isamp
NEWS LETTER

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CONTENTS

Erratum

Following errors have crept in the article ***"A new kind of binding"*** (Vol.1, Issue#2)

1 Page 7, 10th line from bottom **'66.65%'** should be read as **'65.77%'**

2 Page 8, 2nd para, last line **~ 10^{-4}** should be read as **~ 10^{4}** degree Kelvin.

Errors are regretted.

Editor, ISAMP NL

FROM THE EDITOR'S DESK

Water, it is the spring of life. In this issue of newsletter, we have the abstract of a research paper reporting the discovery of cool water (750-900K). Genuinely cool finding, considering it exists in the neighbourhood of violent astrophysical object, a Nova. For confirmation, the authors modelled the molecular lines in the H-band.

An ad of a multinational computer company has *"n is for nanotechnology"* as the punchline. Nanotechnolgy is an emerging field which is likely to impact several facets of our lives in the future. It is the merging and meeting point of chemistry, atomic and molecular physics, and condensed matter physics. In this issue we have an article on nanotechnology, it highlights the techno logical challenges that lie ahead and dwells upon the methods to understand their physical properties.

These two articles in this newsletter indicate the contribution of atomic and molecular physics to other research areas. However, Helium was first discovered in the spectra of Sun and recent advances in atomic and molecular physics made possible with advances in solid state devices.

Talking about helium, accurate Hylleraas-like functions are now available which correctly accounts for the cusp conditions. Interested readers may download this free article from http://www.iop.org/EJ/abstract/0953-4075/38/16/L01/

K.P. Subramanian
EDITOR, ISAMP Newsletter

Dilip Angom
Guest Editor

August 21, 2005

Dr. Dilip Angom, (Physical Research Laboratory, Ahmedabad) has kindly agreed to assist the Editorial Board of ISAMP News Letter. He will act as the Guest Editor of the News Letter.

LETTER TO THE EDITOR

From ssh@astro.umd.edu Fri Jun 26 13:48:44 2005
Date: Sat, 25 Jun 2005 12:10:38 -0400 (EDT)
From: A. Surjalal Sharma (SPP) <ssh@astro.umd.edu>
To: isamp@prl.ernet.in
Cc: ssh@astro.umd.edu
Subject: Re: ISAMP News Letter

Dear Editor,
The ISAMP newsletter is really great. Since plasmas are of interest to ISAMP the following book may be of some relevance. This volume developed out of the workshop in Ahmedabad in 2001.
Best wishes,
Surja Sharma

"Nonequilibrium Phenomena in Plasmas"
Series: Astrophysics and Space Science Library, Vol. 321
Sharma, A. Surjalal; Kaw Predhiman K. (Eds.) 2005, IX, 347 p., Hardcover
ISBN: 1-4020-3108-4

About this book
The complexity of plasmas arises mainly from their inherent nonlinearity and far from equilibrium nature. The nonequilibrium behavior of plasmas is evident in the natural settings, for example, in the Earth's magnetosphere. Similarly, laboratory plasmas such as fusion bottles also have their fair share of complex behavior. Nonequilibrium phenomena are intimately connected with statistical dynamics and form one of the growing research areas in modern nonlinear physics. These studies encompass the ideas of self-organization, phase transition, critical phenomena, self-organized criticality and turbulence. This book presents studies of complexity in the context of nonequilibrium phenomena using theory, modeling, simulations, and experiments, both in the laboratory and in nature.
For more details, look Springer website http://www.springer.ny.com

ABSTRACTS OF RECENTLY PUBLISHED PAPERS

Abstract#1

Near-infrared water lines in V838 monocerotis

D. P. K. Banerjee[1] , R. J. Barber[2] , N. M. Ashok[1] and J. Tennyson[2]

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[2]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK
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V838 Monocerotis had an intriguing, nova-like outburst in 2002 January that has subsequently led to several studies of the object. It is now recognized that the outburst of V838 Mon and its evolution are different from those of a classical nova or other classes of well-known eruptive variables. V838 Mon, along with two other objects that have analogous properties, appears to make up a new class of eruptive variables. There are limited infrared studies of V838 Mon. Here we present near-infrared H-band (1.5 - 1.75 micron) spectra of V838 Mon from late 2002 to the end of 2004. The principal new result from our work is the detection of several rotation-vibration lines of water in the H-band spectra. The observed water lines have been modeled to first establish that they are indeed due to water. Subsequently the temperature and column densities of the absorbing material, from where the water absorption features originate, are derived. From our analysis, we find that the water features arise from a cool ~ 750-900 K region around V838 Mon that appears to be gradually cooling with time.

The Astrophysical Journal Letters, **627**, L141-L144, 2005 July 10

Abstract#2

Amplification without population inversion in molecules

Anindita Bhattacharjee[1], Susmita Sanyal[2] and Krishna Rai Dastidar[1]

[1]Indian Association for the Cultivation of Science, Kolkata-700032, India
[2]Jongipur College, Jongipur, West Bengal, India
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We have studied the feasibility of amplification without population inversion (AWI) in LiH molecule for three-level ladder, V and Λ schemes. We have shown the salient features of AWI in a molecular system in comparison to that in an atomic system, viz. the dependence of gain profile on the choice of different rotational and vibrational transitions. Under different three-level schemes, the effect of homogeneous and inhomogeneous broadening on the gain profile has been studied. We have also studied the dependence of gain on different external parameters. The temporal evolution of gain has been analyzed and it was found that AWI is achievable in both the transient and the steady state regime. For all the three-level schemes and in particular for the ladder scheme, amplification of the weak probe was obtained using a coupling laser of smaller frequency.

J. Mol. Spectroscopy (in press)

Abstract#3

Control of (1+1+1')-photon dissociation dynamics in NaH molecule using three delayed ultrashort pulses

Anindita Bhattacharjee and Krishna Rai Dastidar

Indian Association for the Cultivation of Science, Kolkata-700032, India

Email: spkrd@mahendra.iacs.res.in, krishna_raidastidar@yahoo.co.in

We have calculated (1+1+1')-photon dissociation cross section of the NaH molecule from ν''=0 level of the ground $X^1\Sigma^+$ state to the repulsive $B^1\Pi$ state via the bound $A^1\Sigma^+$ state by using three delayed ultrashort pulses. Two delayed 4 femtosecond pulses have been used for the first step transition to design interfering wavepackets on the intermediate $A^1\Sigma^+$ state and the third delayed ultrashort pulse (either δ-function or 4 femtosecond) excites these wavepackets to the dissociating state. We have shown that control over dissociation dynamics can be achieved by controlling delay between three pulses, the pulse durations and the carrier frequencies. We have considered two values of delay between the first two 4 femtosecond pulses for which it is possible to inhibit and enhance the de-excitation channel to the ground state and hence for these two delays the maximum of the cross section in the dissociation spectrum can be enhanced or diminished respectively for the δ-function transition to the dissociating state by the third ultrashort pulse. The dissociation spectrum also depends on the delay of the third pulse. The dependence of the dissociation cross section on the delays of pulses and on the the carrier frequency of the third pulse has been demonstrated for two step dissociating transition by three delayed 4 femtosecond pulses of gaussian shape. It has been suggested that the oscillation of dissociation cross section with time delay of the third pulse can be realized as time dependent quantum gates and the nature of quantum gates can be controlled by choosing pulses of different shape, duration and photon energy (or carrier frequency) as well as delay between the pulses. This aspect of realization and precise control of time dependent quantum gate in light molecules by using three ultrashort pulses (4 femtosecond) has not been explored before.

Phys. Rev. A (in press)

Abstract#4

Generation of L sub-shell photoionization cross sections for elements 18 £ Z £ 92 at energies 0.320 to 115.606 keV

Ajay Sharma and Raj Mittal*

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Punjabi University, Patiala - 147002 (INDIA)

Email: *rmsingla@yahoo.com, ajay85b@yahoo.co.in*

L sub-shell photo-ionization cross-sections, s_{Li}, for elements 18≤Z≤92 at energies 0.320 to 115.606 keV have been generated from an empirical relation fitted to Scofield's L sub-shell photo-ionization cross-section values. The excitation energy E for an element is constrained by the condition that only L and higher shell vacancies are produced in the elements. The closeness of generated and existing values of Scofield's L sub-shell data recommends the use of generated values in the fields of atomic and molecular physics and for trace elemental analysis. For this purpose computer software 'LSPICS' has been developed. On personal computer LSPICS generates **L** Sub-shell Photo Ionization Cross-Section values in barns just by entering the atomic number of element and excitation photon energy in keV.

J. Quan. Spect. and Rad. Tran., **95**, 49-60, (2005)

Abstract#5

Photon Induced L_3 Vacancy Alignment for elements La to U

Ajay Sharma, Meenu Singh and Raj Mittal*

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Email: *rmsingla@yahoo.com, ajay85b@yahoo.co.in*

Alignment of photon induced L_3 vacancies is studied in rare earth and high Z elements at energies of experimental interest, near thresholds to 60 keV, under non-relativistic dipole approximation. Numerical calculations of the matrix element are undertaken to produce theoretical data for comparison with the experimental findings. The A_2 values being > 0.1 at photo-electron energies < 20 keV are certainly higher than 5 - 8% uncertainties quoted in experimental results. Present findings are from a very basic model, hydrogen like and can further be treated as reference to observe the impact of screening, relativistic, multipole and retardation corrections to the model.

Status: Submitted to PRAMANA (2005)

Abstract#6

Determinations of photon induced atomic inner shell vacancy alignment

Raj Mittal*, Ajay Sharma and Meenu Singh

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Punjabi University, Patiala - 147002 (INDIA)

Email: *rmsingla@yahoo.com, ajay85b@yahoo.co.in*

Alignment of photon induced atomic inner-shell vacancies in a state with $j > 1/2$ is expressed in terms of alignment parameter A_2. The cause of alignment and its influences on subsequent process lead to different methods used for A_2 determinations. Since A_2 is defined as the fractional difference of magnetic sub-state (j) ionization cross-sections of the state, thus, the magnetic sub-state photo ionization cross-sections based upon different models and assumptions have been used to determine A_2 parameter. Further, the vacancy alignment results in anisotropic distribution of x-rays originated from the state, therefore, the distribution measurements of the x-rays lead to determination of A_2. Moreover, the magnetic sub-state ionization cross-sections of an orbital electron depend upon the incident photon energy, which in turn leads to incident energy dependence of x-ray distributions. All this results in a projectile energy dependence of the ratio of differential cross-sections. Thus, the energy dependence of total production cross-sections of lines originating from a same vacancy state predicts vacancy alignment and has been used for alignment determinations. The determinations of A_2 from these three methods are being discussed here.

Status: Submitted to Canadian Journal of Physics (Dec. 2004)

Abstract#7

Computation for photon induced L3 vacancy alignment under non-relativistic dipole approximation

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A computer program in Mathematica **A2NRDPAZ** to calculate L3 vacancy alignment parameter A_2 at energies, threshold to 60 keV, for elements $57 \leq Z \leq 92$ has been described. A_2 is fractional difference of magnetic sub-state ionization cross-sections $\sigma(m_j\text{'s})$ for L3 state. This is accomplished by presenting the elements atomic number and the photon energies in arrays and the basic functions in Mathematica were used to manipulate these arrays. The program has the capability of calculating L3 vacancy alignment for different elements at different energies with minimal overflow problems. The present formulations and numerical calculations of A_2 and the fractional photo-ionization cross-sections are compatible with the earlier reported analytical calculations of Oh and Pratt [Phys. Rev. A 10 (1974) 1198] for Mg and Ca. The A_2 values from non-relativistic dipole approximation at energies < 20 keV were found to lie above the experimental uncertainty limits those were 8 to 10%. This is contrary to the predictions of Mehta *et al.* [Phys. Rev. A 59 (1999) 2723] as well as Yamaoka *et al.* [Phys. Rev. A 65 (2002) 062713-1] that at energies threshold to 60 keV there is no alignment within the experimental uncertainties.

Status: Submitted to Computer Physics Communications, (2005)

Abstract#8

K-shell photoionization cross section generation for the elements $4 \leq Z \leq 95$ at energies 1 to 1500 keV

Meenakshi Bansal and Raj Mittal*

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K shell photo ionization cross-section σ_K (Scofield, 1973) for elements $4 \leq Z \leq 95$ at energies 1 to 1500 keV can be generated from a derived empirical relation. To have the ready values at required energies for an element on computer, the developed computer software KSPICS generates the cross-sections in barns. Observed closeness of generated and the existing values recommended the use of generated values in the field of atomic and molecular physics and for elemental analysis.

Status: Submitted to Applied Radiation and Isotopes (May 2005)

Nanotechnology: A revolution

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"With a revolution in everything from toys to tumors on the horizon, scientists in the nanotechnology arena are working to gain the public's trust.

Hoping to both anticipate pitfalls and head off a publicity fiasco, policy makers and scientists are promoting research and public discussion on environmental, ethical, economic, and other societal implications of the burgeoning field of nanotechnology. Loosely defined as the purposeful creation of structures 100 nanometers in size or smaller, nanotechnology "is a real revolution because it is changing in a fundamental way how we build things," says Mihail Roco, who chairs the White House subcommittee that coordinates the multi-agency National Nanotechnology Initiative (NNI). Scientists predict that applications of nanotechnology will go far beyond their current uses—in sunblock, stain-resistant clothing, and catalysts—to, for example, environmental remediation, power transmission, and disease diagnosis and treatment."

(Physics Today, June 2004)

Presently, the word nano technology, nano structures and molecular electronics are used everywhere but everyone has a different view of what it means and why it is interesting.

For an electrical engineer, the most important device is the transistor and the single most important reason for being interested in nanostructures is that transistors is fast becoming nano devices. Figure 1 shows a common transistor, a dual gate field effect transistor:

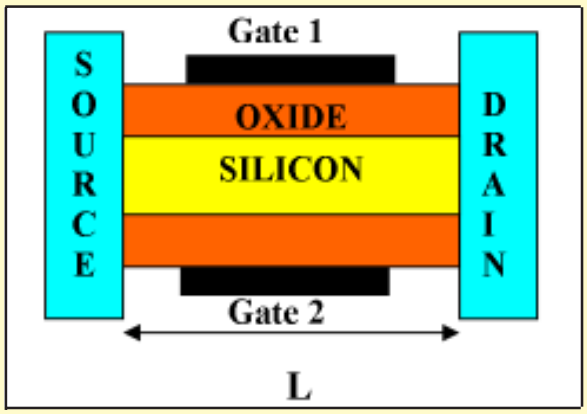

Fig 1. A dual gate FET

Channel length L, has been progressively reduced from ~ 10 μm in 1960 to ~ 0.07 μm in 2004, allowing circuit designers to pack ~ $(143)^2 \approx 20{,}000$ times more transistors into a chip with a given surface area. This increase in packing density is at the heart of the computer revolution.

How much longer can the downscaling continue? Twenty years now, will we build transistors with channel length of the order of nanometers or picometers? Everyone agrees that the path to further downscaling is more difficult since now we are entering the atomic domain.

For example, a channel length of 10 nm spans roughly 40 silicon atoms. For proper transistor operation, the thickness of the gate oxide has to be approximated a tenth of the channel length, means 4 atoms.

Can we reliably fabricate oxide layers that are only 4 atoms thick? May be, fabrication is possible using an insulator with a high dielectric constant, but as shown by the group of researchers from Bell Laboratories, the electrical insulation of the gate oxide breaks down for an oxide thickness of 0.7 nm (*four atomic layers of silicon in the oxides*) causing the chip to fail.

The limit to oxide thickness is fundamental and cannot be overcome by technological improvement. The end of SiO_2 as a gate insulator will be reached in the year 2012, according to the roadmap for semiconductor technology. A simple example of molecular electronics device is shown in fig. 2.

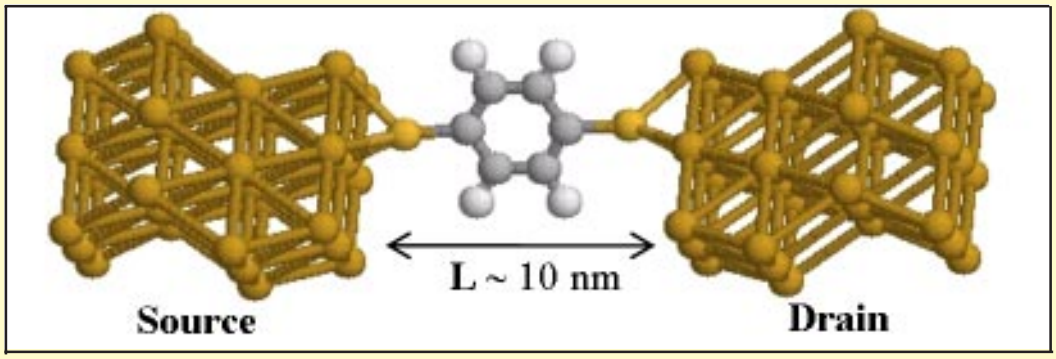

Fig 2. Example of a Molecular Electronics Device

Now, science and semiconductor technology community have come up with a new idea of molecular electronics to avoid a bottleneck in growth. Molecular-electronics (a hot topic of research today), in which, if we sandwich an organic molecule between two metal electrodes and it comprises the dimensions of the order of nanometer ~ 10 nm. These structures contain countable number of atoms and they combine small size, complex organizational patterns, potential for high packing densities and strong lateral interactions and high ratios of surface area to volume.

When we sandwich a molecule between metal electrodes, molecule will be absorbed in electrodes and called extended molecule and with some part of electrodes on both sides, called molecular device. A very simple example of molecular electronics:

A macroscopic quantum system in which size of the device L is larger than any of the internal length scales (Fermi wavelength λ_F, Mean free path L_m, screening length L_s etc.) of the system may be described as a large set of independent subsystems, each described by its own Schrödinger equation. As the system size decreases so that L becomes comparable to the internal length scales, many interesting transport phenomena have been observed including quantized conductance, the quantum Hall effect etc. If $L >> \lambda_F$ (Fermi wavelength $\lambda_F = 2\pi/k_F$), the wave like nature (quantum nature) of the electron can be ignored but if $L \sim \lambda_F$, the quantum nature of the electron comes into play.

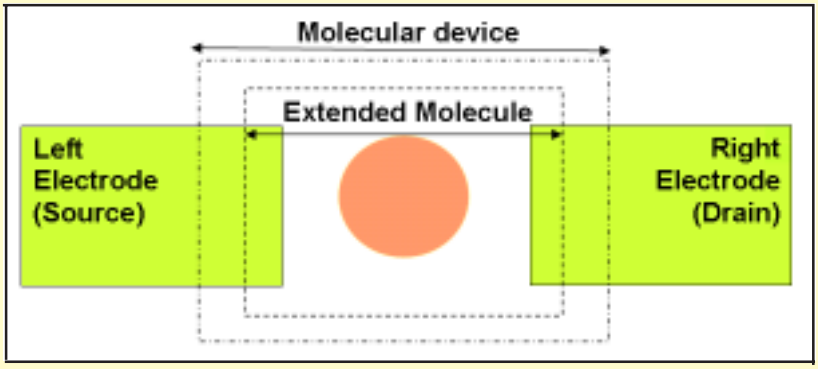

Fig 3. Schematic of a Molecular Electronic Device

Device length of the order of nano meter ≈ 35 nm (k_F = 1.81 Å) than L_m ~ 10 μm and L_s ~ 1 Å. Because device length is larger than the screening length L_s, the perturbation due to the device will be well screened by the electrodes (Source and drain) so the density and effective potential will relax to the equivalent bulk values at the edge of the device. These are the boundary conditions of simulation for molecular electronic devices.

Over the last two decades, the accurate predictions of the properties of atomic and molecular scale devices, including I-V curves, present a difficult challenge, despite the advances and widespread applications of density functional theory (DFT) modeling. DFT-based ab initio condensed

matter simulations frequently used for the studies of finite systems in quantum chemistry and for periodic systems in solid state physics. A molecular electronic device is neither finite nor periodic: it has open boundaries, which are connected to left and right electrodes, where the external bias is applied.

Using ab initio density functional theory and non-equilibrium green's function (DFT-NEGF) approach; we are involved in the development of a simulation method. We have applied this method to investigate the transport properties of molecular electronic devices and carried out calculations for transmission coefficient, density of states and I-V characteristics. Many molecular systems have been studied in recent years as possible candidates for molecular electronics, including n-alkane chains (CH_3–$(CH_2)_{n-1}$), conjugated organic molecules, DNA molecules, fullerenes (C_{60}) and carbon nanotubes.

Presently, we are using simple devices like single benzene or thiophene molecule between Al and Au electrodes. Besides aforementioned research, we have made a theoretical investigation of Metal-Molecule-Interface with different Terminal Groups (Terminal group means atoms, which connects central molecule to left (right) electrodes e.g. H, S, Se, O, CN or NC).

In the far future, interest in nano devices will not be restricted to macro-customer human beings. Micro-robots will have to be equipped and nano-robots may well also be controlled by nano computers. This will extend the range of applications of devices to new domain such as nano-medicine, nano communication and nano-ecology. In biotechnology, new nano scale probes have been developed to monitor and analyze the living process of the cell and nano particles considerably smaller than one micron in diameter have been used in revolutionary ways to deliver drugs and genes into cells. Every discipline has evolved its own separate view of nano sciences and nano technology.

References

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6. "Theoretical Investigation of Metal-Molecule-Interface with Terminal Group", IEEE, Transactions on Nanotechnology, **4**, 422 (2005), Ping Bai, Li Erping, Neerja and Peter A. Collier

DAE-BRNS 3rd National Symposium on Pulsed Laser Deposition of Thin Films and Nanostructured Materials (PLD2005)

November 7-8,2005
Department of Physics
SRI VENKATESWARA UNIVERSITY
Tirupati - 517 502, Andhra Pradesh

3rd National Symposium on Pulsed Laser Deposition of Thin Films and Nanostructured Materials (PLD-05) sponsored by Board of Research in Nuclear Sciences (BRNS) of Department of Atomic Energy (DAE) will be jointly organized by Centre for Advanced Technology (CAT), Indore and Shri Venkateshwara University, Titupati at the above stated venue in Tirupati during November 7 – 8, 2005. This thematic and topical meeting aims to provide a forum for professional interactions amongst the researchers, teachers and students active in this field. The deliberations of the symposium will include invited talks by the leading experts and presentations by young scholars on the growth and properties of thin films and nanostructures of different materials of contemporary and future interest. Some of the classes of these materials are as follows:

- Semiconductors
- CMR and GMR Materials
- Diluted Magnetic Semiconductors
- Ferroelectrics and Dielectrics
- Superconductors
- Polymers and composites
- Nanostructured Materials
- Other new and unknown materials

Deadlines:

Extended abstract	: Sept. 15, 2005
Notification of acceptance	: Sept. 30, 2005
Full Manuscript	: Oct. 15, 2005
Registration	: Nov. 01, 2005

Contact:

Dr. Lalit. M. Kukreja, Convener PLD - 2005,
Thin Film Lab., A-Block
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E-mail: kukreja@cat.ernet.in

Web: http://www.cat.ernet.in/symposiums/conf/pld2k5/pld2005.htm

ANNOUNCEMENTS

The ninth International Conference on Synchrotron Radiation Instrumentation

May 28 - June 3, 2006

Daegu, North Korea

An invitation to SRI 2006

Following the successful conference at San Francisco (2003), the ninth International Conference on Synchrotron Radiation Instrumentation (SRI 2006) will be held on May 28 - June 3, 2006 at EXCO Center, Daegu, Korea. The conference will be hosted by Pohang Accelerator Laboratory (PAL) which has been operating PLS - a 2.5 GeV third-generation synchrotron radiation facility and has recently started construction of a 3.0 GeV Linac-based FEL. SRI 2006 will be also co-hosted by Japan Synchrotron Radiation Research Institute (JASRI), operator of the world largest third-generation machine, SPring-8.

SRI 2006 is the largest and the most important international forum which will seek to promote international exchange and collaboration among all scientists and engineers around the world involved in the developments of new concepts, techniques, and instruments related to the production and utilization of synchrotron radiation. It will feature new developments in synchrotron radiation sources and free electron lasers at photon energies from the infrared to hard X rays, beamline instrumentation to transport the radiation to experimental stations, and experimental techniques to utilize it. Special emphasis will be given to the new and forefront challenges and opportunities provided by recent progresses and expanding interests worldwide in sciences and technologies related to nano dimensions and femtoseconds, which have been putting tremendous pressure on our SRI community to realize new levels of stability, resolution, detectability and accountability.

We will do our best to make the conference most informative, enjoyable and interesting to our SRI community around the world. Please join us at SRI 2006, Daegu, Korea.

- SR-Sources and Advanced Sources
- Beamlines and Optics
- Time-Resolved Techniques
- Nano Science and Technology
- Surface and Interface Analysis
- Magnetism and Spintronics
- Industrial Applications
- Insertion Devices
- Detectors
- Microscopy and Nanoscopy
- Lithography and Micromachining
- Life and Medical Science
- Chemistry and Materials Science

Sincerely yours,

Sunggi Baik
Chair of SRI 2006
Professor and Senior Adviser
PAL/POSTECH
Pohang, Korea

Akira Kira
Co-Chair of SRI 2006
Director General
JASRI/SPring-8
Harima, Japan

Web: http://sri2006.postech.ac.kr/images/1st_circular.pdf

Announcements

Fifth DAE-BRNS National Laser Symposium (NLS-05)

Dec 7-10, 2005
Vellore Institute of Technology (Deemed University)
Vellore, Tamil Nadu

The Fifth DAE-BRNS National Laser Symposium sponsored by the Board of Research in Nuclear Sciences, Department of Atomic Energy will be held at Vellore Institute of Technology, Vellore during December 7 to 10, 2005. The symposium will include plenary talks on recent developments in physics, technology and applications of lasers, invited and contributed presentations by leading experts and young researchers and Ph.D. thesis presentations in the related research areas. The organizing committee of the symposium invites all research scientists, engineers and research students who are engaged in basic or applied research & applications in the broad area of lasers and related fields to participate in the deliberations of the symposium.

Topics of Interest:

- Physics and Technology of Lasers
- Laser Materials, Devices & Components
- Ultrafast Lasers and Applications
- Lasers in Material Science
- Laser Plasma Interaction
- Lasers in Spectroscopy
- Laser based Instrumentation
- Lasers in Nuclear Science & Technology
- Quantum Optics
- Nonlinear Optics
- Tunable Lasers & Applications
- Lasers in Industry & Defence
- Lasers in Chemistry, Biology & Medicine

The Indian Laser Association (ILA) will organize a couple of short tutorial courses on December 6, 2005 preceding the Symposium. Details of this will be announced separately by ILA. ILA will also award prizes for the best thesis and poster presentations. The annual general body meeting of ILA will be held during this symposium.

Manuscripts and abstracts should be sent to:

Mr. S. V. Nakhe
Secretary NLS – 5
Scientific Officer, Laser Systems Engineering Division
Centre for Advanced Technology, Indore-452 013.
E-mail: nls2005@cat.ernet.in

For more details, click
www.cat.ernet.in/symposiums/conf/nls2005

ANNOUNCEMENTS