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2004

CHEMISTRY

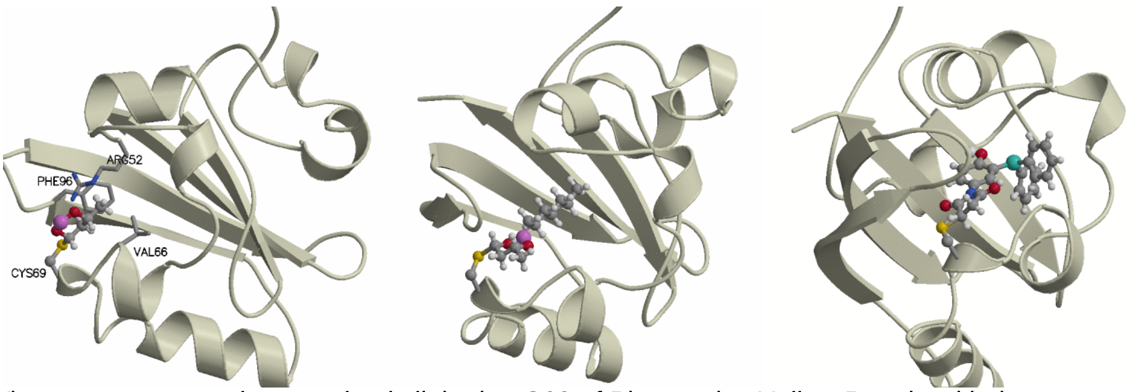
&

PHYSICS

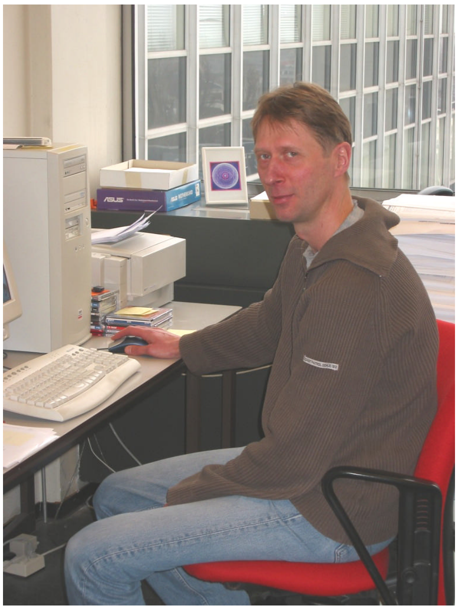
DEVELOPMENT OF LATE TRANSITION METALLOENZYMES AND METALLO-DNAZYMES FOR HIGLY EFFICIENT CATALYTIC PROCESSES

ARTIZYME CATALYSIS

The new group of Prof. Paul Kamer at the School of Chemistry, University of St. Andrews will carry out an exciting range of projects related to sustainable development. Waste-free chemical processes are a must for a sustainable society. In nature, enzymes enable the atom economic synthesis of numerous natural products, but there are no enzymes for the synthesis of the many pharmaceuticals, agrochemicals and fine-chemicals that our society needs. To solve this problem, we seek a paradigm shift in catalysis research by developing transition metal containing "artificial enzymes" for catalytic transformations towards industrial products.We propose a "de novo" design of transition metalloenzymes, using molecular recognition properties of biomolecules to develop (late) transition-metalloenzymes by functionalising oligonucleotides and proteins with phosphino ligands and binding them to late transition metals. Adjusting the structures of the biomolecule and the phosphine ligand will optimise the catalytic performance of these artificial enzymes.Artificial "metallo-DNAzymes" can be developed by complex formation of transition metal prosthetic groups and DNA aptamers as "apo-DNAzyme", starting from large aptamer libraries. The search for efficient "metallo-DNAzymes" will be aided by complex formation with transition state analogues, starting from large dynamic combinatorial libraries.We will create a new class of highly selective catalysts for demanding transformations, like CO insertion, alkene insertion and (asymmetric) C-C bond forming reactions. The biopolymer part will induce the proper substrate orientation to the metal centre. Encapsulating substrates by these "synthetic biopolymers" will then be exploited to achieve clean conversion of unfunctionalised molecules by C-H activation.These new catalysts, like biological systems, will be able to pick out a single substrate, even when it is present at low concentrations in complex mixtures.



A Ni-acetoacetate catalyst covalently linked to C69 of Photoactive Yellow Protein with the surrounding amino acids (left); A growing heptyl chain is inserted into the empty chromophore-binding pocket of PYP (middle); The spatial structure of apo-PYP with the phosphinophenolate covalently attached, occupying a larger part of the cavity (right).



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COSMOLOGICAL IMPACT OF THE FIRST STARS

CIFIST

The first stars which were formed in the Universe were sources of ionizing photons, but also of atomic nuclei more massive than those produced during the big bang. Understanding the nature of these stars and their role in the build up of the chemical elements (nucleosynthesis) is of crucial importance also to understand the formation of galaxies at redshift z~5 or larger. Considering that the Main Sequence lifetime of a star of 0.8 solar masses is of the order of the age of the Universe, the first stars of this low mass are still observable today and they provide the fossil record of the chemical composition of the Young Universe. In this field the European research has taken the lead thanks to the excellent capabities of the ESO-VLT 8.2m telescopes.The Observatoire de Paris, is extremely active in this area. However the complexity of the analysis required and the large amount of data demand an effort which is on a European scale. The CIFIST Team was conceived for this purpose and it will be devoted to the study of the first stars and their chemical composition. The Team will draw from the expertise and know-how present in Paris but also from researchers and expertise from other European countries.

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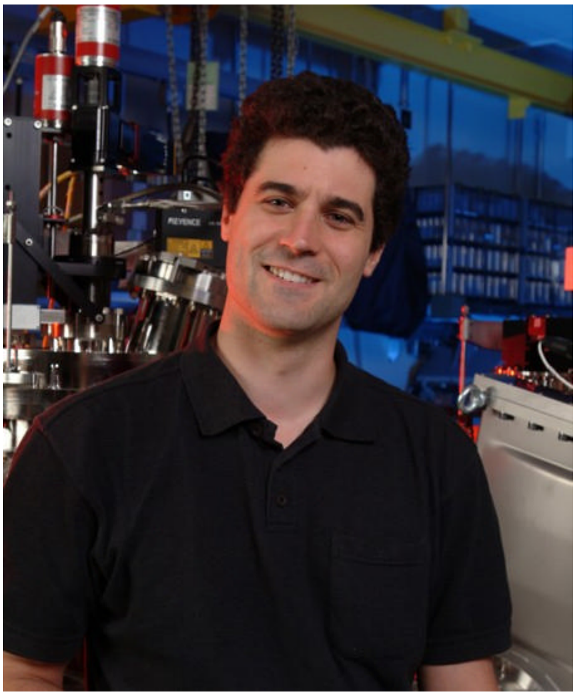
NANO-ENGINEERED MAGNETIC MATERIALS FOR SPINTRONICS AND MAGNETOLOGIC APPLICATIONS

MAGLOMAT

The performance of today's microelectronics is increased by continuous miniaturization, however, the fundamental limits will soon be reached. An alternative approach to increase the computational power is to take advantage not only of the charge of the electron but of the spin as well. This field is nowadays known as "Spintronics". Recently it was demonstrated that the non-volatile magnetic random access memory (MRAM) can in principle serve as reconfigurable magnetologic gate. To employ these MRAM elements for logic operations, materials-related challenges remain to be solved. The goal of this project is to synthesize new heterogeneous materials by Co and Mg doping of oxide semiconductors like ZnO to engineer ferromagnetic electrodes and tunnel barriers from only one type of material. Further, monodisperse ferromagnetic nanoparticles will be incorporated in oxide semiconductors as well forming a magnetically doped oxide-semiconductor where the size and distribution of the magnetic particles is more controllable compared to clustering in highly doped semiconductors. Such granular magnetic semiconductors (GMS) will enable to study the magnetic interaction of magnetic impurities through the semiconductor host under well-defined conditions. These two types of nano-engineered materials will be integrated into all-oxide spin-valve structures to obtain novel reconfigurable magnetologic devices with nanoscale dimensions. Prototypes of such devices, which are expected to offer dramatically increased functionality compared to transistor logic, will be fabricated and tested.



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STANDARD MODEL EXTENSIONS WITH MASSIVE NEUTRINOS :

PHENOMENOLOGY, MODEL BUILDING AND COSMOLOGICAL IMPLICATIONS

NEUTR-COSMO-ACCEL

The research of the team is in the field of Elementary Particle Physics, and focuses on the following topics:(i) An elaborate theoretical study of Standard Model extensions with massive neutrinos and lepton number violation, in association with the generic fermion mass problem.(ii) A detailed analysis of the implications of such models for searches for new particles and interactions in present and future experiments, with particular focus at the LHC (CERN).(iii) A study of related cosmological implications, linked not only to processes that directly involve neutrinos, but to the way in which the breaking of symmetries in this class of Standard Model extensions affects structure formation in the universe.

This work combines analytical calculations with state-of-the art numerical computations, in the interplay between theoretical and experimental physics and between particle physics and cosmology. In this framework, predictions for observables whose study will be in the core mission of present and future experiments will be made. The results will then be used to address fundamental theoretical questions related to the origin of mass, the underlying structure of the fundamental theory of nature, the origin of symmetry breaking, and the short-distance structure of space-time.

The team is hosted at the University of Patras, Greece, where the Team Leader has been appointed as an Associate Professor after spending 15 years in Oxford, Heidelberg and CERN.

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EXPERIMENTAL MANIPULATION OF PHOTONIC ENTANGLEMENT FOR LINEAR OPTICS QUANTUM INFORMATION PROCESSING

PHOTONICENTANGLEMENT

Photonic entanglement plays a crucial role both in fundamental tests of quantum mechanics and in quantum information processing (QIP). Remarkably, recent theoretical and experimental advances have shown the possibility to exploit multi-photon entanglement for efficient QIP using only linear optics together with projective measurement. Building on our long experience in research on entanglement from spontaneous parametric down-conversion, the main purpose of the present project is to perform a number of significant experiments in the field of QIP with particular emphasis on linear optics quantum computation, long-distance quantum communication and new test of multi-party quantum locality. Within the project, we plan to experimentally investigate the potential application of a photonic logic gate with classical feed-forwardability; we plan to exploit free-space entanglement distribution to perform experimental demonstration of long-distance quantum teleportation and quantum cryptography on the order of ten kilometre to penetrate the limit of aerosphere; we plan both to exploit multi-qubit code to experimentally investigate the possibility to overcome the decoherence caused by the channel noise and, to exploit entanglement swapping to investigate the possibility to solve the photon loss in the quantum channel; moreover, we also plan to perform a demonstration of high efficiency quantum cryptography with high-dimensional entanglement; and finally we plan to exploit a high-intensity three-photon entanglement source to perform long-distance third-man cryptography, secret sharing and test of quantum nonlocality. The techniques that will be developed in the above experiments will lay the basis for future large scale realizations of linear optical QIP.

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GAUGE THEORIES OF FUNDAMENTAL INTERACTIONS: THEORY AND PHENOMENOLOGY

STRONG-INTERACTIONS

Gauge theories are the only way we know how to describe the fundamental interactions. In spite of all that has been learned regarding such theories, many fundamental questions remain unanswered. In particular, Quantum Chromo Dynamics (QCD), which is the gauge theory describing the strong interactions between quarks and gluons, continues to pose challenging questions for physicists. Quarks and gluons are confined at low temperature and matter density in the form of hadrons such as protons, neutrons and pions. The origin of confinement within QCD remains unexplained. Our limited progress on this problem is largely due to our ignorance of how to deal with intrinsically non-perturbative regimes of generic gauge theories.The main research objective of the team will be to develop new techniques for the description of both perturbative and non-perturbative regimes of gauge theories and to use these techniques in phenomenological studies directly related to the results of current experiments. The entire project will lead to a deeper understanding of strong interactions and the phase diagram of QCD and QCD-like theories (as function of temperature, matter density, etc.). The confinement mechanism and its relation with chiral symmetry breaking will also be clarified. A detailed knowledge of the QCD phase diagram is essential for a number of physical applications ranging from early universe dynamics to the structure of cold and dense astrophysical objects. A better knowledge of strongly-interacting theories is also needed to model possible extensions of the standard model of particle interactions and for solving fundamental cosmological problems. Finally, we need new and general methods to address the strong interaction problem, which is central in virtually all fields of physics.

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STATISTICAL DATA-MINING IN ASTROPHYSICS

ASTROSTAT

The full exploitation of science data is being impeded by statistical and computational intractability. Scientists are now deluged by large, complex data sets, and the scientific value of these data is presently lessened by the laborious efforts needed to analyze them. Therefore, the goal of this project is to develop and deploy new statistical data-mining algorithms to achieve computer-assisted discovery. Such intelligent systems will unburden scientists, allowing them to focus on understanding their results and formulating new hypotheses. This ambition will be achieved through computational efficiency, scalability and autonomy.These research topics will be addressed in the domain of astrophysics, as astronomers are already overwhelmed by data. This multi-disciplinary (computer science/ statistics/ astrophysics) research will focus on 3 broad areas: Clustering in high dimensional data, e.g., the development of fast n-point correlation function algorithms to fully understand the spatial distribution of galaxies; Anomaly detection, e.g., the automated discovery of new astronomical phenomena in massive, multi-wavelength data sets; Fast kernel density estimation, e.g., the morphology-density relation of galaxies. These algorithms will be exported to distributed Grid systems, especially the UK AstroGrid and the US Virtual Observatory. Dr Nichol is a recognized leader in the development of data-mining algorithms for massive astronomical data sets. He returns to the Institute of Cosmology & Gravitation, Portsmouth, after 12 years in the USA. The Institute has internationally recognised expertise in theoretical cosmology and grid computing, and is a partner in the UK National Cosmology Supercomputer Consortium, with its own advanced computing resources. Nichol will bring a new aspect of high-tech training to students in Portsmouth through his innovative research and teaching ideas. Once established, he will broaden this training throughout Europe

Prof. Bob Nichol

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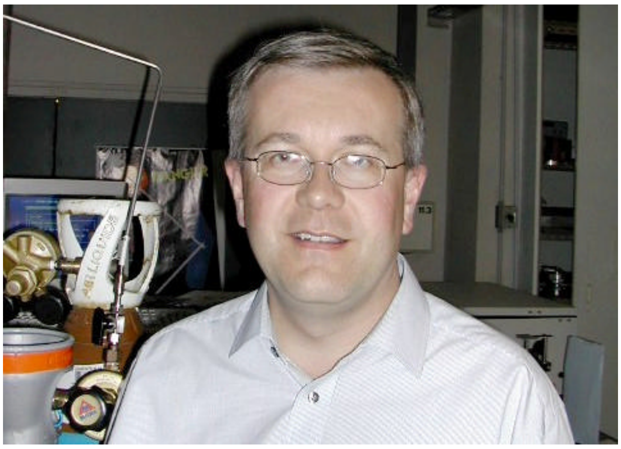
CHEMISTRY AT EXTREMELY LOW TEMPERATURES

COOL CHEMISTRY

An integrated research and training programme will be carried out in the area of chemistry at extremely low temperatures. The research is centred around the use of the CRESU[1] supersonic flow technique to conduct research under three headings: (1) collisional processes at very low temperatures for astrochemistry (T > 10 K); (2) collisional processes at extremely low (T = 1-10 K) temperatures for comparison with theory; and (3) the growth of clusters/nanoparticles at a molecular level. The training programme involves PhD thesis supervision in this area, as well as lectures at undergraduate, postgraduate and public level.

The chair holder is Professor Ian R. Sims (IRS), Professor of Physics at the Université de Rennes 1, in Brittany, France. IRS studied Natural Sciences at the University of Cambridge (UK) before undertaking a PhD in gas phase kinetics with Professor Ian WM Smith (IWMS) at the University of Birmingham (UK). This was followed by two periods of postdoctoral research, the first at Caltech (with Professor Ahmed Zewail, studying femtochemistry) and the second at the Université de Rennes 1 with Dr Bertrand Rowe. It was during this second period that, in collaboration with IWMS, he performed the first measurements of neutral-neutral reactions in the CRESU apparatus which showed that an unexpectedly wide range of chemical reactions actually become faster at very low temperatures, contrary to the then accepted view. IRS returned to Birmingham, first on an EPRSC Advanced Fellowship, and later as Lecturer and then Senior Lecturer. In collaboration with IWMS he constructed a new CRESU apparatus at Birmingham, and continued to work in collaboration with the Rennes team of Dr Bertrand Rowe. This collaboration resulted in the award to both teams of one of the first EU Descartes prizes in 2000. In 2003 IRS accepted a chair in physics at the Université de Rennes 1.



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[1] Cinétique de Réaction en Ecoulement Supersonique Uniforme, or Reaction Kinetics in Uniform Supersonic Flow