SEVENTH FRAMEWORK PROGRAMME
THE PEOPLE PROGRAMME

Grant agreement for:

Initial Training Networks

Annex I - "Description of Work"

"This document refers to PEOPLE Work Programme 2008"

Project acronym
LASSIE

Project full title
LABORATORY ASTROCHEMICAL SURFACE SCIENCE IN EUROPE

Grant agreement no.
238258

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by Research Executive Agency
November 24th, 2009

PART A

A.1 List of Beneficiaries and Project summary

A.1.1 List of Beneficiaries

Beneficiary Number	Beneficiary Name	Beneficiary Short Name	Country	Date enter Project	Date exit project
1 (Coordinator)	Heriot-Watt University	HWU	UK	1	48
2	Aarhus University	AU	DK	1	48
3	Paris Observatory	OBSParis	FR	1	48
4	University of Münster	UM	DE	1	48
5	Max-Plank-Gessellschaft	MPG	DE	1	48
6	National Institute for Astrophysics	INAF	IT	1	48
7	Leiden University	LUO	NL	1	48
8	Chalmers University	Chalmers	SE	1	48
9	University of Gothenburg	UGOT	SE	1	48
10	University College London	UCL	UK	1	48
11	The Open University	OU	UK	1	48
12	Queen's University, Belfast	QUB	UK	1	48
13	Strathclyde University	SU	UK	1	48

List of Associated Partners

Associated Partner Number	Associated Partner Name	Associated Partner Short name	Country	Level of Participation (Level 2 or 3)	Organisation Status
1	Graphic Science	Graphic Science	UK	2	Enterprise/SME
2	Gridcore AB	Gridcore	SE	2	Enterprise/SME
3	Hiden Analytical Ltd.	Hiden	UK	2	Enterprise/SME
4	Kore Technology Ltd.	Kore	UK	2	Enterprise/SME
5	HITEC2000	HITEC	IT	2	Enterprise/SME
6	Quantel SA	Quantel	FR	2	Enterprise
7	SPECS GmbH	SPECS	DE	2	Enterprise/SME

A.1.2 Project Summary

Free Keywords: Astronomy; Astrophysics; Molecular Physics; Chemical Physics; Surface Science; Solid State Science; Computational Chemistry; Molecular Solids; Chemical Reactions; Simulation; Gas-Grain Interaction

Abstract: Astronomical observations are revealing in ever increasing detail how our Universe works. Existing and planned European investment in sophisticated observational platforms approaches many billions of Euros. However, the observations that can be made on these telescopes would be little more than "pretty pictures" were it not for the efforts of the experimental and theoretical laboratory astrophysics communities in collaboration with their astronomical colleagues in developing models of our Universe firmly grounded here on Earth. These models recognise the importance of chemical processes in the astronomical environment and the young science of Astrochemistry seeks to understand the rich variety of this chemistry in such a way as to make a significant contribution to truly understanding the evolution of the modern day Universe. The LASSIE (Laboratory Astrochemical Surface Science in Europe) Initial Training Network seeks to address the key issue of the interaction of the astronomical gas phase with the dust that pervades the Universe. The gas-grain interaction, as it is known, has been recognised by astronomers as crucial in promoting chemistry. The LASSIE ITN brings together the leading European players in experimental and computational surface and solid state astrochemistry, astronomers seeking to understand the detailed role of chemical species in our modern Universe, industrial partners engaged in the development of relevant laboratory instrumentation and experts in public engagement. Through this combination LASSIE will develop capacity in astrochemistry in Europe, produce researchers equipped with a range of specialist and generic skills necessary to engage in a wide range of knowledge-based careers and to reach out to all aspects of European society to deliver a positive message in relation to the scientific and technical advancement of Europe.

PART B

B.1 Description of the Joint Research Training Project

This Initial Training Network (ITN) brings together Europe's 13 leading research groups engaged in the study of one of the most topical areas of modern astronomical research - **the role of the gas-grain interaction in the evolution of the Universe** - combined with 7 micro, small and medium-sized enterprises (MSME) from across Europe to provide a unique interdisciplinary and intersectorial training environment. The ITN's members have an outstanding track record in training both Early Stage Researchers (ESRs) and Experienced Researchers (ERs) in a wide variety of skills and knowledge transfer covering both fundamental and applied physical sciences. ***This ITN will prepare both ESRs and ERs for careers not only in astronomy and astrochemistry (for which there is an urgent need) but provide them with a skills base that is relevant in a wide range of knowledge-based enterprises across Europe, so contributing to the integration of the European Research Area (ERA).***

B.1.1 Project Overview

The LASSIE (Laboratory Astrochemical Surface Science in Europe) Initial Training Network (ITN) has the goal of providing a training and research environment uniquely equipped

- *To conduct a scientific research programme that addresses one of the key issues of modern astronomy and astrophysics - hence supporting the major investment of the ERA in observational astronomy and space exploration.*
- *To enhance the European knowledge economy via the provision of trained and mobile researchers equipped with the skills necessary to pursue successful careers across a wide range of employment sectors in the face of increasing global competition.*
- *To enhance the global standing of European culture.*

To achieve these aims, the LASSIE ITN will use a broad and coherent range of 'training through research' activities that will:

- *Produce highly trained researchers with a range of practical, theoretical and computational skills relevant to astrochemistry.*
- *Produce researchers with an ability to independently analyse problems and formulate suitable strategies for their solution.*
- *Produce researchers capable of both independent research and of working as part of a multi-disciplinary team.*
- *Produce researchers experienced in a SME research and development environment.*
- *Produce scientists with a broad portfolio of non-scientific skills relevant to the wider career goals of these individuals. In particular, through integrated training with a range of industrial partners, the network will provide its researchers with skills in presentation, management, business and entrepreneurship.*
- *Produce researchers with experience in the communication of science to a wide range of people both inside and outside of the scientific community.*

The LASSIE ITN brings together Europe's 13 leading theoretical and experimental surface and solid state astrochemistry research groups supported by a partnership of 6 high technology MSME partners and an internationally recognised MSME outreach partner. The network has a combined experience in excess of 250 years in research and training; has a publication record in high quality journals numbering over 1000 papers; and has trained over 100 ESR and ER who are now fully integrated into a wide range of knowledge-based enterprises in Europe. Furthermore this strong interdisciplinary and intersectorial team provides:

- *A large inclusive network that will allow interactions across the surface and solid state astrochemistry communities in Europe to be developed.*
- *The necessary knowledge base and human resources to ensure that the past, present and future multi-billion Euro support for observational astronomy is capable of being fully exploited by providing the necessary scientific support to allow astronomers to interpret their observations based on realistic and well-understood laboratory chemistry and physics.*
- *A much needed infrastructure for developing a coherent programme of astrochemical research within the EU that will allow the ERA to compete more effectively globally.*

At national level the need for, and the benefits of, such collaboration in furthering research in astrochemistry has been recognised in France, the Netherlands, Sweden and the UK. In the latter, the AstroSurf Network (http://www.chem.ucl.ac.uk/astrosurf/home.html), funded by the UK Engineering and Physical Sciences Research Council, is an ideal example of how cooperation and collaboration may be brought together in a wider European programme. Whilst aspects of astrochemistry form part of other European-funded programmes such as the EuroPlanet consortium (which requires astrochemical data for the study of planetary atmospheres) and the European Astrobiology Network Association (EANA), neither of these have the goal or structure for training the much needed next generation of astrochemists which is the main purpose of this ITN. However both of these consortia have indicated a willingness to collaborate with the LASSIE ITN. Furthermore, ASTRONET (http://www.astronet-eu.org/-Astronet-), the European consortium of astronomy and astrophysics funding agencies, has recently declared that astrochemistry is crucial in underpinning the major investment in telescope development expected in the next 20 years (http://www.astronet-eu.org/-Science-Vision-) and must be supported if Europe is to successfully utilise that investment.

B.1.2 Concept and Project Objectives

The Universe is littered with the debris of dead and dying stars. This debris includes large quantities of micron and sub-micron-size dust grains. For generations astronomers seeking to unravel the complexity of the Universe have been frustrated by such dust blocking their view of many galaxies and the oldest parts of the universe (**Figure 1**). However, we now recognise that these cold dusty regions are in fact the progenitors of evolution in the modern Universe. Rich in chemical complexity, they are known to be the sites of star and planet formation and even the host for molecules that are necessary for the development of life itself.

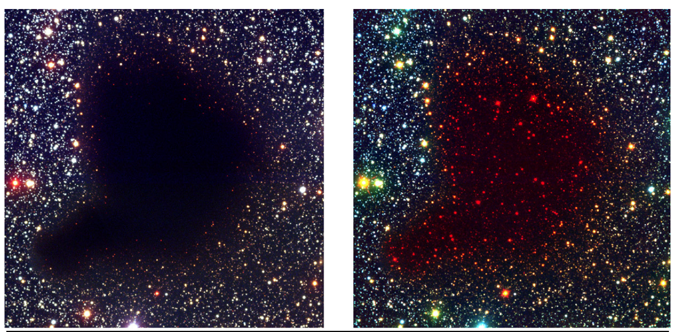

Figure 1: The quiescent object Barnard 68 viewed in the visible (left) and infrared (right). Visible light is scattered by dust in the object, but infrared light is transmitted. Image copyright European Southern Observatory (ESO).

The young interdisciplinary science of ***Astrochemistry***, lying at the interface of Astronomy, Astrophysics, Physics and Chemistry has evolved in order to explore the products, mechanisms and rates of the chemistry that dominates the Universe. Such astrochemistry is distinct from the chemistry occurring in the terrestrial and industrial environments for the following reasons:

- *Due to the low densities encountered in many astronomical regions, the time scale of the chemical evolution of astronomical objects may be tens of thousands (or even millions) of years.*
- *The chemistry often takes place at much lower temperatures than those commonly encountered on Earth, emphasizing so-called barrierless chemical reactions.*
- *Chemical species not commonly found on Earth play a key role in astrochemistry e.g. the molecular ions H_3^+ and HeH^+, both of which are believed to have taken part in the first chemical reactions to occur in the Universe.*

Thus astrochemical research requires a multidisciplinary approach, bringing together researchers from astronomy, quantum physics/chemistry, surface science, condensed matter physics, low temperature physics as well as physical chemistry and chemical physics. This in turn requires the training of interdisciplinary researchers capable of assimilating techniques, ideas and practices from a wide range of scientific disciplines. In an earlier FP6 Research Training Network *The Molecular Universe* (http://molecular-universe.obspm.fr/index.php?page=home) aspects of the gas phase chemistry in these regions were explored. However, such chemistry cannot explain the overabundance of small hydrogen-rich species such as molecular hydrogen (H_2) and water (H_2O) or the presence of more complex organic molecules, including those of potential biological significance, such as glycolaldehyde ($CH_2(OH)CHO$, a sugar precursor), acetamide (CH_3CONH_2) and polycyclic aromatic and heteroaromatic species, that recent observations have shown are present in large abundances in such regions.

It is now recognised that if we are to understand the complex chemical synthesis prevalent in these dusty regions of the universe we must understand the heterogeneous chemistry that takes place on the surface of the micrometre-sized grains. Indeed, while Gould and Salpeter first proposed atomic recombination on dust grain surfaces as the most efficient mechanism for H_2 formation in the 1960s, the true role of such heterogeneous chemistry has only become apparent with the recent data recorded by the Hubble, ISO and Spitzer space telescopes. This data has opened up the study into the so-called ***Gas-Grain Interaction***, which may ultimately explain the formation of the chemical progenitors of life (**Figure 2**). Dust grains are thought to have many roles including:

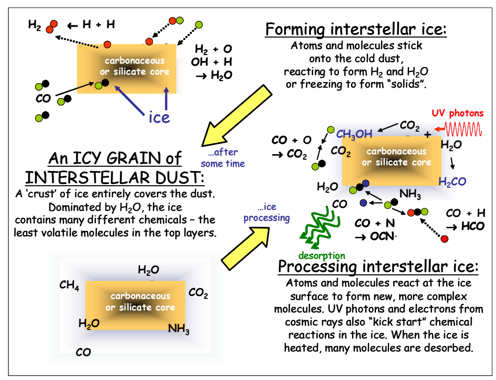

Figure 2: A cartoon illustrating some of the complexity of the gas-grain interaction in the ISM[4].

- *Acting as catalysts for the formation of small hydrogen-rich molecules, including H_2 itself.*
- *Acting as a reservoir for volatile gases through the accretion of icy mantles that are formed both by reaction on the grain surface (e.g. H_2O) and condensation from the gas phase (e.g. CO). These mantles are returned to the gas phase during star formation to radiatively cool a collapsing gas clump.*
- *The icy mantles act as chemical nanofactories driven by light, electrons and cosmic rays to convert small molecules into more complex chemical species e.g. CO and H_2O react to give carbon dioxide (CO_2), H_2O and methane (CH_4) react to form methanol (CH_3OH) and ammonia (NH_3) and CH_4 form methylamine (CH_3NH_2), seeding the Universe with the potential for life.*
- *Grains and their icy mantles are the building blocks from which comets, planets and other rocky bodies in the universe are assembled.*

The Scientific Programme of the LASSIE ITN therefore seeks to address the cyclic role of dust in the chemical evolution of the Universe, from its synthesis in aged and dying stars, through its roles in the gas-grain interaction in increasingly dense environments in the interstellar medium (ISM) through to grain-grain collisions and the first steps in the construction of new stars and planetary systems. A combination of state-of-the-art computational and experimental chemical physics and molecular astronomy and astrophysics will be used to address these issues. The network brings together leading theoretical and experimental surface scientists working to unlock the secrets of the gas-grain interaction with astronomers engaged in observing and understanding star and planet formation and the role of icy dust grains in these processes. The network also includes several industrial partners who are producing the necessary state-of-the-art equipment to allow such research to be pursued.

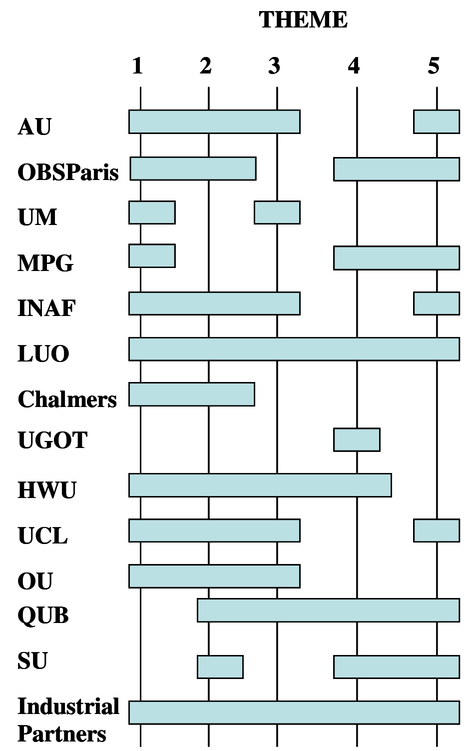

Figure 3: Scientific themes and their connectivity within the LASSIE ITN.

The research programme of the LASSIE ITN is organised around five interconnected interdisciplinary themes (**Figure 3 and Table 1**) which have been internationally agreed as being the most urgent research topics for current astrochemical research and that aim to understand

1. ***the formation and destruction of interstellar dust.***
2. ***the formation of simple molecules, and hence icy mantles, on realistic models of (icy) dust grain surfaces.***
3. ***the physical processes that result when an icy grain mantle is heated or irradiated with light, electrons or ions.***
4. ***the chemical processes that result when an icy grain mantle is heated or irradiated with light, electrons or ions.***
5. ***the role of these processes in observations of grains, ices and the molecules formed by the intermediary of grains and their icy mantles in the evolving Universe.***

The work packages (WPs) are described in detail in section B.1.3 and the logistics are summarized in Table 1.

B.1.3 Scientific and Technological Objectives of the Research and Training Programme

Research Programme

These research themes stated above form the basic structure of the scientific programme of the LASSIE ITN. Each theme addresses clearly defined scientific aims and objectives that constitute the separate research sub-programmes. These, in turn, will provide the ‘training by research projects’ for ERs and ESRs employed by the LASSIE ITN that will be developed under our implementation plan. **Figure 3** illustrates the depth and breadth of the interconnections between these themes and the LASSIE ITN partners.

WP1 1 - Formation of Grains, Small Molecules and Ices

Observations have shown that vast clouds of molecules and dust exist between the stars and the gravitational collapse of these clouds is the first step in the formation of new stars. Observational evidence further shows that in these clouds the dust grains are coated with icy mantles of small molecules, such as H_2O, CO, CO_2, NH_3 and CH_3OH. How do we account for the presence of the dust?

What is it made of and what does it look like? How can we be sure of the veracity of observations that indicate the presence of these small molecules and their ices? These are questions that cannot be addressed by observation and modelling alone and laboratory measurement is crucial to help us identify what is out there and to understand its origin. It has become apparent in recent years that the neglect of heterogeneous chemistry in these clouds is a major shortcoming in the traditional "gas-only" models of interstellar chemistry. Hence we must address these questions from the standpoint of investigating heterogeneous processes at the gas-solid interface using realistic models of the relevant interfaces. Fortunately, we are now in a position where such heterogeneous processes can be studied in the laboratory in great detail, using a range of highly sophisticated techniques. These experiments can probe phenomena as varied as the structure of condensing carbon or silicate grains; the disposal of energy into the translation, rotation and vibration of newly formed molecules; and the rates of reactive accretion of icy layers and the morphology of those growing ice layers.

Aims and Objectives: Theme 1 will focus on the formation and optical properties of dust grains, the formation of small molecules on grains and the reactive accretion of icy layers and the morphological and spectroscopic properties of the resulting icy films. The theme will focus on experiments aimed at providing a basic understanding of grains and ices. For each task the primary contractor responsible for delivery is clearly identified by underlining. The primary contractor will be responsible for coordinating with the secondary contractors where multiple contractors are contributing to the effort.

- *The mechanism of formation of interstellar dust grains from their initial condensation through to grain aggregate formation via grain-grain collisions (MPG, OU, UM).*
- *The release of reaction energy into product translation, rotation and vibration in the heterogeneous formation of small molecules on model dust grain surfaces (AU, Chalmers, INAF, OBSParis, UCL, UM).*
- *The rates of molecule and ice formation on dust grain surfaces, including studies of isotopic fractionation (AU, Chalmers, HWU, LUO, INAF, OBSParis, UCL).*
- *The morphology of ices formed reactively on model grain surfaces (AU, Chalmers, HWU, INAF, OBSParis, UCL).*
- *The infrared, optical and ultraviolet (UV) spectroscopy of ices formed reactively on model dust grain surfaces (Chalmers, HWU, LUO, OU, UCL).*

WP2 - Physical Processes in and on Icy Grains

The dominant ice in the Universe is water ice. However observations tell us that icy grain mantles contain more than just water ice *e.g.* CO, CO_2, and CH_3OH. Furthermore, it is likely that these ices will be doped with small amounts of polycyclic aromatic and heteroaromatic hydrocarbons (PAHs) that are believed to be prevalent as a sink for carbon in the Universe. Moreover, some of these icy mixtures may exist in the form of crystalline solids such as clathrates. Understanding the physical processes that can occur in such an icy material is central to the LASSIE ITN. In particular, we are interested in the destruction of grains and their icy mantles as a mechanism for returning material to the gas phase. Physical destruction processes, driven in part by electromagnetic and particle irradiation, consist of thermal or photon/particle-induced desorption and evaporation, differentiation by selective evaporation, and sputtering. Grain-grain collisions may also play an important role, leading to both disruption of icy mantles and fragmentation of a grain cluster itself, and represent an important physical process undergone by grains (see theme 1). The groups involved in this research theme have excellent track records regarding the application of surface science in astronomy. Indeed, they have championed the application of ultrahigh vacuum methods within the community. Their contributions in studies of the thermally driven desorption from model icy grain mantles have had a major impact in astrochemistry in highlighting the role of ice morphology in modifying the thermal behaviour of ices, resulting in a paradigm shift within the community. In addition, their detailed studies of the infrared spectroscopy of

CO and CO_2 in and on water ices have been able to address long standing problems in comparing laboratory spectral data with observations.

Aims and Objectives: Our primary aim is to contribute to the understanding of the physical processes occurring when an icy mantle is subjected to electromagnetic radiation or bombarded with charged and/or neutral particles. For each task the primary contractor responsible for delivery is clearly identified by underlining. The primary contractor will be responsible for coordinating with the secondary contractors where multiple contractors are contributing to the effort.

- *Understanding the thermal desorption of simple ices, complex mixed ices and clathrates as observed in the cold, dense regions of the ISM associated with star formation (Chalmers, HWU, LUO, OBSParis, SU, UCL).*
- *Understanding desorption of simples ices, complex mixed ices and clathrates induced through interaction with electromagnetic radiation (Chalmers, HWU, LUO, OU, SU, UM, UCL).*
- *Understanding desorption of simple ices, complex mixed ices and clathrates induced via interaction with low energy electrons and models of cosmic rays (AU, Chalmers, HWU, INAF, OU, QUB).*
- *Understanding the role of heat, electromagnetic radiation and cosmic rays in promoting changes in ice morphology (HWU, LUO, INAF, OBSParis, OU, UCL, SU).*

WP 3 - Chemical Transformations in and on Icy Grains

More than 150 different molecules have been identified in star-forming regions. These range from simple diatomic species such as CO to exotic radicals (*e.g.* linear HC_5) and complex organic molecules like CH_3OCH_3 and CH_3CH_2CN. This chemical complexity has been explained for many years by gas-phase processes driven by cosmic-ray ionization, but new models show that such processes only reproduce observed abundances of the smaller, open shell, species. New evidence shows that icy dust grains with temperatures as low as 10 K can act as catalytic sites for molecule formation and that the formation of the more complex species involves surface processes in ices adsorbed on interstellar grains. Two routes to complex organics have been proposed. First generation species are produced on surfaces through elementary exothermic hydrogen additions and reactions possessing activation-energy barriers of closed-shell species with H-, N-, O- or C-atoms. The reactivity is further enhanced by simultaneous energetic processing, due to UV irradiation and cosmic ray exposure. Later in the star formation sequence, during the 'hot core' phase, grains warm up to temperatures between 20 and 100 K and molecules desorb from the ices, bringing into the gas phase a new class of molecules that acts as a starting point for second generation species.

Aims and Objectives: The topic of research theme 3 is to study this evolution and to simulate the formation of complex molecules of astrophysical interest on grains and in interstellar ices under laboratory controlled conditions at an unprecedented level of detail and sensitivity. The majority of the participating groups in this theme have experience in growing interstellar ices on dust grain equivalents under high or ultrahigh vacuum (UHV) conditions dependent on ice morphology (chemical composition, amorphous *versus* crystalline structure, in pure, layered or mixed configurations), ice temperature and ice thickness. Within this theme the influence of different chemical trigger mechanisms will be quantified under conditions typical for inter- and circumstellar matter. The work plans for this theme is as below. For each task the primary contractor responsible for delivery is clearly identified by underlining. The primary contractor will be responsible for coordinating with the secondary contractors where multiple contractors are contributing to the effort.

- *UV photon-induced chemical transformations (HWU, LUO, OU, UCL).*
- *Low energy electron-induced chemical transformations (AU, HWU, INAF, OU, UCL).*
- *VUV, XUV and X-ray photon- and cosmic ray-induced chemical transformations (AU, HWU, LUO, INAF, OU, UM, QUB).*

- *Chemical transformations following atom, radical or thermal molecular ion bombardment, using e.g. special thermal cracking and microwave discharge sources (HWU, INAF, LUO, OBSParis, UCL).*

WP 4 - Modelling the Gas-Grain Interaction

Computational modelling of the gas-grain interaction provides further insights into the physics and chemistry underlying the relevant processes and relates macroscopic processes to interactions between individual atoms and molecules. Generally, the rates of surface reactions do not show a simple Arrhenius-like behaviour, since they are determined by a collection of different events such as deposition, diffusion, desorption, and chemical reaction parameters that cannot be easily controlled in the laboratory, but may be isolated and probed in computational models. Understanding these separate processes is of critical importance as we attempt to translate the total reaction rate to interstellar conditions, where fluxes are much lower than used in laboratory experiments. In this theme we will adopt quantum, Monte Carlo and classical modelling of icy systems to obtain information about the structure, spectroscopy and dynamics and allow the data obtained on laboratory timescales to be corrected for interstellar conditions. This theme therefore fulfils a key role in the scientific programme as it couples the experimental work of themes 1, 2 and 3 to the observation and modelling programme of theme 5.

Aims and Objectives: Our computational modelling programme is based around the work plan and identifiable tasks given in the table below. For each task the primary contractor responsible for delivery is clearly identified by underlining. The primary contractor will be responsible for coordinating with the secondary contractors where multiple contractors are contributing to the effort.

- *Developing models of amorphous ices and dust grains (LUO, OBSParis, QUB, SU, UGOT).*
- *Calculating IR and UV absorption spectra for water and adsorbates on and in crystalline and amorphous ices (HWU, UGOT).*
- *Understanding the dynamics of photon-driven processes in amorphous ices, including photodesorption and photodissociation (HWU, LUO, OBSParis, UGOT).*
- *Understanding molecular hydrogen and small molecule formation on silicates, carbonaceous, graphite and amorphous ice (AU, LUO, OBSParis, QUB, UGOT).*
- *Understanding the hydrogenation and deuteration reactions of CO in various types of ice, particularly CH_3OH formation (LUO, OBSParis, QUB, UGOT, SU).*
- *Calculating diffusion and desorption rates of H atoms, O atoms and simple molecules on amorphous and crystalline ices of various compositions (OBSParis, UGOT).*
- *Modelling coupled grain growth and chemistry under interstellar conditions (MPG).*
- *Simulating the growth and evolution of water ice and other solids under interstellar conditions (LUO).*

WP 5 - Observations and Astronomical Models Involving Dust and Ices

The laboratory experiments and theoretical calculations described in themes 1 through 4 are the key to understanding the chemistry in interstellar clouds in which new stars and planets are formed. A particular strength of this network is the close interaction of chemists, physicists and astronomers, both within the various institutes and across nodes. Astronomical observations and modelling define the needs for laboratory experiments. In turn, the basic chemical data allow a much deeper understanding of the astrophysical data than otherwise possible.

In the vicinity of forming stars, in so called 'hot cores' ($T > 100$ K), many of the complex molecules observed in the gas phase are likely due to ices which have evaporated from the grains. The cores are warmed by the radiation as the star turns on, so that ices deposited on dust during the star-formation process are released to the gas phase and their emissions detected. *Therefore, hot cores represent the* *integrated history of the physical conditions during the formation of the star*. However, a key question is how these complex molecules form, whether by successive hydrogenation and oxidation of accreted gas-phase species, especially CO, or by processing of the ice by UV photons and charged particles, or by gas-phase reactions between evaporated species at high temperatures. A combination of these three processes is most likely the answer. The laboratory experiments described in themes 1 through 3 are essential to distinguish between these scenarios.

Following the star formation process, many young stars exhibit emission bands believed to originate from carbonaceous particles. These bands are often observed strongly in emission from the photon-dominated regions (PDRs) that surround massive star formation regions. The origin of these bands is, as yet, unresolved. We will make detailed observations of the strengths and relative intensities of these bands as a function of astrophysical environment, in order to correlate them with our laboratory investigations of surface chemical reactions on carbon surfaces.

Aims and Objectives: The primary goal of this theme is to obtain quantitative astronomical constraints on the role of grains in interstellar chemistry. This will be achieved through a combination of observations and modelling. The observational and molecular astrophysics groups within our network have a number of goals that closely link into the programme of laboratory science. These are summarised below. For each task the primary contractor responsible for delivery is clearly identified by underlining. The primary contractor will be responsible for coordinating with the secondary contractors where multiple contractors are contributing to the effort.

- *Large and small scale maps of infrared lines of H_2 and deuterated species will be constructed to trace H_2 formation on grain surfaces under different conditions (AU, OBSParis).*
- *An inventory of ices in different environments will be assembled using infrared spectroscopy from the Spitzer Space Telescope (INAF, LUO, UCL, SU).*
- *Constraints on ice formation will be obtained by ice mapping with the AKARI satellite (UCL, SU).*
- *A line survey of massive- and intermediate- star forming regions with the Submillimeter Array will be conducted in order to search for complex molecules, which may point to formation routes on grain surfaces (MPG, QUB).*
- *A determination of the formation and lifecycle of water from gas to solid and back again will be performed by combining infrared spectroscopy of water ice with submillimeter spectroscopy of water gas from the Herschel Space Observatory (LUO, UCL, SU).*
- *A study of the formation and composition of silicate and carbonaceous grains in disks and envelopes around young and old stars will be undertaken using infrared spectroscopy (MPG, UCL).*
- *High spatial resolution IR spectroscopy of PDRs in nebulae and around stars will be recorded, looking at how the emission band strengths and relative intensities vary with distance from the exciting source as a diagnostic of PAH formation and excitation mechanisms (OBSParis, UCL).*
- *Modelling of the gas-grain chemistry in hot cores and disks using the new laboratory data and comparison with observations (UCL, LUO, MPG, OBSParis, QUB, UCL, SU).*