Foreword

The Indian Association for the Cultivation of Science (IACS) is on the threshold of a momentous occasion — the celebration in the year 2001 of its 125 years of functioning. Looking back through the vista of time, to the inception of IACS and the role it has played in the growth and development of Indian Science, is indeed a very stimulating experience. Its glorious history spans the pioneering achievements and dedication of its founder, the visionary and patriot Mahendra Lal Sircar, of the renowned scientists C V Raman, K S Krishnan, M N Saha and a host of other luminaries, who all contributed to the great heritage that is the bedrock of IACS of the present time. Inspired by these titans, the scientists of today have continued to uphold the excellence in research, and have made major strides in the various fields. Apart from making significant contributions in the mainstream areas of Chemistry and Physics, IACS has also diversified into several frontier areas with technological potentiality and the biology-inspired sciences.

In this new millennium, IACS stands poised between the two worlds : its vibrant present evolving from its past with rich heritage and a future pregnant with possibilities in a rapidly changing global scenario. An important strength of IACS is the confluence and synergy of the activity of its various wings. IACS is thus in a unique position not only to consolidate and expand its current activity but also to venture in the emerging cross—disciplinary areas.

This booklet tries to capture the goals and aspirations nurtured by us in the course of time, the pleasures and pains experienced along the way and the spirit of our undying dreams.

D. Mukherjee
Director

A Century : An Outline

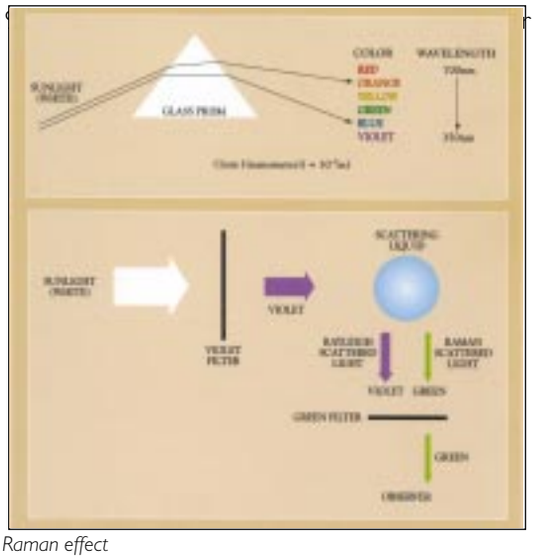
The Indian Association for the Cultivation of Science (IACS) is symbolic of the intellectual awakening that swept Bengal in the nineteenth century. It was a time of practical dreamers who wanted to substantiate their dreams. Born in 1833, Mahendra Lal Sircar became a Doctor of Medicine but his dream was to establish an institution where, 'lectures on scientific subjects will be systematically delivered…'

It was a time when facilities for teaching of science were virtually nonexistent in this country. Mahendra Lal realised that if the country is to advance, 'it can only be by means of science.' Many were aroused by the idea and Mahendra Lal's dream institution finally took shape in the form of the Indian Association for the Cultivation of Science which was formally inaugurated at 210 Bow Bazar Street in Central Calcutta on Saturday July 29, 1876.

Mahendra Lal became the first Honorary Secretary of IACS, a position he held till his death in 1904. A remarkable galaxy of men taught at IACS in the early years – Rev. Father F. Lafont, Jagadish Chandra Bose, Asutosh Mookherjee and Chunilal Bose, to mention a few. Prafulla Chandra Ray, then a student of Presidency College, attended such classes much to his profit.

Pandit Iswar Chandra Vidyasagar and Keshab Chandra Sen were among the Members of the first Trustee Board of 1876. Also associated closely with the IACS were persons like Guru Dass Banerjee, Rajendra Lal Mitra and Surendra Nath Banerjee. In 1912, Raja Peary Mohan Mookherjee became the first Indian to become the President of IACS. Years later Nilratan Sircar, Jnan Chandra Ghosh and Satyendra Nath Bose adorned this position. Satyendra Nath also held the National Professorship at IACS.

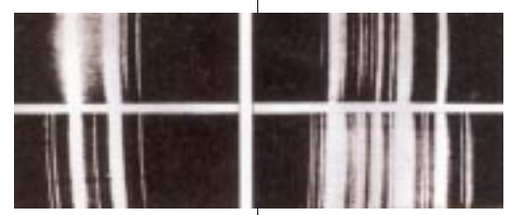
Nearly thirty year after the inauguration, the young Chandrasekhar Venkata Raman, still in his teens, enrolled himself as a member of IACS in August 1907 and started carrying out research in his spare time. The rest is history. The Raman effect was discovered in 1928 and Nobel recognition came in 1[illegible] research



Raman effect

in Physics, the fortyfive year old Raman left Calcutta for Bangalore in 1933. In 1998 the American Chemical Society eulogised the discovery of Raman effect by installing an International Historic Chemical Landmark plaque at IACS.

In the year Raman left Calcutta, K. S. Krishnan joined IACS as the first Mahendra Lal Sircar Professor and started his celebrated work on magnetic anisotropy. In 1942 Krishnan also left for Allahabad and the mantle was ably carried forward by K. Banerjee who became an early pioneer of the direct method in crystallography.



First Raman spectra

The building and space at Bow Bazar Street were becoming increasingly inadequate for the activities of IACS. In 1946, the year before independence, Maghnad Saha became the President of IACS. Nearly ten acres of land were promptly acquired at Jadavpur, then the southern fringe of Calcutta city. The foundation stone of the new building was laid on September 26, 1948 by Dr Bidhan Chandra Roy. The new campus became functional in 1951 and in 1953 the Association found its first whole-time Director in none other than Meghnad Saha. Things were moving fast and the mood and mantra were of development and progress. Then came a brutal tragedy – the sudden demise of Saha in 1956.

Things were moving fast and the mood and mantra were of development and progress. By 1957 eight departments of physics and chemistry were making their impact felt : (1) General Physics and X-rays, (2) Magnetism, (3) Optics, (4) Theoretical Physics, (5) Physical Chemistry, (6) Organic Chemistry, (7) Inorganic Chemistry and (8) Macromolecules. Leading researchers included S. C. Sircar, B. N. Srivastava, A. Bose, P. Rây, N. K. Dutt, S. R. Palit, Sadhan Basu and P. C. Dutta. By 1975 the departments had produced more than two thousand research papers and more than three hundred doctorates in science.

IACS became hundred-year-old in 1976. It was a time for celebration of heritage, of achievements past and present and of future possibilities. The work of the hundred years has been chronicled in detail in the book 'A Century' published by IACS in the centenary year. A few glimpses are recorded i

Raman's Spectrograph

PHYSICAL SCIENCES

- Discovery of Raman effect
- Magnetic anisotropy of graphite and rare earth compounds (critical torque method)
- Early work on direct methods in crystallography
- Proof of singularity in the evolution of big bang universe
- First observation of dinuclear magnetic exchange interaction
- Excited state symmetries and exciton splitting (electronic absorption and luminescence spectra)
- Hydrogen bonding, rotamers and librational modes (Raman and IR spectra)
- Dielectronic relaxation in polar liquids (radio- and microwave spectra)
- Electronic structure of transition metal compounds (Zeeman splitting in pulsed magnetic field)
- Photodissociation of molecules
- Charge transfer in ion-atom and rotational excitation in atom-molecule collisions
- EPR spectra of copper compounds with a home-built K-band spectrometer
- Early work on air liquifaction (multistage turbine method)
- Metallic thin films
- Band structure of metals, semiconductors and alloys
- Structural phase transitions at low temperatures
- Transport and galvanometric properties of graphite
- Transport properties of gases in fractional distillation of petroleum
- Calculation of pion-nucleon and kaon-nucleon scattering cross sections
- Variational methods for ion-atom collision problems
- Efficient analytic algorithms for calculating matrix elements in ion-atom scattering

CHEMICAL SCIENCES

- Kinetics and mechanisms of free radical polymerization reactions
- Free radical intermediates in redox reactions
- End group analysis of polymers by dye techniques
- Chemistry of rubber vulcanization
- Thermodynamics of liquid mixtures and polymer solutions
- Micelles, self-assembly, hydrophobic interaction and long-range water structure
- Quantum mechanical free-electron model : structure and reaction of delocalized systems
- New strategies in stereocontrolled organic synthesis
- Polycyclic aromatics, quinolines and isoquinolines
- Bridged-ring sequiterpenes, diterpene resin acids, ophiobolin sesterterpenes
- Bicyclooctanone systems and tetracyclic core of gibberellins
- Novel reactions : catalysed ring juncture isomerisations, annelations, keto-carbenoid additions and insertions, diazomethyl ketone cyclisations
- Coordination chemistry : synthesis, stereochemistry and reactions of new species
- Ligand design : biguanides, b-diketones, Schiff bases and hydroxamic acids
- d-Block and rare earth compounds : unusual oxidation states, stability constants and thermodynamics
- Mechanisms of substitution reactions of planar and octahedral species
- New analytical reagents, electroanalytical techniques and thermogravimetry
- Isolation and chemistry of new carbohydrates from Nature
- Structure of polysaccharides of plant origin
- Immunochemistry of capsular and cell-wall polysaccharides from pathogenic bacteria
- Characterization of leech connective tissue glycoprotein
- Structure of carbohydrates of humic and fulvic acids from soil humus

Twentyfive Years

An Overview

The centenary celebrations which spread over a full year (1976-1977) was a landmark event in the history of IACS. Inaugurated by the Prime Minister Smt. Indira Gandhi on July 29, 1976, the celebrations were marked by major national and international symposia and conferences attended by many distinguished physicists and chemists from India and abroad. The centenary proceedings had a highly positive impact on the image, function and vitality of IACS.

Availability of increased funding and the desire to instill a fresh scientific look induced IACS to search for scientists who were relatively young but already eminent, scientists who could provide leadership and open up new areas of research. This search was very successful and led to the appointment of a number of such distinguished physicists and chemists in a short span of time. These and other scientists of IACS have since contributed very significantly in keeping IACS at the frontier of research – primarily basic research but with forays into fields having technological and social relevance. National and international recognition, major prizes and medals, fellowship of distinguished scientific academies, editorship of leading journals have been normal outcomes of the impact made.

The accelerated activity of IACS soon called for certain structural changes so as to optimise outputs. To achieve this a review was necessary. The Review Committee having C. N. R. Rao as the Chairman visited IACS in 1983 and held detailed discussions with faculty, staff and students. The proposed restructuring led to renaming and realigning certain departments and to the creation of some units. Subsequently some further changes were required and in 1997 another Review Committee visited IACS. In addition to the Review Committees, the work of IACS is now overviewed on a regular basis by the Research Advisory Committee (RAC) which is reconstituted from time to time. Six visits have so far been made by RAC's. This has considerably helped in focusing and consolidating the research activities.

The topography of the campus has changed significantly over the years. The second floor of the main building was completed fulfilling the original plan of Meghnad Saha. The boys hostel has been extended and a new ladies hostel constructed. Other constructions include the energy research building and housing for the liquid He plant and a Level IIII Computer Centre (ICOSER facility). Some staff quarters and a canteen building have been erected. The new library building is coming up which will finally house the vast IACS treasure of journals and books. The campus has now been fully networked and hooked with the internet facility available round the clock. These developments apart, the free space now available at IACS is virtually nil. A new campus is the need of immediate future — a need for forging ahead with the plans of diversifying research activities in the new millennium.

The eight current departments of IACS are (1) Material Science, (2) Solid State Physics, (3) Spectroscopy, (4) Theoretical Physics, (5) Biological Chemistry, (6) Inorganic Chemistry, (7) Organic Chemistry and (8) Physical Chemistry. The three active units are (1) Energy Research, (2) MLS Professor and (3) Polymer Science. The activities of these departments and units will be briefly presented in the following section. More than four thousand research papers and nearly six hundred doctorates have been produced.

It is noteworthy that the activities of the departments and units are interlinked and more often than not, are interdisciplinary in nature. Indeed the contributions can be categorised under four interdisciplinary thematic areas : (1) Molecular Sciences, (2) Physics and Chemistry of Materials, (3) Biosciences and (4) Theoretical Sciences. The matrix of linkages of the departments and units to the thematic areas is shown on the right.

Two events of celebration at IACS deserve special mention. In 1984 the 150th birth anniversary of Mahendra Lal Sircar was remembered through seminars, exhibitions and setting up of a Janakalyan Kendra at village Paikpara, Howrah, the birthplace of Mahendra Lal. Raman Centenary was celebrated in 1988 and as part of it an International Conference on Raman Spectroscopy was held in the campus.

Departments	Areas of activity			
	Molecular science	Physics and chemistry of materials	Biological sciences	Theoretical sciences
Materials Science	•	•		•
Solid State Physics	•	•		•
Spectroscopy	•	•	•	•
Theoretical Physics	•	•	•	•
Biological Chemistry	•		•	•
Inorganic Chemistry	•	•	•	•
Organic Chemistry	•		•	•
Physical Chemistry	•	•	•	•
Energy Research Unit	•	•		•
Polymer Science Unit	•	•	•	•
MLS Professor's Unit	•	•		•

Energy Research Unit Building

ICOSER facility at Computer Centre

New Library Building

Energy Research Unit

Origin

The Energy Research Unit was established in 1986 following the recommendation of the Third Review Committee.

Activity Profile

The Unit had initially focused on the development of advanced solar photovoltaic technology. In 1987, it received generous funding from UNDP and DNES/MNES for the development of a-Si solar cell. Since then the Unit has maintained balanced activity in basic as well as technological research.

Research Highlights

A Development of Materials and Fabrication Technology of Amorphous Silicon Solar Cell

As a result of the dedicated effort by the team in Energy Research Unit, it has been possible to

(i) develop plasma processing technique for deposition of thin films and fabrication of devices,

(ii) develop state-of-the-art hydrogenated amorphous silicon, it's alloys like SiGe:H, SiC:H, etc. and microcrystalline silicon films,

(iii) develop transparent conducting oxides like indium tin oxide, tin oxide and zinc oxide by the magnetron sputtering method,

(iv) develop fabrication technology for single and multijunction a-Si solar cells.

Our expertise in the field led to our active participation in the development of process, commissioning and operation of the pilot plant set up by Bharat Heavy Electricals Ltd. at Gwalpahari, Harayana.

B Polycrystalline / Microcrystalline / Nanocrystalline Silicon Thin Films for Application in Solar Cells

Recently, polycrystalline silicon thin film solar cells are drawing considerable attention due to their inherent advantage of performance, stability under light exposure and high conversion efficiency. Using the PECVD technique, device quality poly-Si films have been developed at low temperature (200^0) on low cost substrates like glass. Undoped microcrystalline and nanocrystalline films with very low degradation have been prepared using novel techniques and subsequently used in solar cells.

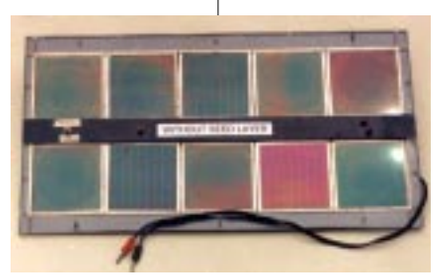
C Setting up of a Plasma Diagnostic Facility

Optical Emission Spectroscopy and Langmuir probe arrangement have been incorporated with the PECVD deposition system. The objective is to study silane plasma which is used for the deposition of photovoltaic grade amorphous silicon. An accurate knowledge of the plasma helps to improve material properties.

Faculty:

A K Barua
D Das
P Chaudhuri
P Chatterjee
S Ray

a-Si Solar cell driven appliances developed at ERU (i) calculator (ii) radio (iii) battery charger



Double junction amorphous silicon solar module fabricated at IACS with 6% stabilised efficiency (without laser scribing)

D Computer Modelling of Solar Cells

At integrated electrical-optical model for the simulation of the performance of solar cells has been set up. The model can take into account both diffused reflection and transmission due to interface roughness and specular interferential effects. It has been used to analyse and optimise the performance of a-Si:H based double junction solar cell having a microcrystalline silicon window layer.

Multichamber PECVD system for fabrication of a-Si thin film solar cell

E Thin Films by Photo-CVD Technique

Photo chemical vapour deposition technique has been used to develop different thin film materials like 'Diamond like carbon' and alloys of silicon. To the best of our knowledge no other group in India has developed this deposition technique. Using low temperature deposited SiO_χ passivation layer improvement in efficiency of C-Si cell has been obtained.

MLS Professor's Unit

Origin

MLS Professor's Unit came into existence in July, 1987. Since then it has functioned with a lone faculty member.

Activity Profile

The focal theme of research activities of the unit has been science and technology of nano-materials. Significant contribution has been made in the fields of Glass-Metal and Glass-Semiconductor nano-composites.

Research Highlights

A Nonconventional Glasses by Sol-Gel Route

Some of the systems investigated are:

SiO_2 - Sb_2O_3, SiO_2 - As_2O_3, Fe_2O_3 - SiO_2. The first two are characterized by high dielectric constant over a limited temperature range around room temperature.

B Preparation and Characterization of Ferrites-Soft and Hard

Both sol-gel and glass ceramic methods were used.

C An inhomogenous Conductor model

The model was developed and applied successfully to a large number of glass systems prepared both by melt quench route as well as by the sol-gel method.

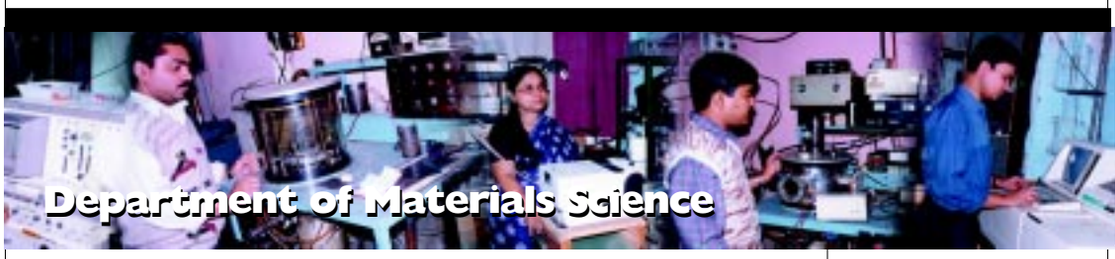
D Investigation on Nanocomposities

Glass-Metal and Glass-Semiconductor nanocomposites of different compositions were synthesized by a variety of soft chemical routes. Electrical, Optical and Magnetic properties were studied. Some of the significant observations were: fractal growth of metallic phase under the influence of electric field-the metal phase comprising of an assembly of interconnected nanosized metal particles, quantum confinement effect as evidenced by the electrical transport and optical properties; large electronic polarization in nanosized metallic strands; core-shell structure effect on the magnetic behavior of nanosized ferromagnetic-ferrimagnetic composites.

The future research efforts would be directed to develop molecular-level templates for growing nano scale phases of different kinds to study their physical properties.

Faculty:
D Chakravorty

Fractal growth of a metallic phase



Department of Materials Science

Origin

The Department of Materials Science, previously known as the Department of General Physics & X-Rays, was created in 1986 with a view to concentrating on the science and technology of advanced materials.

Activity Profile

The profile of activity over the last two decades points to gradual diversification of the research activities of the department into the challenging areas of advanced tailor-made materials and consolidation of activities in areas where our past record has been impressive. In fact, now the Department presents an admirable blend of research in basic and applied sciences.

Research Highlights

I Materials Science and Condensed Matter Physics

A Low Temperature Experiments and Condensed Matter Theory

A sophisticated low-temperature laboratory has been set up to measure electrical properties down to 0.3 K and in magnetic fields upto 8 Tesla. The transport properties of magnetic/metallic multilayers and intermetallic compounds, colossal magnetoresistance and low temperature electrical properties of polyaniline blends have been extensively studied. Computational techniques, based on first principle electronic structure calculation have been developed for strongly correlated many electron systems.

B Synthesis and Characterization of Thin Films for Fundamental Studies and Device Fabrication

(i) Synthesis of binary and ternary semiconductors for the fabrication of thin film solar cells.

(ii) Synthesis of nanostructured materials in thin film form.

(iii) Hard coating materials : Diamond and nitride (c-BN and AlN) films.

(iv) Preparation of stress-relieved diamond-like carbon films for practical application.

(v) Surface and interface properties of multilayer thin films using AES and scanning probe microscopic techniques.

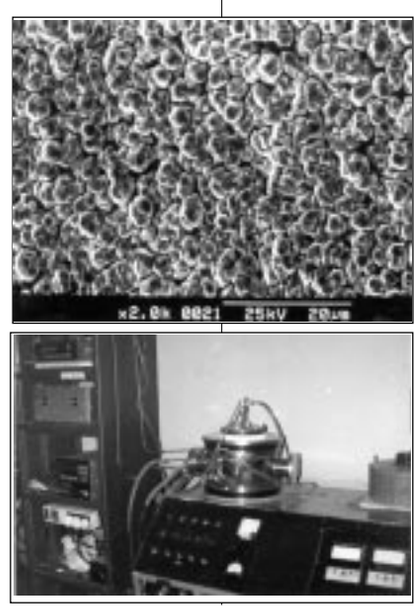
The following are the important achievements:

Rapid thermal processing (RTP) of absorber layer for the fabrication of large-area solar cells.

Fabrication of pressure sensors with diamond/diamond-like carbon

Faculty:

A K Pal
B K Sarkar
M De
S C Saha
S K Sen
S P Sengupta
S S Bhattacharyya
S K De
S Chatterjee
S Chaudhuri
T Kar



Diamond coating by plasma CVD

films.

Deposition of diamond films at low substrate temperature by hot filament chemical vapour deposition (HFCVD) technique from a low-cost precursor material (camphor).

Conduction mechanism in nanocrystalline composite films with nanocrystalline II-VI semiconductors embedded within a dielectric (SiO_2) matrix.

Nondestructive technique was developed for the studies of mechanical properties of thin films from below band gap optical absorption process.

Pseudopotential formulation to explain the composite experimentally obtained interfacial diffusion parameters.

- Synthesis and in-depth study of conducting transparent ZnO film.

C X-ray Diffraction Studies for Structural Crystallography, Microstructures, Crystal Defects and Growth

Major activities include determination of X-ray crystal structure of some nucleosides, natural products and organic crystals,

morphology and growth of efficient non linear optical materials like KDP, ADP, KTP, LAP, LAHCl, LAHB to be used for devices in the ultraviolet to infrared range of frequencies,

characterization of lattice defects from X-ray powder profile analysis of metals, Alloys, thin films, composites and industrial materials, and determination of amorphous structures in semiconducting materials by X-ray radial distribution analysis.

2 Atomic, Molecular and Optical Physics

The following is a glimpse of our activities in this area:

Clear evidence obtained for single electron capture into excited states in N_2^{++} - N_2 collisions in Ion Beam Scattering experiment.

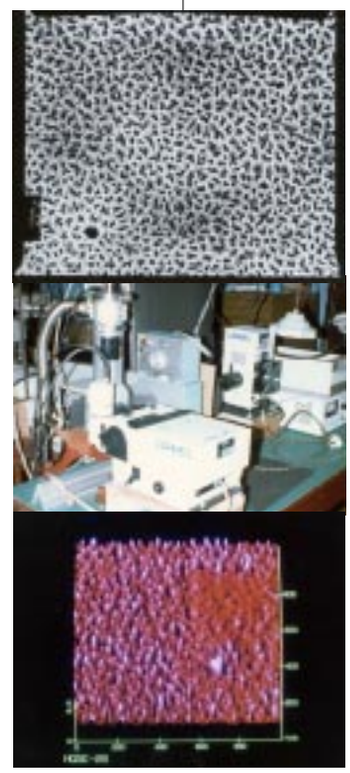
Calculation of rotational excitations and modeling of dark interstellar clouds.

Extensive study of multiphoton infrared absorption in polyatomics including analysis of the role of intramolecular relaxation.

Spontaneous and stimulated Raman processes and two-photon dissociation studied.

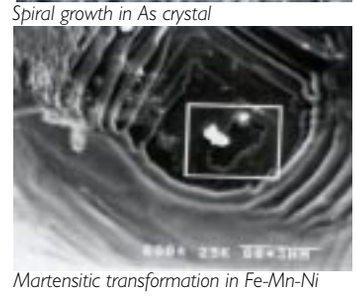
Intense field effects in and laser control of multiphoton dissociation processes examined.

New theory of two-photon autoionization of molecules proposed.



Room temperature visible luminescence from nano-CdTe/SiO_2 composite

Spiral growth in As crystal



Martensitic transformation in Fe-Mn-Ni system

Department of Solid State Physics

Origin

Professor K S Krishnan initiated work on magnetism in IACS in the 1920's. After him Professor K Banerjee came to head the Department of X-Ray and Magnetism, later called the Department of General Physics & X-Rays, and Magnetism. Subsequently, the Department of Magnetism was carved out of it with Professor A Bose as the head in 1956. It was renamed as the Department of Solid State Physics in 1986.

Activity Profile

In the last twenty five years or so, the department has diversified its research activities considerably. In addition to EPR and optical spectroscopy including Zeeman studies on solids, new experimental methods like ultrasonics, Mossbaüer and photoacoustic spectroscopy were introduced. The field of investigation also broadened to cover both crystalline and amorphous solids.

Research Highlights

A EPR, Magneto-optic, Magnetic and Mossbaüer Studies at Low Temperature

Single crystals, both diamagnetic and paramagnetic, undergoing different kinds of phase transitions have been studied. Studies on low dimensional magnetism in different types of 1D Cu(II) paramagnetic crystals have been made from EPR line width measurements showing the importance of exchange coupling. A high pulsed magnetic field (~10T, ~10ms duration) has been set up and low temperature study of Zeeman spectra of several transition and rare-earth doped compounds have been made. Low temperature studies of magnetic susceptibilities, anisotropies, and specific heat of magnetic ordered states and Mossbaüer spectra of minerals and rare earth compounds have been investigated. Crystal field and hyperfine effects have also been studied.

B Preparation and Characterization of High Temperature Superconducting and CMR Materials

A new glass to ceramic technique suitable for making high Tc superconducting material in different forms have been developed. Superconducting properties of many high Tc materials have been studied. Recently metal-semiconductor transitions in rare-earth manganates showing CMR and giant magneto-resistance have been investigated from the study of transport, thermal and magnetic properties. Phonon-drag effect, polaron hopping conduction and contribution of magnetic polarons have been elucidated.

C Acoustic and Photoacoustic Properties of Solids and Liquids

An ultrasonic pulse echo interferometer was developed and ultrasonic properties of several alloys and glasses have been studied. Suitable

Faculty:

A J Pal
A K Pal
A Ghosh
B K Chaudhuri
C Basu
D Ghosh
M Mukherjee
R K Mukherjee

models have been developed to analyze the elastic behavior of binary glasses. Photoacoustic spectrometer (PAS) has been developed for the nondestructive characterization of materials and for direct measurements of optical band gap, thermal diffusivity, optical absorption coefficient etc. in narrow gap semiconductors and, dilute magnetic semiconductors etc. Superconducting transitions in high Tc materials are also studied using the PAS technique.

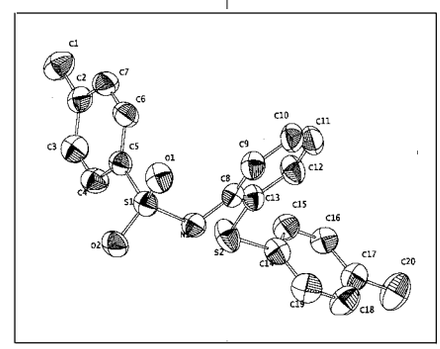
D Dielectric Spectroscopy

The technique has been developed to measure frequency dependent relaxation behavior of glasses, polymers and gels, etc. Various computer programs for the analysis of the experimental data have been developed.

E Single Crystal Growth and Crystal Structure Study by X-ray

Different techniques (Bridgeman, Zone melting, Holden etc.) for growing high temperature melting single crystals have been developed in the department. High temperature melting Bi-Te, Bi-Se, $CsCdCl_3$, $CsCdBr_3$ etc. crystals have been grown for different studies. Many solution grown ferroelectric and antiferroelectric KDP-ADP, NH_4Cl-KCl, Rochelle salt, ADP, etc. crystals have also been grown and their ferro and antiferroelectric properties studied.

The existing direct method using the real space and reciprocal space concept for the ab initio crystal structure studies of macromolecules has been modified. Studies of disorder in metal complexes using X-ray crystallographic technique, conformation of several organic compounds as well as inorganic complexes have been made. New settings in some space groups have been theoretically worked out.



Molecular diagram of an organic compound revealed by X-ray diffraction

F Melt-Quenching and Sol-Gel Processing of New Materials and Study of Conductivity Spectra and Scaling Behaviour in Glassy Materials

Sol gel technique has been developed in the department for the preparation of several oxide glasses, and ceramic materials including superconducting and ferroelectric materials. Structural, optical and electrical transport properties, dielectric and conductivity relaxation have been studied in several glasses. A new scaling formalism for the conductivity spectra indicating a correlation of relaxation dynamics with structure, has been developed.

G Light Emitting Diodes: Operation Mechanism and Device Physics - Molecular Electronic Devices

Different types of semiconducting materials have been used to fabricate LEDs. Charge injection mechanism, barrier heights for the charge carriers, dielectric constant of the LED materials etc. have been studied. High frequency (400kHz) luminance has been obtained from these devices which are thin on a molecular level. The intrinsically accumulated

charge has been shown to result in an instantaneous EL at the beginning of first voltage pulse.

H Experimental and Theoretical Study of Phase Transitions

Structural characterization of some macrocyclic complexes, and thermally induced phase transition (between 370 to 170K) have been carried out by X-ray structural analysis. A unified theory for studying structural phase transitions called pseudo-spin lattice coupled mode (PLCM) model has been developed. Soft mode, central peak, central dip, deuteration induced phase transitions in some single crystals have been explained in many ferreolectric and H-bonded crystals. A conduction type calorimeter has been developed for studying heat capacity down to LN2 temperature and phase transitions of a number of magnetic and non-magnetic crystals and mixed molecular crystals have been studied. A cryostat for measuring heat capacity at liquid helium temperature has also been constructed.

I Pressure Induced Phase Transitions of Ferroelectric and Antiferroelectric Liquid Crystals

AvH Foundation, Germany, has sponsored the study of dielectric relaxation behavior, piezoelectric properties, etc. of ferroelectric and antiferroelectric liquid crystals of technological importance. A high pressure cell has been designed to study dielectric constant and polarization of FLC and LC under pressure.

Pulsed high magnetic field setup

Department of Spectroscopy

Origin

The Department of Optics was established in 1948 with Professor S C Sirkar, as the Head. In 1986 it was renamed as the Department of Spectroscopy.

Activity Profile

During the last two decades and a half, the department has broadened its research horizon to encompass many of the emerging areas of non-linear spectroscopy, surface-mediated phenomena, photo-induced conductivity, fast photodynamics, etc. In addition, topics like physics of liquid crystals, spectral diffusion in disordered molecular solids, lasing without population inversion, laser assisted multiphoton processes and non-linear optical properties of atoms and molecules have received increasing attention of the faculty.

Research Highlights

A Laser Raman Spectroscopy

Under the "National Laser Program" of DST, a Laser (Ar ion) Raman Spectroscopy laboratory was set up. Normal Raman, resonance Raman, surface enhanced Raman and surface enhanced resonance Raman spectroscopy have been used as tools to study solvent induced vibrational relaxation, phase transitions in organic crystals, lattice phonon mediated solid state photoreaction, and silver-water interfacial phenomena. Necessary interfaces have been locally designed and computer programs developed for data acquisition and analysis in Raman / luminescence spectroscopy / CARS / Pico-second degenerated four wave mixing.

B Experiments with Langmuir Blodgett Films

Spectroscopy of organic molecules and energy transfer in molecular systems in restricted geometry of frozen organic glasses, polymers, sol-gel glasses, micelles, electrooptic and Second Harmonic generation on Langmuir Blodgett films have been extensively investigated. Percolation model has been successfully applied to triplet energy transfer, and experimentally evaluated critical exponents have confirmed the presence of two and three dimensional percolation . On the technology front a fully automated programmable Langmuir-Blodgett (LB) film deposition apparatus has been designed and fabricated. The technology has been transferred to NRDC, Govt. of India.

C Molecular Electronics and Biosensors

Under "Technology Mission Initiation" scheme of DST, research on molecular electronics and biosensors was undertaken and four biosensors, two for ethanol and two for monitoring fish freshness, have been developed. The technology has been transferred to NRDC for patent sealing and commercialization. One patent (alcohol) has been sealed and another (fish freshness) is under processing.

Faculty:

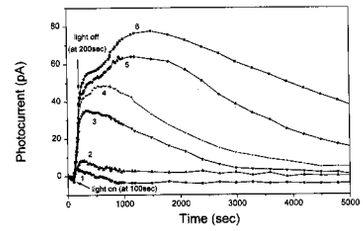
A K Das
B Mallik
G B Talapatra
K Rai Dastidar
P K Mukherjee
S Chakravorti
S K Roy
S Chattopadhyay
T Ganguli
T N Misra

Laser Raman Spectrophotometer

D Dark, Semi and Photoconductivity Measurements

Photoinjection of carriers from electrodes and direct electron-hole pair production and recombination via shallow traps at short time, second order decay through exponential traps at long time have been confirmed. Ultrathin organised assemblies of conducting polymers have been studied to understand conduction mechanisms and dimensionality of charge transport in varied assemblies.

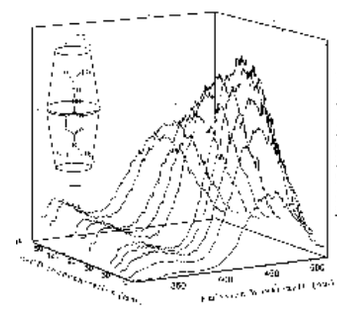
Studies on spectroscopic, semi and photoconductive properties of some biologically active organic and organometallic compounds important for developments of gas vapour sensors, molecular electronics, molecular photonics and optoelectronic devices have led to the confirmation of the formation of charge transfer complexes, the validity of compensation effect in semiconduction processes, adsorption induced phase transition, low frequency electrical current oscillations in vapour adsorbed state, photoinduced phase transition, and electrical current instabilities in the relevant materials after withdrawal of photosource .



Persistent photocurrent in ferrocene-doped PMMA thin films containing chloroform as impurity

E Spectroscopy and Excited State Photodynamics

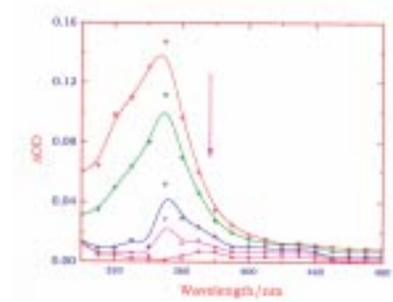
The symmetry forbidden $^1B_{2u} \leftarrow {}^1A_{1g}$ transition in a series of organic molecules have been analysed in relation to excited state geometry. Vibrational assignment in different aromatic molecules from Raman and infrared spectra enabled as to predict their molecular configurations. The dynamics of optical changes in cholesteric liquid crystals with guest molecule was investigated using single laser beam excitation. A few potential photosensitizers have been identified by spectroscopic experiments. Theoretical calculations were done for designing molecules with similar properties. Our studies on photodynamics in general, established understanding of N-heteroatomic photophysics, formation of twisted intramolecular charge transfer excited state in some new molecules and shed light on various aspects of excited state proton transfer processes.



3-dimensional plot of emission spectra of 4-N,N-dimethylaminocinnamic acid in aqueous solution with different concentration of α-cyclodextrin

F Photoinduced Electron Transfer and Relaxation Dynamics

Photoinduced electron transfer, excitation energy transfer and relaxation dynamics in some bichromophores have been studied using nano and picosecond time resolved techniques with a view to designing highly efficient polymeric photoconducting materials.

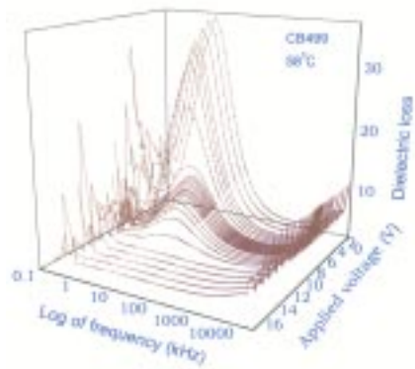


Transient absorption spectra of p-chloroacetophenone in acetonitrile solution at different delay times obtained using nanosecond laser flash technique. (λ_{ex}=355 nm)

G Physics of Liquid Crystals

Orientational order parameters, birefriengence, dielectric anisotropy, layer thickness and intermolecular distance in nematic and smectic phases of liquid crystal molecules, molecular dynamics, spontaneous polarization, tilt angle pitch in ferroelectric smectic C^* phase were determined. Dependence of spontaneous polarization (Ps) on

transverse component of dipolar group present near or at the chiral centre was examined vis a vis Goldstone and soft mode contribution to Ps, molecular tilt., quadrupole coupling between tilt and Ps. The dependence of SmC^*-SmA transition temperature on bias electric field has been established. Microwave absorption and relaxation mechanisms of some organic molecules and their potential energy barrier for reorientation processes, number of rotational isomers, their structure and the percentage composition were also determined.



Behaviour of Goldstone mode and domain mode, with the application of bias electric field, of a ferroelectric liquid crystal material

H Miscellaneous Experimental Work

Experimental and Monte Carlo simulation studies have been done on the exciton dynamics and spectral diffusion in organic disordered molecular systems. Surface plasmon resonance technique was successfully applied for the study of dielectric and non linear optical properties of different materials. Translational energy spectroscopy was used for studying charge transfer processes

I Theoretical Sciences

Calculation of frequency dependent linear and non-linear polarizabilities of molecules by the time-dependent coupled Fock method, Monte Carlo simulation of the processes operating in organic light emitting diodes fabricated using LB film deposition technique, normal coordinate analysis and force field calculations of heterocyclic molecules, studies on lasing without population inversion, laser assisted multiphoton processes, development of a new model of nonlocal quantum electrodynamics, studies on the interaction of swqeezed light with matter highlight some of the theoretical activities of the department. Other notable theoretical activities include static and time dependent perturbation calculations on multipole polarizabilities of closed and open shell atomic systems, understanding the atomic Rydberg states and autoionizing states of two electron atoms, spectroscopy of highly stripped ions, studies on excited states and spectroscopic parameters of small molecules by Half Projected Hartree Fock method and hyperspherical harmonic calculations of ground and excited states of atomic systems.

Department of Theoretical Physics

Origin

The Department came into being in 1951 with a broad spectrum of research activities spanning gravitation and cosmology on one hand and physics of atomic collision processes on the other.

Activity Profile

In the post 1976 period, the Department kept up its excellence in the calculation of cross-sections of atomic and molecular collision processes and made forays into experimental work and analysis of data relating to astroparticle physics. From mid-nineties, the Department has further broadened its activities to encompass topics in statistical physics, non-linear dynamics and fluid mechanics.

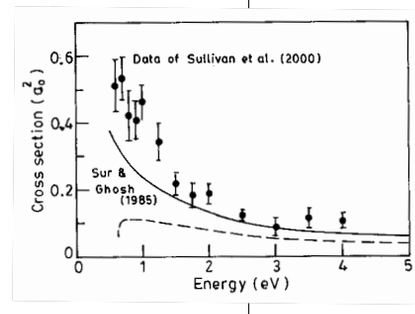
Faculty:

A S Ghosh
D P Bhattacharyya
C Sinha
J K Bhattacharjee
J Chakrabarti
K Roy
V P Gautam

Research Highlights

A Atomic and Molecular Physics

The discovery of mono energetic positron source in 1972 led to extensive studies of positron atom and positron molecule scattering. Scattering cross-sections, calculated at low and intermediate energies agreed very well with the experimental data. The inclusion of the effect of positronium formation was a notable achievement. Calculation of the cross-section for positron-molecule scattering was equally successful. More recently the focus has shifted to positronium-atom scattering and a long standing puzzle in the experimental data at low energies has been resolved. The theory group has calculated ionization cross sections in heavy particle collisions and found agreement with experiments at low energies.

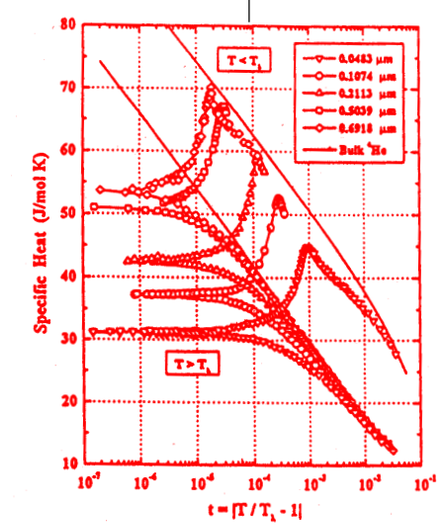


B Solid State Physics

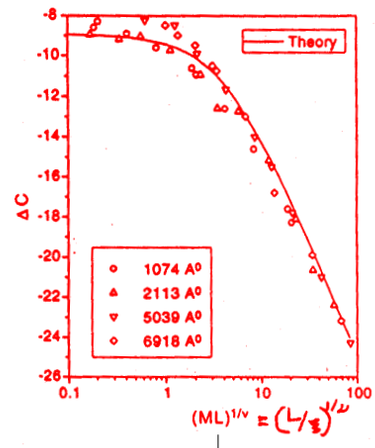
A particularly elegant derivation of the Froelich Hamiltonian was given in the early eighties. Fermions on a lattice have been extensively studied from the point of view of bosonization. The effects of an applied field have also been investigated.

C Statistical Physics

How close can one get to the critical point in an experiment? If the experiment is on gas-liquid system or a binary liquid mixture, the limitation is produced by the density stratification produced by gravity. The density and hence temperature is not constant throughout the cell and this sets a limit to how big the correlation length can get. Conducting critical phenomena experiments in NASA space shuttles has removed this constraint. In a gravity free environment, it is possible to approach Tc to the point, where correlation lengths can become several microns. Performing the experiment in a cell of size few microns, now lets the experimentalists explore a domain where the system size is smaller than the correlation length. This leads to deviations from the thermodynamic limit. With system size L and the correlation length ξ as the two competing parameters, response functions like

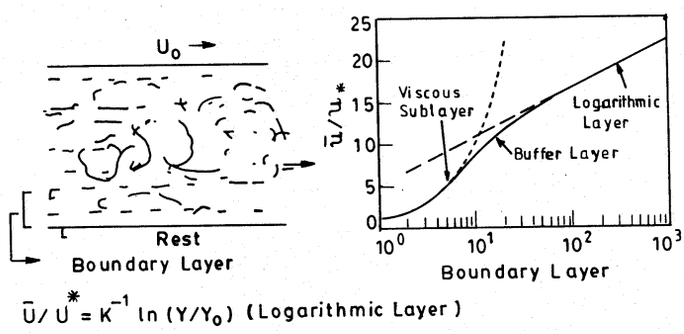


susceptibility and specific heat depend on both ξ and L. With proper extraction of critical parts, the response functions depend on the single scaled variable ξ/L. The purpose of the experiments is to test this scaling and of theory to actually calculate the function. For specific heat near the lambda transition of helium, the data and the two-loop scaling function obtained in our group are shown in the figure.



D Non-linear Dynamics

Turbulent Shear Flow



κ is an universal number (Von Karman's constant) measured to be κ = 0.40. While this number has been known for the last 100 years, its calculation has never been attempted. Calculations done in the theory group yield κ >> 0.50 at one-loop level.

E Dynamical System for Marangoni Convection

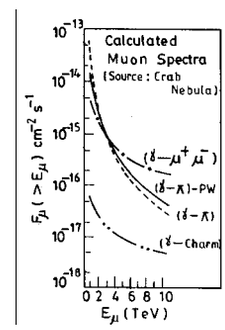
While the buoyancy driven Rayleigh convection was the more studied phenomenon in the seventies and eighties, the experimental importance of thin films has made the surface tension driven Marangoni convection a major field of study in the nineties. Our primary contribution is establishing a dynamical system for studying the effects of nonlinearities in Marangoni convection.

Keep it short!

As an open polypeptide chain undergoes a folding process, it passes through a metastable state which has properties of a spin glass. In this state, the evolution is extremely sensitive to the specifications of the initial bonds. Consequently, it was shown that synthesizing shorter proteins is easier than synthesizing longer ones.

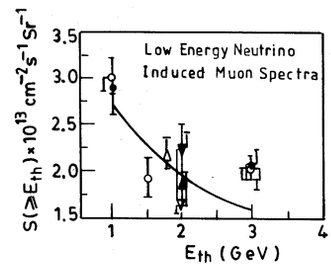
F Large-N Quantum Mechanics

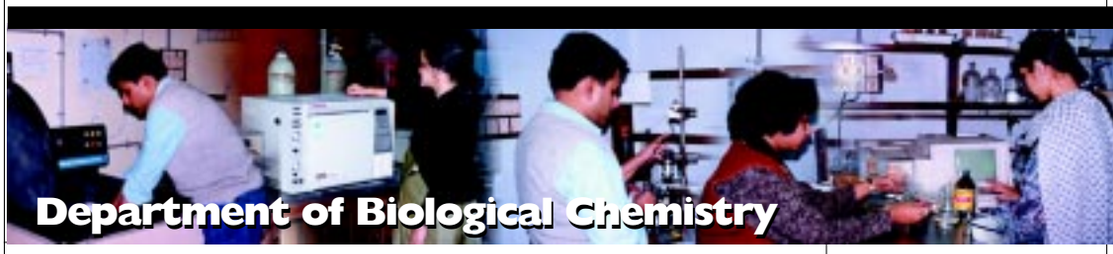
An approximate method of constructing radial wavefunctions that follow the classical orbit for a central potential was set up by exploiting the properties of Schroedinger equation in a N-dimensional space with N >> 1.



G Astro Particle Physics

The vertical muon spectrum showing the intensity vs. depth below a standard rock has been calculated using primary nucleon spectrum and data on hadron-nucleus collisions. The abundance of Ne to Ni nuclei above 4.1 Gev near the top of the atmosphere has been found using balloon borne passive detector results.





Department of Biological Chemistry

Origin

The Department of Biological Chemistry was previously known as the Department of Macromolecules, which came into existence in 1958 with Professor P Bagchi as the Head. It was renamed as the Department of Biological Chemistry in 1986,

Faculty:

A Banerjee
A K Guha
B P Chatterjee
M Ray
N Roy

Activity Profile

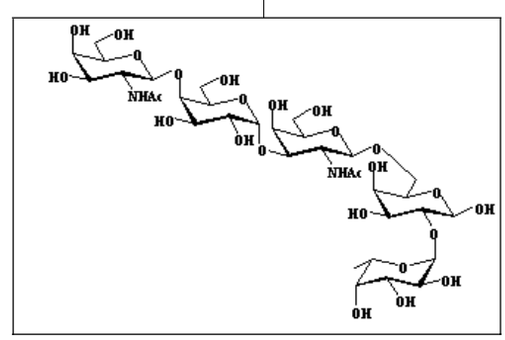
During the last two decades and a half, the Department has made significant contributions in the fields of characterization of polysaccharides from bacterial and plant sources, synthesis of oligosaccharides, molecular level characterization of lectins from plants, animal and microbial species, microbial biochemistry, biochemistry of tumour cells, molecular enzymology and peptide design. A detailed presentation is made in what follows.

Research Highlights

I Molecular Sciences

A Structure and Immunochemistry of Plant and Bacterial Polysaccharides

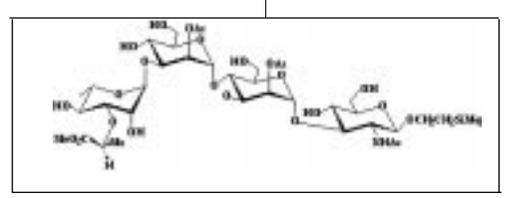
With a view to developing vaccines against bacterial infection, it is important to know the primary structure of bacterial antigens and their immunological specificities. That motivated us to determine structures of several bacterial antigens of *Streptococcus pneumoniae*, *Shigella dysenteriae*, *S.boydii*, *Klebsiella*, *Vibrio cholerae* and *Escherichia coli* and also to determine the immunodominant fragments in these antigens. Lipopolysaccharides from virulent plant pathogens, *namely Pseudomonas solanacearum*, *Erwinia carotovora* and polysaccharides from other sources like, *Arucaria cookii*, *Mirabilis jalapa*, *Madhuca indica*, *Poinciana pulcherrima*, *Pongamia glabra*, *Pterosprmum suberifolium*, *Spondius dulcis* and bael gum were accomplished with respect to their structural and immunochemical aspects. Glycoproteins from bael seed, human milk, goat submaxillary gland mucin, ant egg, *Epidermophyton floccosum*, *Trycophyton rubrum* dermatophytes also received attention.



Structure of E. coli *O126 O-antigenic polysaccharide*

B Synthesis of Oligosaccharides of Biological Interest

The critical role of oligosaccharides in biological processes and the promise of therapeutics based on them prompted us to synthesize oligosaccharides of biological interest on one hand and to develop newer techniques of the synthesis of carbohydrate derivatives on the other. Several di-, tri- and tetrasaccharides related to the antigens from *S. pneumoniae*, *Klebsiella* , *S. dysenteriae* and *E. coli* have been synthesised. Newer methods for the synthesis of partially methylated galactoses, TF-disaccharide and ethyl thioglycosides of sugars as well as for the synthesis of oligosaccharides having galactofuranosides and



Oligosaccharide related to Shigella dysentariae *type 5*

galactofuranosiduronic acids and chemoselective glycosylation have been conducted.

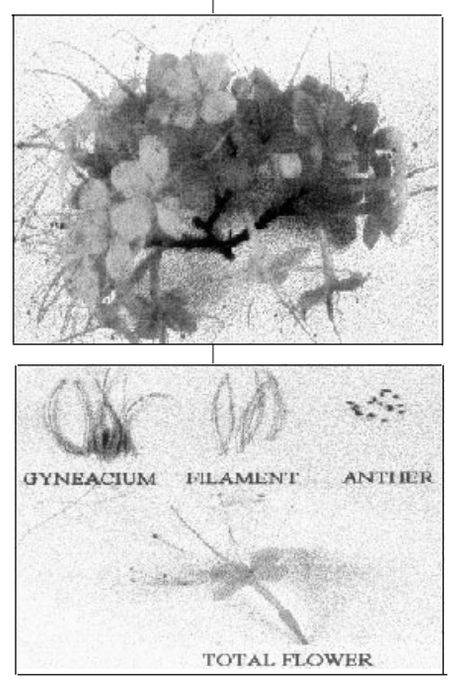
C Peptide and Pseudo-Peptide Design Using Noncoded (Unusual) Amino Acids

Small molecular mimicry of protein structures is a great challenge to scientists. Various types of reverse turns (viz. Alpha- beta- and gamma-turns) play vital role in protein structure and folding. An alpha-turn has been successfully designed in a model pseudo-peptide, Boc-Aib-beta-Ala-N-(N,N"-dicyclohexyl)-Urea. The terminally blocked tetra-peptide, Boc-ϒ-Abu-Aib-L-Ala-Aib-OMe adopts multiple turn structure in solid state involving one novel turn (12-membered ring H-bonded structure) and one typical β-turn (10 membered ring H-bond structure).

2 Biosciences

A Lectins and Allergens

In the last twenty five years lectin-carbohydrate interaction, allergy and immunology have been topics of major research interest. Several lectins from plant, animal and microbial sources were characterized on molecular level. Of them, anti TF-lectin, jacalin from jackfruit seed was a major breakthrough for its unique property to separate IgA_1 and IgD from other Igs. Jacalin was effective as ligand in the affinity matrix to separae several polysaccharides and glycoproteins and as a growth inhibitor of Ehrlich Ascites tumor cell. Lectotyping of different serogroups of *Pseudomonas aeruginosa, Shigella dysenteriae* and *Klebsiella pneumoniae*, a valuable method for epidemiological survey, discovery of anti-A lectin, crotalarin, a substituite of anti A serum used in blood typing, apoptosis by Ashok flower lectin are landmark in bioscience. Immunogenic component has been separated from allergenic counterpart in dust and cotton allergens by lectin affinity chromatography, could be the choice of a more reliable immunotherapy for respiratory allergy. Specific reactivity of excretory-secretory antigen of *Ascaris lumbricoides* helminth with IgG_4 in ascaris infected patients' sera and lack of cross-reactivity with other nematode infected patients' sera leads to a rational approach for serodiagnosis of ascariasis in epidemiological survey.



Saraca indica *(Ashok) flower and it's different parts*

B Biotechnology of Agro Wastes

Production of lactose, lactic acid and single cell protein from whey, the largest by-product of dairy industries causing environmental pollution, has been made possible. Investigation on the production of edible mushroom and organic acids by microbial fermentation of whey are under way. Studies are in progress to produce different qualities of chitin and chitosan and their oligomers from waste products (shell) from shell fish industries.

C Biochemistry and Bioenergetics of Tumor Cells and Molecular Enzymology

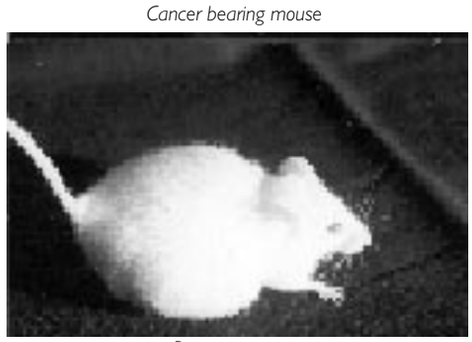
Tumoricidal effect of methylglyoxal and its potential regulatory role

Methylglyoxal , a normal metabolite has been shown to inhibit strongly respiration of a wide variety of malignant cells form both human and animal sources, whereas respiration of normal cells remain unaffected. Furthermore, methylglyoxal made cancer cells nonviable within a short period of incubation and showed strong inhibitory effect on glycolysis, mitochondrial respiration and energy metabolism of malignant cells. These findings have led to the understanding of a very significant biochemical difference between normal and malignant cells. Studies with human tissue samples have been specially important, for designing new and effective anticancer drugs. Based on these results a novel hypothesis that "excessive ATP in cells may lead to malignancy" has been proposed. Evidences have been obtained in support of the proposed hypothesis.

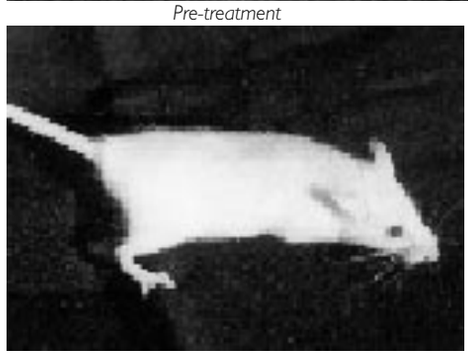
Therapy of Cancer by Methylglyoxal

Methylglyoxal alone or in combination with other anti oxidants and vitamins has strong anticancer effect as evidenced from animal model systems. Appropriate dose, toxicity, and effective delivery systems have been designed for different types of cancer and tumor bearing hosts of different species. With these experiments successfully implemented, methylglyoxal is now on the way to be put on clinical trial. With methylglyoxal as leading ingredient novel formulation has been developed which is highly effective in the treatment of cancer and apparently has no toxic effect, which are in contrast to other drugs now widely used in the treatment of cancer patients.

Cancer bearing mouse



Pre-treatment



Post-treatment

Department of Inorganic Chemistry

Origin

The Department was established in 1951. Professor P Ray was the first Professor. In the early years important contributions were made on the coordination chemistry of d-block and rare earth elements and on analytical chemistry and techniques. The activities of the period starting from 1977 are outlined below.

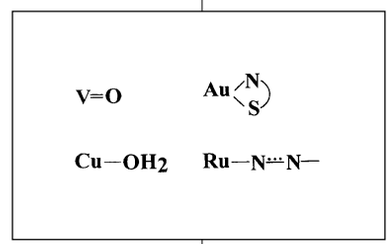
Activity Profile

The chemistry of transition metals is the mainspring of the work. The design and synthesis of new compounds is the primary hub from which major activities radiate. These encompass structure, spectra, magnetism, redox, valence manipulation, cooperative phenomena, mediated reactions, reaction pathways and bioinorganic models. A battery of chemical, physical and theoretical techniques are used in concert to extract and rationalize information. Discrete molecules constitute the mainstay of activity but extended-structure solids and materials are receiving attention. The metals of major concern are those of the 3d series, platinum metals, coinage metals, Mo, Re and Cd. Ligand donor atoms include H, C, N, P, As, O, S and halogens in the form of many functionalities. Ligands are generally tailored to achieve desired binding goals.

Research Highlights

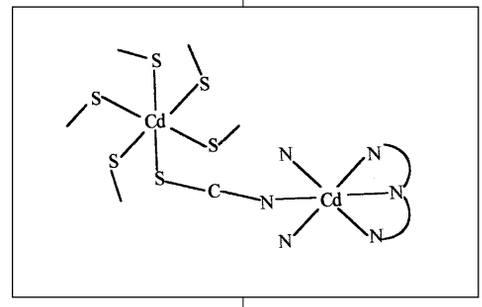
A Mononuclear Systems

Presence of just one metal site per molecule is useful for addressing basic problems of electronic structure and bonding, metal and ligand oxidation state manipulation, isomerism, spin state and bond activation. Recent studies include : conformational isomers of V(IV)O species, polyol-chelated V(V)O, spin control of thioether coordinated Mn(II), nitro-nitrito isomers of Ni(II), sulfur coordinated Ni(III, IV), Cu(I)-water binding, Au(II) aminothiophenolates, crystalline Re(VI)-imidospecies, azo anion radical stabilization by platinum metals, spectroelectrochemical correlations in complexes of noninnocent ligands, redox-driven geometrical isomerization and delayed fluorescence in Cu(I) species.



B Polynuclear Compounds

These are important in modelling intermetal interactions, multiple redox, mixed-valence states and multimetal reaction sites. The cores Ru_2Ag_2 and Ru_2Cu_2 have been assembled. Symbiotic electron and proton transfer has been realized in certain tailored Ru_2 and Os_2 species. Other interesting systems include : isovalent and delocalized mixed-valence poly-VO, mixed-valence oximato Cu_3 and Fe_3 and mixed-spin Mn_3, oxo-phenoxo Mn_4, acetato Zn_2, oximido Re_2, azooximato Ag_2, carbonato Cd_2, thiocyanated bridged two-dimensional and three-dimensional Cd Polymers. Zeolite-like cyanobridged Cu(II)Ni(II) polymer that reversibly accommodates molecules like H_2O and MeCN



Faculty:

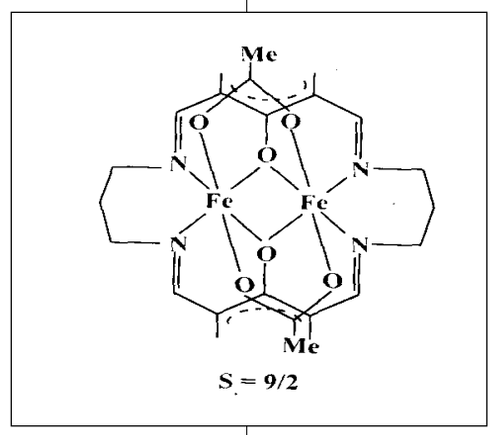
A Chakravorty
D Dutta
K Nag
M Chaudhury
N Ray Chaudhuri
P Banerjee
S Ghosh
S Goswami

as guests has been characterized.

C Macrocyclic Species

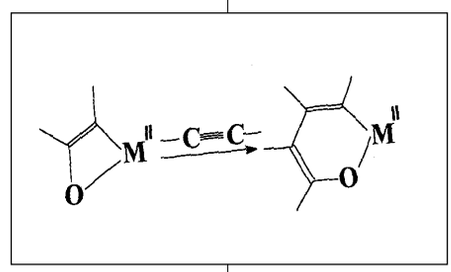
Of interest here is cavity-size manipulation and juxtaposition of multiple metal centres providing a model chemical environment for scrutiny of intermetal communication. This has been extensively achieved by tailoring polyaza/aminophenol macrocycles so as to accommodate 1-4 metal sites. Two examples are cited. In Cu_2 and Ni_2 systems stepwise electrogeneration of oxidation states +1 to +3 has been achieved.

Unusual mixed-valence high-spin Fe_2 (S = 9/2) and Fe_4(S = 9) systems displaying valence delocalization vis-à-vis chemically tunable spin-induced double exchange leading to the observed parallel alignment of spin have been realized. A triazacyclononane with two imino N atoms has been prepared.



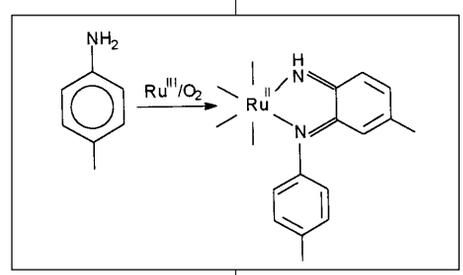
D Organometallics

The main interest is the design and reactivity of ortho-metallated compounds. Systems realized include Ru(III) cyclometallates, acyl compounds of Rh(III) and zwitterionic four-membered metallacycles of Os(II) and Ru(II). Among numerous reactions of the latter, regiospecific alkyne insertion leading to two-carbon metallacycle expansion is particularly noteworthy. Peracids have been found to insert an oxo atom into the Pd-C bond of sulfur functionalized azobenzene palladacycles. Organometallics of Co(III) have been assembled via thioether activation by base.



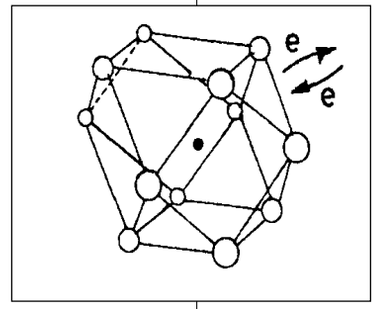
E Mediated and Catalytic Transformations

Metal mediated reactions is an important area of inorganic research. Oxidative coupling of aromatic amines has afforded hitherto inaccessible diimine chelates of Ru(II) and Os(II) and regiospecific aromatic ring amination has furnished unusual tridentate ligands suited for low-spin Mn(II) binding. Nucleophilic addition of alcohols and thiols to nitriles coordinated to Ni(II) and Pd(II) and cycloaddition of alkynes to similarly coordinated azide have been achieved. Other notable findings include Ru(II, III) and Re(III, IV) promoted oxidation of aldimines to amides by water, Ru(II, IV) promoted oxidation of water oxygen, oxygen atom transfer from Re(V)O moieties to phosphines, sulfoxide deoxygenation by Os(IV) affording thioether complexes and Cu(II) mediated benzimidazole synthesis. Mechanisms of many these transformations have been scrutinized.



F Mechanism of Electron Transfer and Substitution Reactions

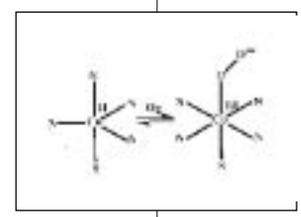
Electron transfer reactions of cage molecules of the type $CoW_{12}O_{40}^{z}$ (z = -5/-6) with organic and reagents have been scrutinized revealing a catalytic role of alkali metal cations. Marcus cross-reaction relationship applies well to the reactions. The z = -6 species transforms to the z =



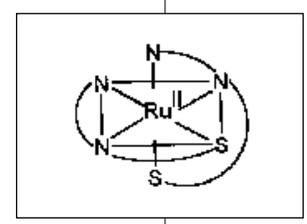
-5 analogue by oxo and perxo reagents without perturbation of the core. Oxidation of histidine with a seven-coordinate Mn(III) species leading to β-imidazolyl pyruvic acid and NH_3 involves C-H bond fission. Formation of H-bonded adduct occurs in the electron transfer reactions of oxime-imine Ni(III, IV) complexes with organic and inorganic electron donors. Ring opening occurs in the substitution reaction of some Pt(II) complexes by N-heterocyclic bases.

G **Bioinorganic Models**

Oxo-transfer pathways of oxidoreductase Mo-enzymes have been explored in terms of Mo-O(terminal) reactivities to substrates having symbiotic proton and electron transfer properties. Trigonal bipyramidal Co(II) compounds capable of reversibly binding O_2 and undergoing transient transformation to Co(III)-superoxide are model of



O_2 reactivity. The active sites of some nonheme iron proteins have been modelled by synthesizing carboxyl and phenolato bridged Fe_2 cores held in macrocycles. Crystalline sugar vanadates have been characterized and these display supramolecule formation via O…O hydrogen bonding. A catalytic catecholase reaction of a vanadate ester system incorporating monoionized catechol chelation has been defined. Thiosemicarbazone complexes of Ru(II) have been shown to possess significant antitumor activity.



H **Concepts and Computation**

Notable contributions include : a new route to electronegativities of ionic and neutral groups, prediction of reaction direction, bond valence summing for negative oxidation states, limits of electron addition to atoms in the gas phase and estimation of cone angles of alkyl groups. Extended Hückel molecular orbital methods have been used to define electronic structure and frontier orbitals of chelated noninnocent ligands having low-lying π^* levels. Algorithms for computing exchange integrals in spin clusters have been developed.

Department of Organic Chemistry

Origin

The Department of Organic Chemistry came into being in 1949 with two faculty members and soon became a leading centre of synthetic organic chemistry in India.

Activity Profile

The focal theme has been synthesis of natural products belonging to the terpenoid family and often displaying pronounced biological activity. In the process novel C-C bond formation and annulation processes have been developed employing skeletal rearrangement, free radical cyclisations and fragmentations, metal catalysed heteroannulations and photoinduced processes. Methodologies of general applicability for chem-, regio- and stereoselctive reductions, selective protection and deprotection of hydroxy and carbonyl groups, improved reactions on solid surface etc. have been developed. Several heterocyclic systems related to uracils and benzothiophenes have been synthesised for evaluating biological activities and photoinduced electron transfer in specific tricyclic systems leading to regioselective bond scission has been demonstrated.

Research Highlights

A Stereocontrolled Synthesis of Complex Multi-chiral Centred Natural Products

Synthesis of complex natural products have paid rich dividends and the synthesis of a host of compounds belonging to the terpenoids family encompassing a variety of structural features and often displaying pronounced biological activity has been realised. Some representative members are the anti-HIV compound avarol (1), the insect antifeedent aplysin (2), the diterpene xanthoperol (3). Pioneering studies into the synthesis of the tricarbocyclic system of the ophiobolin group of sesterterpenes and the anticancer compound taxol are worth mentioning. Other successful efforts include the synthesis of anti-tumour antibiotic methylenolactocin (4), the antimicrobials protolichesterinic acid, roccellaric acid, the biologically active lignans sesamin (5), samin.

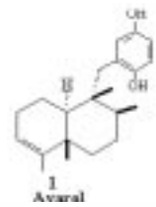
B Development of Novel Synthetic Methods and Reagents of General Applicability

Evolution of the complex structural networks of the molecules cited above required the development of novel carbon – carbon bonds and ring annulation processes. A spin-off has been in the generation of innovative methods involving intramolecular cyclisations through keto-carbenoid and other reactive intermediates, skeletal rearrangements (Scheme I) through ionic and free-radical fragmentations, radical induced cyclisations, metal catalysed heteroannualtions, etc. How palladium catalysis facilitates generation of variety of heterocycles is illustrated (Scheme II).

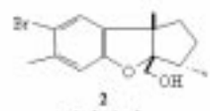
Considerable efforts have also been directed to the development of

Faculty:

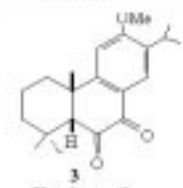
A De
B C Ranu
D Mukherjee
N G Kundu
R V Venkateswaran
S Lahiri
S C Roy
S Ghosh



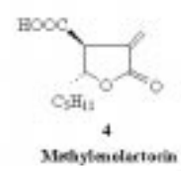
1
Avaral



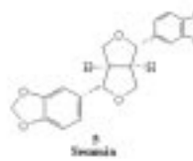
2
Aplysinol



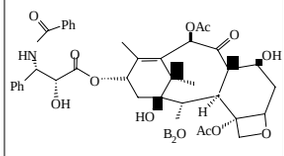
3
Xanthoperol



4
Methylenolactocin

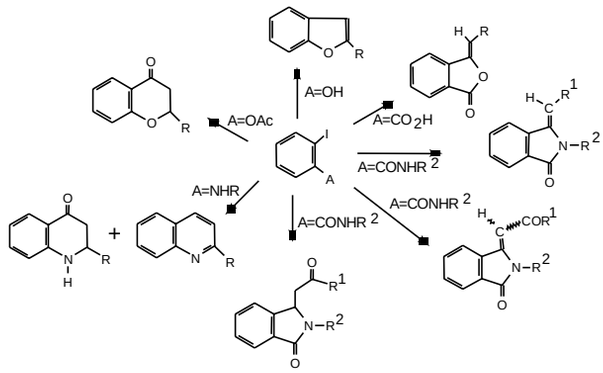


5
Sesamin



Taxol

efficient processes for functional group transformations, the key process in any organic synthesis, leading to the realization of many methods for chemo-, regio-, and stereoselective reduction, regioselective protection and deprotection of hydroxy and carbonyl groups, improved reactions on solid surfaces, etc.



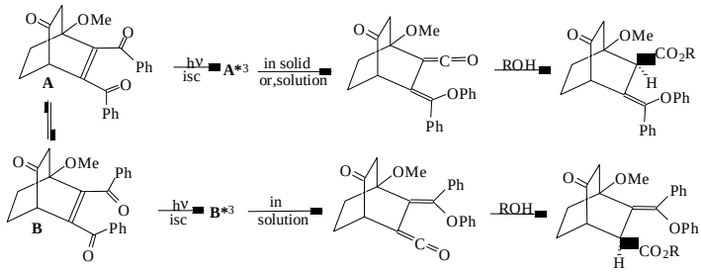
SCHEME - II

C Heterocyclic Chemistry

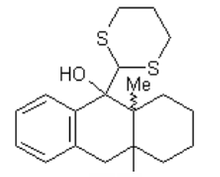
Novel 5-substituted uracils (6) and the corresponding 2'-deoxyribonucleosides were synthesized for evaluation of their potency against tumor cells. Several polycondensed systems incorporating a fused thiophene ring (7-8) were prepared for studies on their potential biological activity as well as physico-chemical studies for comprehension on the transmission of substituent induced electronic effects across the thiophene ring.

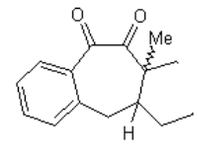
D Photochemistry

The structure-activity relationship in bridged enones has been explored. Regio-selctive bond scission in certain tricyclic systems under single electron transfer (SET) and photoinduced electron transfer (PET) has been studied. A conformational control leading to topochemical selectivity has been observed in rigid *cis*-dibenzoylalkene photorearrangement (Scheme-III). Photochemistry has been also extensively applied to synthesis involving cycloadditions, remote hydrogen abstraction, ring contraction, etc. for developing the carbocyclic frame-work of natural products.

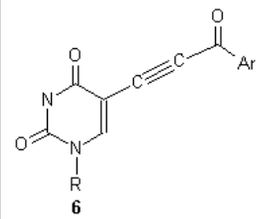


SCHEME - III

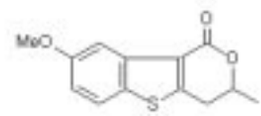




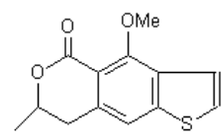
SCHEME - I



6



7



8

Polymer Science Unit

Origin

IACS was the forerunner in research in the field of polymer science in India where it was started as early as 1947 in the Department of Physical Chemistry. Subsequently, research in the field of rubber chemistry also began in the Department of Macromolecules. However, following a reorganization of Departments in 1986 these groups were brought together under one administration with the new name 'Polymer Science Unit'.

Activity Profile

During its 16 years of existence the unit has made significant contributions in the fields of (1) thermodynamics of polymer blends, (2) conducting polymer colloids and nanocomposites, (3) dispersion polymerization of water soluble monomers, (4) polymer crystallization, (5) polymer gels, (6) chemistry of rubber vulcanization, (7) elastomer blends and (8) surfactant-surfactant as well as polymer-surfactant interactions. In what follows descriptions of the important contributions are presented under the headings Molecular sciences and Technology Development.

Research Highlights

I Molecular Sciences

A Novel Polymerization Processes

A polymerization process for preparing polyacrylamide, an important water soluble polymer, in dispersion form was developed and studied in detail. The work is the first such study reported in the open literature. Systematic investigation on the mechanism of phase transfer catalysed free radical polymerization shed new light on the phenomenon.

B New Initiator Systems for Vinyl Polymerization

Transition metal laurates (Fe^{+3}, Mn^{+3}, Cu^{+2}) in combination with suitable reductants (amine, thiol, a-hydroxy ketone etc.) in non-aqueous medium were successfully used as initiators for redox polymerization of vinyl monomers.

C Proton-transfer Complexes

Proton-transfer complexing equilibria involving some donors and acceptors such as p-nitrophenol, p-nitrosalicylic acid and ethylene diamine in aquo-organic and micellar media were studied in order to understand the nature of such interactions which are operative in various biological systems comprising proteins, lipids, membranes, etc.

D Mixed Surfactant Systems

Detailed physicochemical investigations on some surfactant-surfactant, dye-surfactant and polymer-surfactant systems have revealed interesting insights into the molecular interactions controlling the association

Faculty:

A R Das
A K Nandi
B M Mandal
D K Basu

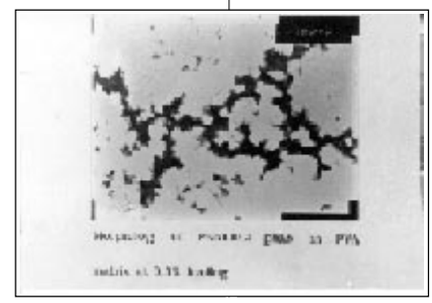
Differential scanning calorimeter

processes in varied environments.

2 Physics and Chemistry of Materials

A Studies on Polymer Blends and Alloys

Judicious blending or alloying of polymers leads to materials with improved physical and mechanical properties and of lower cost. The study of polymer blend thermodynamics resulted in the discovery of several miscible amorphous polymer blends the kind of which are not available in plenty. The study also led to a prediction capability as to which polymers will blend homogeneously with which others. Most of the instruments used in this study were designed and fabricated in the laboratory.



Transmission electron micrograph of a polyaniline-poly(vinyl alcohol) nanocomposite film

B Conducting Polymers and Their Composites

Novel dispersions of some conducting polymers were developed which could be blended with a variety of commercial nonconducting polymers to yield conducting nanocomposites. The electrical conductivity threshold of the latter is reached at an extremely low concentration of the conducting polymer through the self-assembly of the conducting polymer nanoparticles resulting in a fractal structure of the conducting polymer phase in the composite. These composites are technologically attractive in view of their optical transparency and also cheapness in cost.

C Chemistry of Rubber Vulcanization

Systematic studies were carried out on some binary systems of accelerators for rubber vulcanization in order to understand their synergistic activity. It has been established that formation of several compounds in the early part of vulcanization play a vital role for the significant cure synergism of the combinations studied. In the study concerning modification of cure of natural rubber brought about by retarders in the presence of accelerators several effective cure retarders were prepared in the laboratory. Additional light on the mechanism of cure retardation was thrown.

Most rubber additives (sec. amine based accelerators and antioxidants) are detrimental to health due to the formation of carcinogenic nitrosoamines. Suitable rubber additives were selected which are safer because of their low volatility. They were prepared and their activity in practical vulcanization was investigated. This study led to the development of several less hazardous rubber accelerators which have great technological usage potential.

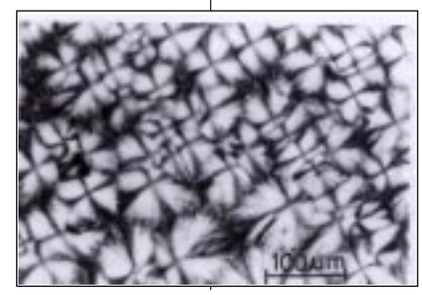
D Novel Rubber Blends

Several thiophosphoryl disulphides and poly-sulphides have been prepared and successfully used as coupling agents for polar carboxylated nitrile rubber and nonpolar diene rubbers. In this area a novel technique of 'two-stage vulcanization' has been developed. Improved physical as

well as chemical properties of vulcanizates have been obtained using this technique.

E Polymer Crystallization

Blends of a crystalline polymer, poly(vinylidene fluoride) (PVF_2), with the amorphous polymer poly(methyl acrylate) (PMA) was studied. The lower the head to head (H-H) defect of PVF_2 higher is its compatibility with PMA. From the study of crystallization kinetics of the blends it was concluded that polymer chain extension occurs on blending. The cocrystallization of PVF_2 samples differing in H-H defect content and of VF_2-VF_4 copolymers was found to be limited to blends in which the components have only small difference in structural defects. The physical properties e.g. melting point, d-spacing and crystallization kinetics of cocrystals were studied and it was concluded that cocrystallization is an entropy driven process.



Optical micrographs of the KFE PVF_2 blend with PMA (w_{PVF2}=0.50) crystallized at 150° C for 3 days

F Polymer Gelation

Gelation mechanism of thermoreversible PVF_2 gels in different solvents has been explored. It has been shown that three dimensional percolation is a suitable model for all the gels. The gelation is a two step process of conformational ordering and crystallization. Formation of polymer-solvent complexes during gelation has been proved from thermodynamic study and also using molecular modeling. Thermoreversible gels of polyaniline and poly(3-hexyl thiophene) are under investigation.

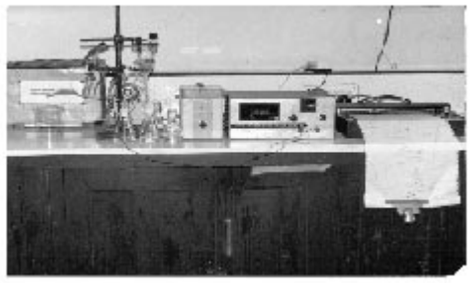
G Dispersed Molecular Aggregates

Colloidal dispersions of some metal salts such as copper ferrocyanide, lead chromate, tungstic acid etc. have been prepared in the microdomains of the water pools of water/AOT/n-heptane water-in-oil microemulsion. X-ray diffraction and FT-IR studies established the formation and characterization of the nanosized particles while scanning and transmission electron microscopic studies yielded the shape and size of the colloidal dispersions.

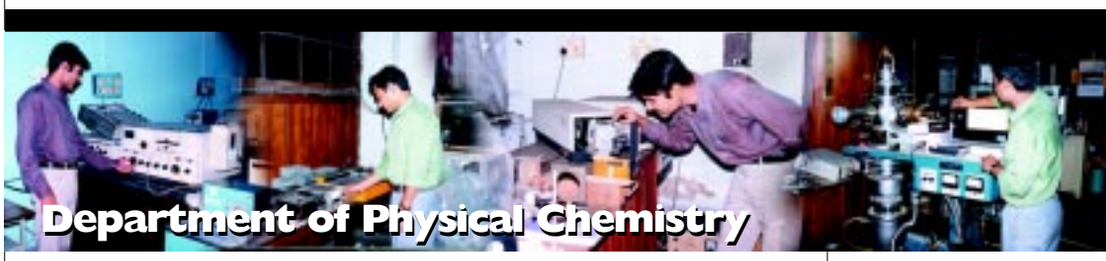
3 Technology Development

Know-how of microbial BOD sensor was developed.

Precision calorimeters for measuring enthalpy of mixing of liquids, gas chromatograph, apparatus for measuring cloud points of polymer blends were des e help of the institute v



Microbial BOD sensor developed at Polymer Sciense Unit



Department of Physical Chemistry

Origin

The Department of Physical Chemistry came into being in 1947 with Professor S. R. Palit as the Head of the Department. Pioneering contributions were made during 1947-76 in the fields of Polymer and Solution Chemistry.

Activity Profile

Since 1976, there has been a marked shift in the focus of research activities of this Department. Explorations of bulk-chemistry has been replaced by microscopic probing of both structure and dynamics of molecules by state-of the-art tools. While experimentalists searched for the finer details of microscopic systems, quantum and statistical mechanics provided the insight for the theoreticians for their activities, often with a degree of synergistic enrichment of one by the other. Our major activities have been confined to molecular and theoretical sciences.

Research Highlights

I Molecular Sciences

A Non-linear Spectroscopy

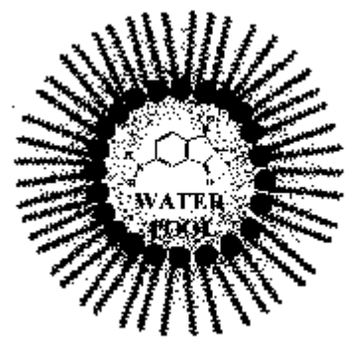
The high intensities affordable with pulsed dye lasers may allow a molecule to absorb two photons simultaneously giving rise to two-photon absorption spectrum (TPA) which was exploited for deriving information that is complementary to what is revealed in the standard one-photon spectra of both organic and inorganic molecules. It was during this period that Resonance Second Harmonic was observed in Gd^{III} single crystals, Later on, Resonance surface second harmonic generation was exploited for probing liquid surface-air interface. It provided insight as to how water-structure makers and breakers determine the surface population of organic molecules in water.

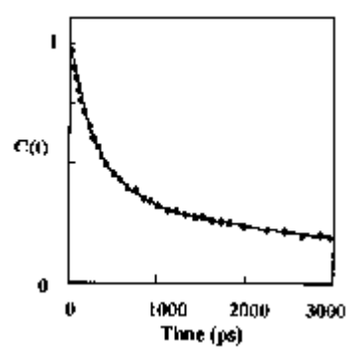
B Fast Photodynamics

Laser can provide very short light pulses which can be used as triggers for setting off of fast process like conformational relaxation of a molecule, intramolecular proton transfer in excited state, etc. Initially, attention was focused on these elementary processes in solution and a host of molecules were studied. ESIPT was used to gather information on the nature of surfactant-protein binding. With the setting up of a laser facility with picosecond time-resolution, attention was turned on to the dynamics of liquids confined in self-organized assemblies. Solvation dynamics in such assemblies, e.g. micelles, reverse micelles, micro-emulsions, lipids, polymer hydrogels, sol-gel mixtures and zeolites have been studied in this laboratory. These studies unequivocally established dramatic retardation of solvation dynamics in confined systems, an important observation which we believe, we have been the first to make. In addition significant retardation of TICT process in

Faculty:

D Mukherjee
D Nath
D S Ray
K Bhattacharyya
M Chowdhury
S Mukherjee
S P Bhattacharyya





Solvation Dynamics in Microemulsion

various organized assemblies have been discovered. We are planning to extend our investigations into the Femto-second domain.

C Vibronic Spectroscopy of Jet Cooled Molecules

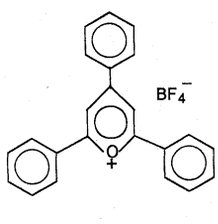
It is possible to produce cold molecules in extreme isolation in seeded supersonic jets, where the band width gets dramatically reduced. The potential energy surfaces with respect to large-amplitude displacement coordinates of many floppy molecules have been mapped by recording the vibronic frequencies observed in LIF and SVL spectra of the target molecules.

D Circular Dichroism (CD) Spectroscopy

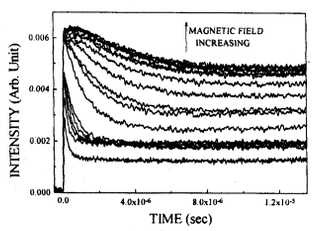
The single crystals of Ln^{III} complexes offer an excellent opportunity for correlating the Ln^{III} chiral environment with the circular dichroism of transitions between crystal-field split levels. Several crystals with O,T and D_3 symmetry of the unit cell were studied under high resolution. The contributions of magnetic dipolar and electric quadrupolar transition moments in CD were estimated.

E Magnetic-field Effect (MFE) on Chemical Dynamics

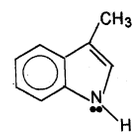
In the last two decades, it has been firmly established that a small magnetic field can indeed affect the dynamics of chemical reactions in which radical pairs(RP) are formed as intermediates. This laboratory has investigated MFE on RP recombination dynamics by transient absorption and emission spectroscopy and observed a large MFE for a



[$TPP^+BF_4^-$]



Transient decay obtained at 555 nm for TPP in aqueous SDS in presence of various external fields

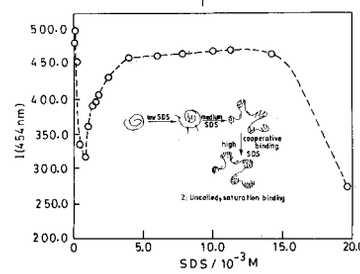


[Skatole]

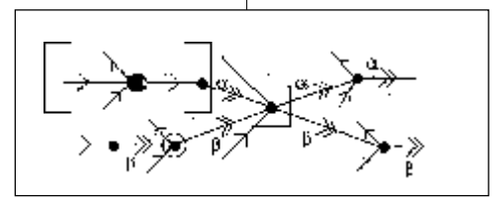
2 Theoretical Sciences

A Many Body Theory

Theoretical work over the last two decades have established quite a few landmarks in the area of many-body theories of electronic structure and dynamics. Of then closed and open-shell coupled-cluster theory, coupled-cluster based linear response theory have become standard tools for size consistent calculation of excitation energies and response properties of atoms and molecules ab-inito, understanding and interpreting Auger and Core-ionization spectra. The state-specific multi-



Probing protein-surfactant interaction



A connected diagram in the many-body theory for core-holes

reference coupled cluster theory developed in this laboratory has led to the formulation of a dynamic linear response approach for computing excitation energies for systems with strongly quasi-degenerate ground state. Time-dependent generalization of coupled-cluster theories have paved way to the understanding of the dynamics of strongly correlated systems.

B Quantum Optics

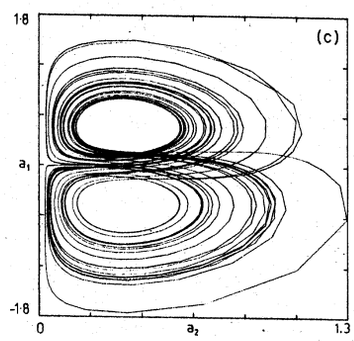
Theoretical investigations of matter interacting with high intensity radiation systems have led to the prediction of spectral modifications of Raman lines in a cavity, optical phase transitions, photon-localization in quasi-periodic media, optical chaos, etc. Studies in few atoms-photon systems have brought in new methods for generating, manipulating and exploiting non-classical field states.

C Non-equilibrium Statistical Mechanics

In the realm of non-equilibrium statistical mechanics generalizations of master equations and the associated stochastic formulations relating to chemical kinetics or quantum optics worth special mention.

D Non-linear Dynamics and Chaos

In this emerging and hotly pursued area of theoretical research, a notable contribution form this department has stemmed from the idea of treating chaos as a statistical mechanical problem of a few-degrees of freedom system and a demonstration of realizability of chaotic diffusion, an existence of fluctuation- dissipation type of relations in chaotic systems.



A Raman Attractor

Background

The IACS Library is the oldest research library in India, offering bibliographical facilities to a wide class of scholars. It has a vast collection of very old scientific journals of immense historical and archival values – a collection that has no parallel in any other library of a Research Institute. The First volume of the first Scientific Journal - 'The Philosophical Transaction of the Royal Society', published in May, 1665 is available in this Library.

Services

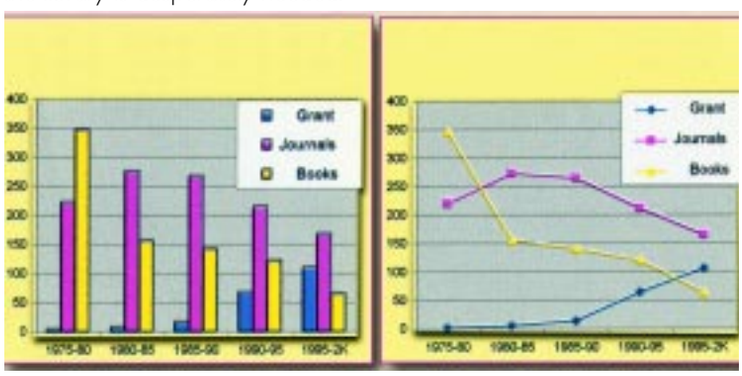
It extends one of the most liberal usage facilities in the region — all potential users have direct access to the shelves of the books and journals and offers extensive reprographic services to users from all over India. The resource of the library is shared by many Academic Institutions such as The Calcutta University, Jadavpur University, Saha Institute of Nuclear Physics, Bose Institute, CSIR Laboratories and other research Institutes. Industrial Organisations often make use of this library. The outstation users cover wide area starting from Institutes such as IIT, Kharagpur, Burdwan University, Visva Bharati, North Bengal University, and the Universities of Eastern, North Eastern and Southern Region.

The Library : Space and Funding

The Library has been passing through a difficult time for over a decade due to dwindling resources — inadequate funds for procuring books and journals, lack of facilities and space for the maintenance of the invaluable bibliothic treasure of the library.

A separate air-conditioned Library building is coming up. The Ground floor would soon be completed, though the space available would just about hold the present collection.

Perusal of (Charts no.1 & 2) the Bar Diagram and Line Diagram respectively showing the growth rate of collection of books and journals against Grant (Rs in Lakhs) received during the past 25 years in five yearly blocks, would seem to indicate an increased flow of funds to the library. In reality, the steep rise in price of journals coupled with devaluation of rupees has more than offset the increased allocation leading to a steady decline of the holding of the library. Much higher allocation of funds for the library is desperately needed.



Computer Centre

Background

Although Indian Association for the Cultivation of Science is 125 years old, the Computer Centre is a relatively new addition to its facility. In 1989 VAX computer system was procured and round the clock operation started in 1990. The computer culture existed in the Association since early sixties. At that time no computer suitable for research in natural science existed in the city and the scientists were forced to travel to other parts of the country namely TIFR, IIT Kanpur, IIT Madras for using computing facility.

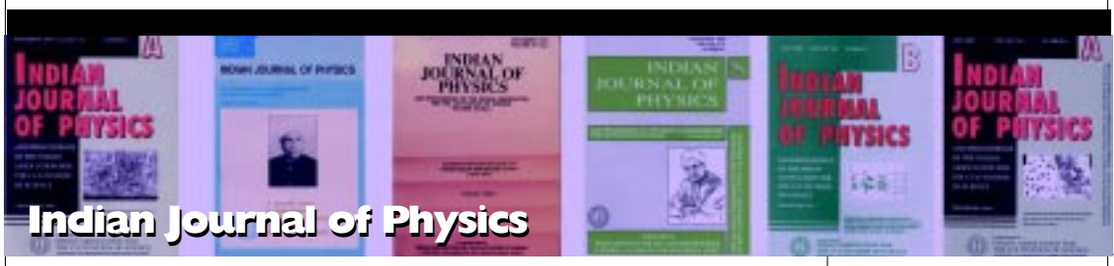
Services

In 1991 e-mail facility became available through dial-up telephone line and full internet facility was established in 1998 through a radio link between IACS and VSNL.

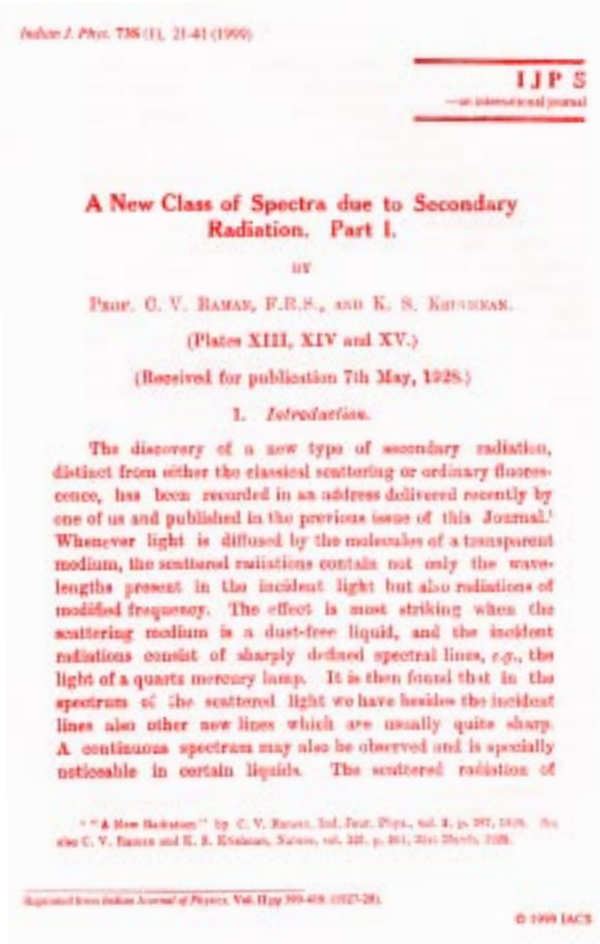
ICOSER Facility

Department of Science and Technology, Government of India, under their ICOSER project decided to establish a few LEVEL III computer centres throughout the country and IACS was chosen as one of these centres. DST procured a number of compute-servers and these machines were installed in 1998. Since then IACS is functioning as one of the level III computer centres of the country. Side by side, work related to local area network was undertaken and all these three inter-related works, namely installation of servers, internet connection and LAN were completed in July, 1998 and the centre was formally inaugurated in August, 1998. Computing facility and internet access are available round the clock through LAN and dial-up telephone line through modem. Besides serving as the computing facility of IACS, the centre is also offering computing facility to universities and sister research institutes.

Faculty:
S Ray



Indian Journal of Physics, the oldest Indian research journal in Physics, will achieve the 75th (Platinum Jubilee) year of its publication in 2001, as IACS completes 125 years of existence. This journal was C V Raman's contributions to scientific journalism in India. It began as a Bulletin of IACS, later transformed into Proceedings of IACS which finally evolved as Indian Journal of Physics in 1926. Raman strongly believed that the best work done in India should be published in Indian Journals and demonstrated it by publishing all his early works in this journal. His Nobel prize winning work 'A New Radiation', later known as Raman Effect was published in IJP in 1928 (Vol. 2, pg. 387, 1928). Apart from C V Raman's contributions, this journal published many important papers of M N Saha, K S Krishnan, K Banerjee, S K Mitra, S Bhagavantam and others. The journal, with its uninterrupted publication, has grown into an international journal, publishing papers in two sections A and B covering almost all branches of physics. Special issues commemorating Golden jubilee, birth centenaries of C V Raman, M N Saha and K S Krishnan have been published. An active Editorial Board comprising of eminent physicists from all over the country oversees its publication.



Indian J. Phys. 73B (1), 21-41 (1999)

IJPS

—an international journal

A New Class of Spectra due to Secondary Radiation. Part I.

BY

PROF. C. V. RAMAN, F.R.S., AND K. S. KRISHNAN.

(Plates XIII, XIV and XV.)

(Received for publication 7th May, 1928.)

1. *Introduction.*

The discovery of a new type of secondary radiation, distinct from either the classical scattering or ordinary fluorescence, has been recorded in an address delivered recently by one of us and published in the previous issue of this Journal.[1] Whenever light is diffused by the molecules of a transparent medium, the scattered radiations contain not only the wavelengths present in the incident light but also radiations of modified frequency. The effect is most striking when the scattering medium is a dust-free liquid, and the incident radiations consist of sharply defined spectral lines, *e.g.*, the light of a quartz mercury lamp. It is then found that in the spectrum of the scattered light we have besides the incident lines also other new lines which are usually quite sharp. A continuous spectrum may also be observed and is specially noticeable in certain liquids. The scattered radiation of

[1] "A New Radiation" by C. V. Raman, Ind. Jour. Phys., vol. 2, p. 387, 1928. See also C. V. Raman and K. S. Krishnan, Nature, vol. 121, p. 501, 31st March, 1928.

Reprinted from *Indian Journal of Physics*, Vol. II pp 399-419 (1927-28).

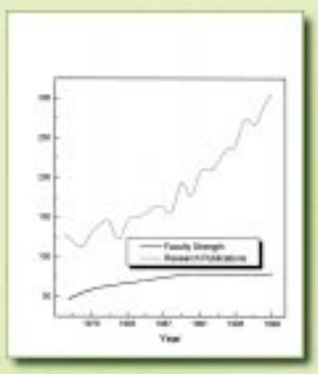
Third World Academy Prize	1
S S Bhatnagar Prize	7
INSA Research Professorship	1
Fellowship of Indian National Science Academy (New Delhi), Indian Academy of Sciences (Bangalore), Indian National Science Academy (Allahabad)	20
Fellowship of West Bengal Academy of Science	7
Fellowhship of International Academy of Quantum and Molecular Academy	1
Honorary Professorship, Jawaharlal Nehru Centre for Advanced Scientific Research	2
Medals:	
CSIR New Millennium Medal	1
INSA Medal	1
Other Awards: Indian Science Congress Association Material research Society of India Chemical Research Society of India	12
Faculty Members on the Editorial Board of Major Journals	17
Lecture Awards of the Indian Chemical Society	
Acharya J C Ghosh Lecture	1
D N Agarwal Award	1
INSA Young Scientist Award (New Delhi)	8

Looking Ahead

In the beginning of the new millennium, IACS is poised to initiate research in the emerging areas of science. It plans to develop research groups on the emerging frontiers in all the umbrella areas where active research is going on in IACS. An important strength of IACS is the co-ordination and confluence of research activity in the design of novel materials at the molecular and at the nanoparticle levels. IACS is thus in a unique position to venture into the fertile area of molecular science of materials. IACS is also moving ahead with time to the emerging fields of biology-inspired sciences and bioinformatics. It also envisages building centres for theoretical and mathematical sciences to carry its theoretical activity to new heights. At the same time, we want to consolidate and expand its present activity.

In the year 2001 IACS will celebrate 125 years of its functioning. The types of research frontiers it wants to pursue require vibration free surroundings, facility to synthesise materials of ultra-high purity and sophisticated buildings. The need of the day is to acquire a new land for establishing centres in the selected emerging areas of science. Action plans and proposals are being framed to generate the infrastructure for the new laboratories. At the same time, refurbishing and modernising the laboratories of the present campus is also of prime importance. It is evident from the accompanying graphical summary that IACS is not in the best of financial health at the moment - but that has not dampened our spirit. We are looking forward to generous funding from the funding agencies which is crucial to launch IACS to the sciences of the new century.

Growth of faculty and research publications during the period 1982-1999



Total amount of external funding and total strength of externally supported scholars during the period 1982-1999

Grant received during the period 1976-77 - 1999-200