will be responsible for proposing networking activities for scientific synergy in the EUROCORES Programme. They will also advise and support the EUROCORES Programme Coordinator in the coordination of networking activities.

Programme Networking

Networking activities are designed to strengthen the science objectives of this EUROCORES Programme by promoting coherence in the activities of the science community involved. This will provide the European added-value which is the central objective of any EUROCORES Programme.

Networking and collaboration within EUROCORES Programmes takes place at two levels:

1. between the various Individual Projects within each Collaborative Research Project (CRP) and
2. between the funded CRPs within the programme as a whole.

The intra-CRP activities are supported through the research grants each participant receives from the participating funding organisations in the given CRP. The cross-CRP activities are funded through contributions to the EUROCORES Programme.

The intra-CRP collaboration is motivated by the nature of the CRP's research objectives, i.e., by the scope and the complexity of the questions it deals with. In a CRP, the participating groups have the opportunity to gather the required critical mass to successfully address the objectives and challenges of their project.

The cross-CRP networking and collaboration is stirred by the aims and the nature of the particular EUROCORES Programme. The theme which was the basis of this EUROCORES Programme has been selected for its clear need of collaboration in the proposed field. The funded CRPs will collectively set up and further streamline this new collaboration. To this end, the CRPs will engage the programme participants and, when of clear benefit, colleagues from outside the programme in joint activities such as:

- Working Group meetings for the exchange of information and results across the CRPs;
- Joint scientific meetings or summer schools;
- Short term visits;
- Development and delivery of joint training schemes;
- Seminars, Workshops, symposia, invited sessions either stand-alone or as part of other larger events;
- Common web-facilities and publications.

Through active participation of scientists in the above mentioned activities, not only existing collaborations are enhanced but new and strategic partnership opportunities are also identified.
Furthermore, these activities may provide opportunities to explore aspects of the programme which are not covered by the funded research projects.

The integrative activities between the CRPs will help to strengthen the field by building coherence within this emerging research community and will serve as a platform for the research work which is done in the programme.

Project members are expected to participate annually in at least one cross-CRP activity.

When submitting your proposal, please note that the costs for networking within your CRP should be budgeted for in your proposal. Funds for

networking between the CRPs will be centrally managed by the ESF through contributions from the participating funding organisations.

Programme evaluation

A Mid-Term evaluation, conducted by the Review Panel, will evaluate the overall progress of the Programme, based on the progress of the funded CRPs. Here, the Review Panel has a steering function and can comment on the CRPs' work plan in relation to the objectives of the overall Programme. A final evaluation will assess the achievements of the whole EUROCORES Programme.

Contacts in the participating organisations

As it is currently not known which Funding Organisations will support this programme, please contact your National Funding Organisation or Research Council to inquire about this programme.

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