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# *Research Update*



*Abstracts of  
research publications of  
Thapar University*

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*This issue of 'Research Update' includes extended abstracts of research publications in SCI journals from July-December 2011 of the Thapar University faculty. We aim at sharing globally about Thapar University's research facilities, and the research conducted by its faculty. This research communication is published twice a year in hard as well as electronic form.*

*This time the 'Research Update' includes 'Research Profile' of the Department of Biotechnology and Environmental Sciences. The profile covers briefly the issues such as main research areas, research funding, research facilities, faculty initiative, contributions and achievements. We always look forward for your constructive feedback. Our email ID: [update@thapar.edu](mailto:update@thapar.edu).*

*I sincerely thank members of the editorial board for their support to bring this issue. My thanks are also due to G.S.Lotey for the technical support, Mr Abhista for designing, and Ms Parveen for secretarial support.*

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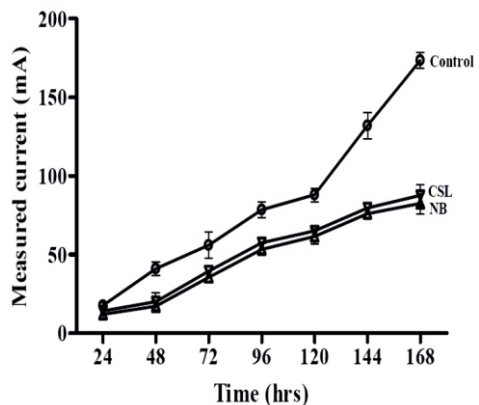
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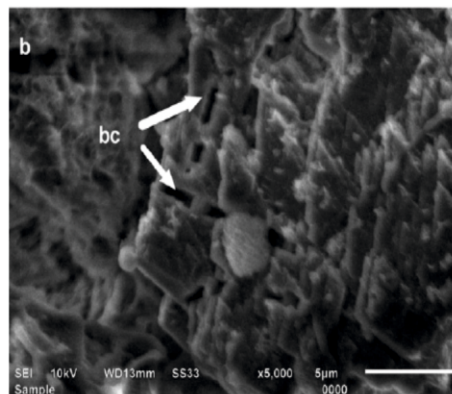
# Role of bacterial calcite in prevention of corrosion in reinforced concrete and improvement in strength properties of ash bricks

Microbially induced calcite precipitation (MICP) on concrete or mortar is an important area of research to enhance the durability of construction materials. The effectiveness of MICP in reducing reinforcement corrosion is investigated. Reinforced concrete (RC) specimens were treated with bacterial strain *Bacillus* sp. CT-5, isolated from the cement sample and subjecting the specimens to accelerated corrosion. The results showed that bacterial-treated RC specimens reduced the corrosion rate four times more than the control specimens. A considerable reduction in mass loss and increase in pullout strength is observed with MICP-treated specimens. Corn steep liquor, an industrial pollutant, was used as a nutrient source to grow the bacterial cells for MICP in cementitious structures. This is a step toward the development of microbial concrete that provides a greener and more ecofriendly option.

In another study, we investigated the potential of *Bacillus megaterium* to produce calcite and improve properties of ash bricks (Fly ash bricks and Rice husk ash bricks). The treated bricks showed significant reduction in water absorption, better frost resistance and increased compressive strength due to calcite deposition on the surface and voids of bricks. Scanning electron micrographs revealed extracellular deposition of calcite crystals by the bacteria on the surface of the bricks. These observations suggest that this technology has the potential of producing durable and eco-friendly building blocks.



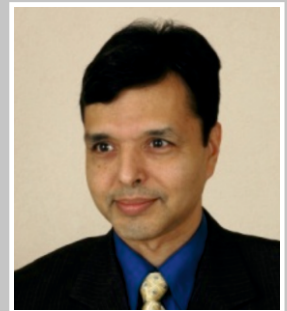
**Figure** Current-time relationship at constant voltage of reinforcing bar (control and bacterially treated specimens in nutrient (NB) and CSL media)



**Figure** Scanning electron micrograph of microbiologically induced calcite precipitation by *B. megaterium* in Fly ash bricks. Rod shaped impressions consistent with the size of bacterial cells (bc) spread around the calcite crystals

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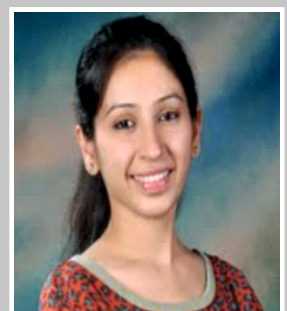
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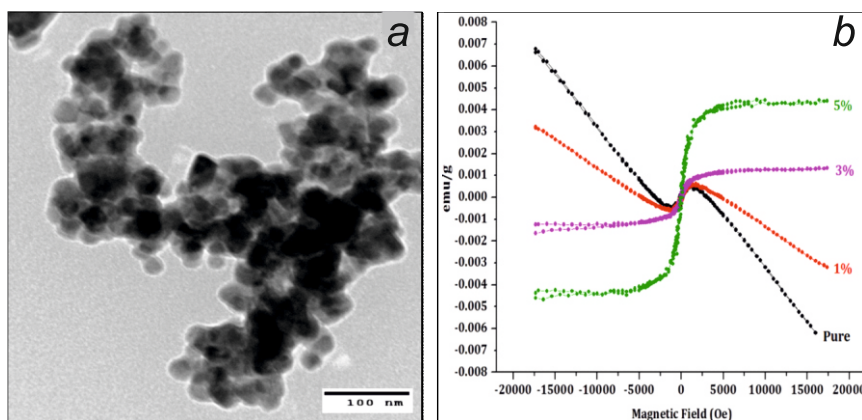
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## Dilute Magnetic Semiconductors: Materials for 'Spintronics'

The term "spintronics" stands for spin transition electronics. As well known today, integrated circuits and high-frequency devices, used for information processing and communications, have had great success through controlling the charge of electrons in semiconductors. Mass storage of information using electronic spins in ferromagnetic materials. It is then quite natural to ask if both the charge and spin of electrons can be used at the same time to enhance the performance of devices. This is the main idea of spintronics, which is widely expected to be the future solution to downsize current microelectronic devices into size of even nanometers. The realization of functional spintronic devices requires materials with ferromagnetic ordering at operational temperatures compatible with existing semiconductor materials. There is a wide class of semiconducting materials which is characterized by the random substitution of a fraction of the original atoms by magnetic atoms. The materials are commonly known as semimagnetic semiconductors or diluted magnetic semiconductors (DMS). These materials are very promising for spintronic device applications.



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**Figure (a)** Magnetization versus magnetic field (M-H) hysteresis loop of pure and Cr-doped CdSe nanoparticles and TEM images of (b) pure CdSe (c) 1% Cr-doped CdSe nanoparticles

**Jaspal Singh et al. [1]** report the synthesis of Cr-doped CdSe nanoparticles by solvothermal technique. The effect of Cr doping on structural, morphological, optical and magnetic properties has been explored. XRD study clearly reveals that Cr-doped CdSe nanoparticles possess wurtzite structure having hexagonal phase. Pure CdSe nanoparticles are spherical in nature having particle size 28.87 nm, which further decreases to 18.75 nm with increases in Cr concentration up to 5%. UV-Vis spectroscopy shows clear blue-shift in energy band-gaps. Pure and 1% Cr-doped CdSe nanoparticles are found to possess diamagnetic behaviour. However, with further increase of Cr-content from 1 to 5%, the doped-CdSe nanoparticles exhibit ferromagnetic behaviour.

**Sanjeev Kumar et al. [2]** The CdS nanoparticles co-doped with Ni and Cu have been synthesized using wet chemical method and mercaptoethanol as capping agent. The Ni- and Cu co-doped CdS nanoparticles have been studied morphologically and structurally by HRTEM and XRD giving particle size  $\approx$  5 nm. Co-doping with Cu results in an increase in ferromagnetic moment in Ni-doped CdS nanoparticles. Therefore, a defect-mediated exchange mechanism, such as the F-center (sulfur vacancy)-mediated exchange mechanism reported previously by others, may appear to present a better clarification for the ferromagnetic ordering observed in transition metal (Ni and Cu)-co-doped CdS nanoparticles.



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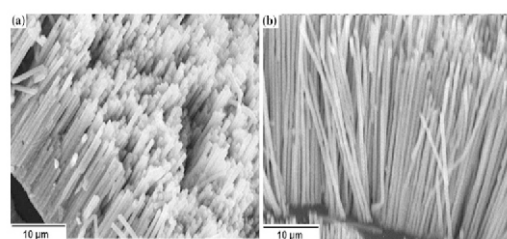
## Fabrication and characterization of highly ordered nanowires and their heterojunctions

One-dimensional (1D) nanostructures such as nanotubes, nanorods, nanowires, nanobelts have been extensively studied not only for their novel physical, chemical, electronic, magnetic, and electrical properties but also for their prospective applications in future-generation nanodevices. Among the various hierarchical structures, 1D nanostructure arrays, perpendicular to the substrate, are of significant interest. The 1D nanostructures are ideal building blocks for nanoelectronics since, in the architecture of nanodevices, they can act both as interconnects and device components.

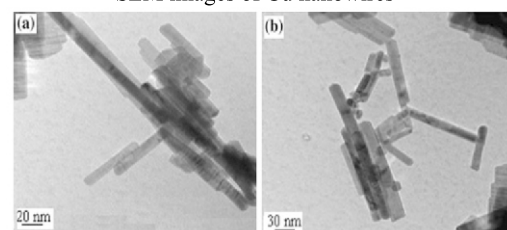
**Gurmeet Singh Lotey et al.** [3] have synthesized highly ordered and dense crop of copper nanowires using a template-assisted electrodeposition technique; the nanowires have been found to be of average size, 100 nm, and preferentially grown along the direction, [111]. The non-linear I–V characteristics suggest formation of tunneling potential barrier in copper nanowires. The nanowires register rise in impedance above 1 kHz due to the inductive effect. The nonlinear I–V characteristics clearly show the possibility of the synthesized copper nanowires finding potential applications in future nanoelectronics.



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SEM images of Cu nanowires

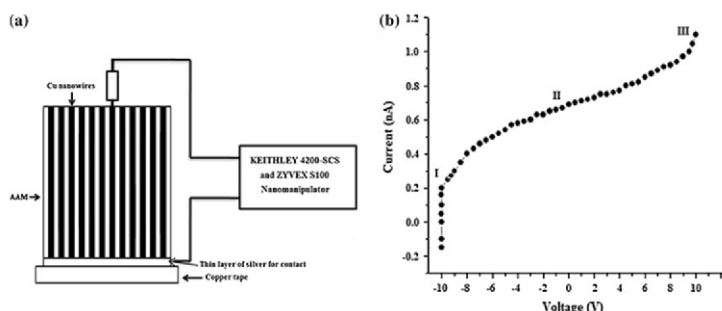


TEM images of CdS nanorods

**Sanjeev Kumar et al.** [4] fabricated 20 nm diameter copper nanowires using the electrodeposition technique. These are found to be highly dense, uniform and parallel aligned. Face centered cubic structure of copper nanowires was found using XRD. EDXRF confirmed the purity of copper nanowires. The decrease in impedance in copper nanowires has been observed after 10 kHz, due to capacitive effect. Because of highly ordered nature of nanowires, they can be directly patterned for fabrication of nanodevices.



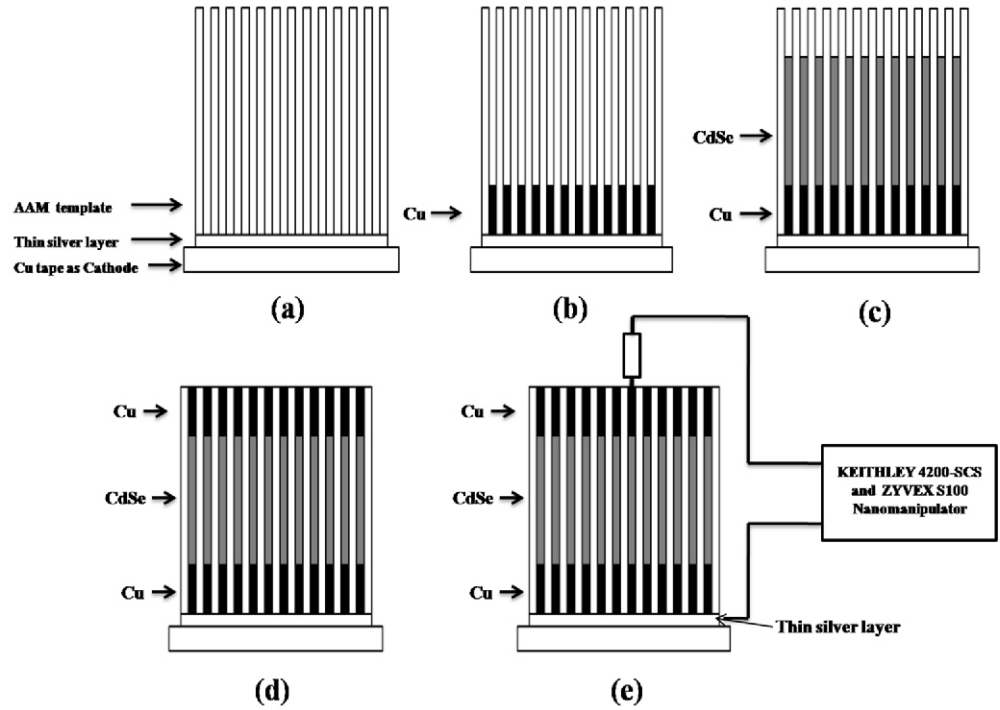
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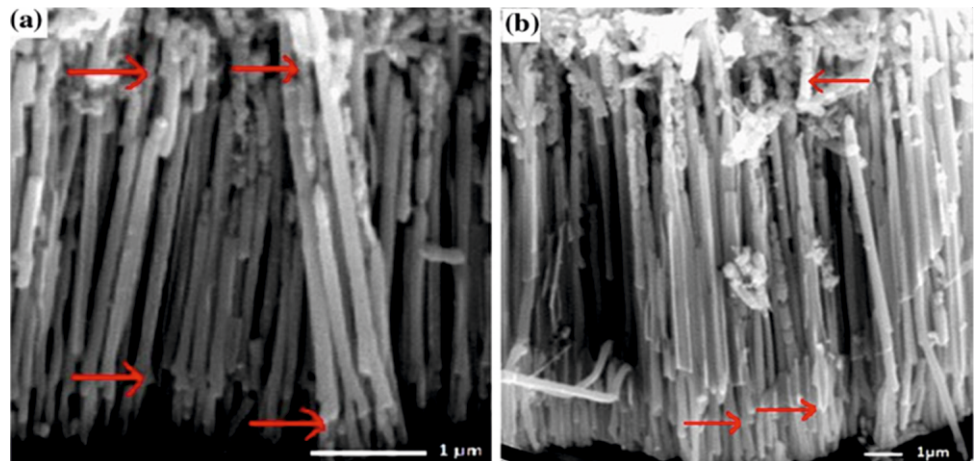
**Figure (a)** The schematic of collective I–V characteristics measurement set up and **(b)** I–V characteristics curve of copper nanowires



**Gurmeet Singh Lotey et al.** [5] fabricated the highly ordered and uniform Cu–CdSe–Cu nanowire heterojunctions by template-assisted electrochemical deposition technique. The SEM and HRTEM micrographs reveal their growth and morphology. UV–Visible spectra reveal blue shift for 100 nm but not for 300 nm nanowire heterojunctions confirming quantum confinement effect for the former. The I–V characteristics reveal the rectifying and the asymmetric behaviour for the 100 and 300 nm nano-wire heterojunctions, respectively. This study establishes the potential of template-assisted fabrication technique for patterned nanowire heterojunctions for nano-sized device applications.



**Figure** Schematic diagram showing various steps involved in growth of Cu–CdSe–Cu nanowire heterojunctions. (a) AAM on which one side is coated with silver conductive layer, (b) electrodeposition of Cu metal, (c) electrodeposition of CdSe semiconductor, (d) electrodeposition of Cu metal and e collective I–V characteristics measurement set-up.



**Figure** SEM micrographs of Cu–CdSe–Cu nanowire heterojunctions of diameter: (a) 100 nm and (b) 300 nm. The arrows in figures indicate junctions present in nanowires

**Sunil Kumar et al.** [6] have investigated the effect of Eu doping on the structural and optical properties of solvothermally synthesized CdS nanorods. The resultant cylindrical nanorods have diameter 10–12 nm with varied lengths of 50–100 nm. The sharp XRD spectra suggest the wurtzite structure of the nanorods with a directional growth along the (002) direction. The spectra also confirmed the doping with no separate peaks due to Eu which is supported by EDS. The PL spectra showed the red peaks at 613 nm due to  $5D_0-7F_2$  transitions of  $\text{Eu}^{2+}$  and it increases with increasing the Eu concentration. The blue shift in peaks in UV–Vis spectra with increase in Eu concentration may be attributed to decrease in crystal defects or quantum confinement.

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## Structural, thermal and electrical properties of $\text{Ti}^{4+}$ substituted $\text{Bi}_2\text{O}_3$ solid systems

In the present study, the effect of  $\text{TiO}_2$  doping on  $(1-x)\text{Bi}_2\text{O}_3 \cdot (x)\text{TiO}_2$  ( $x = 0.05, 0.10, 0.15, 0.20$ ) materials is investigated using X-ray diffraction (XRD), differential thermal analysis (DTA), ac conductivity, scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). XRD results show the formation of single phase  $\text{Bi}_{12}\text{TiO}_{20}$  at  $x > 0.15$  concentration of  $\text{TiO}_2$ . It is observed that, the lower concentration of  $\text{TiO}_2$  leads to the formation of mixed phase. The  $x = 0.15$  and  $x = 0.20$  samples exhibit regular and uniform distribution of the grains as compared to  $x = 0.10$  sample. The highest conductivity is observed for  $x = 0.15$  specimen, e.g.,  $9 \times 10^{-7} \text{ Scm}^{-1}$ .

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# A framework for efficient enterprise resource planning (ERP) implementation in technical educational institutions



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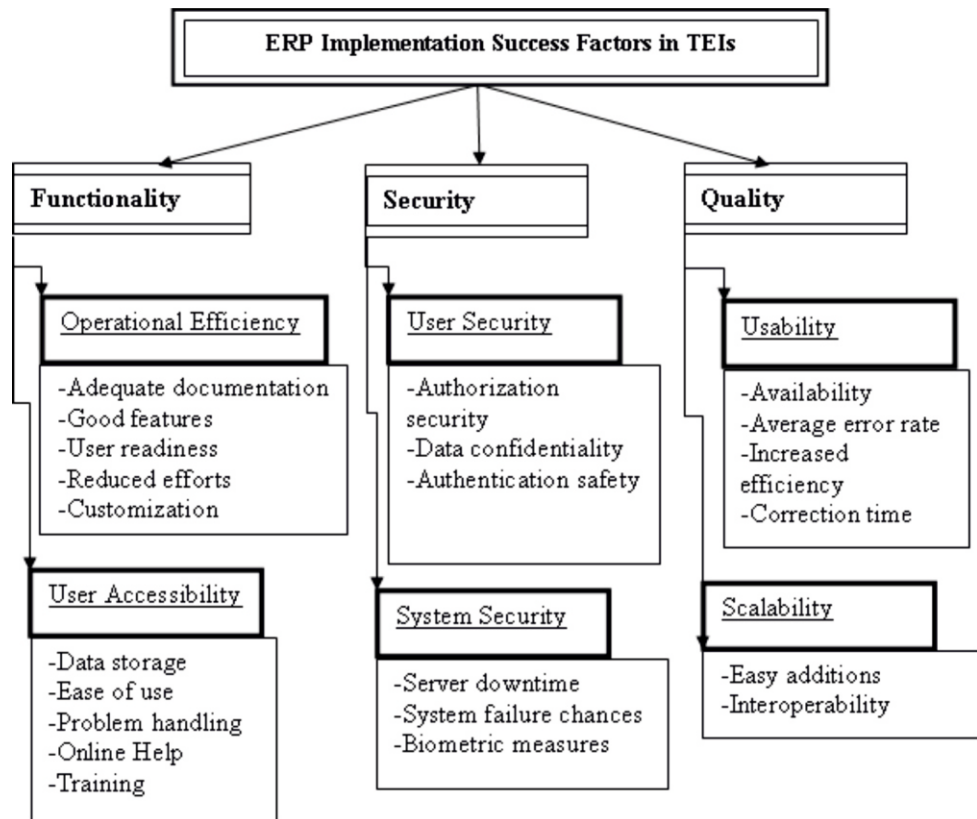


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Technical educational institutions (TEIs) can use enterprise resource planning for an integrated, better and efficient system for management of all the information related to many users in these Institutions. Though ERP is used in many TEIs in India, but it has not been found to be completely successful. This paper aims at assessing the efficiency of implementing an ERP system from users' perspective. The study uses a survey of 900 users in four categories in technical educational institutes in India to gain feedback in their experience of applying ERP. The focus of paper is on three features for efficient ERP: functionality, security and quality. The present research identifies the success factors for efficient ERP implementation. The study also identifies the problems faced in ERP implementation and finally suggests a framework for efficient implementation of ERP in technical educational institutions. The framework designed will help the technical educational institutions in successful and efficient implementation of ERP. The ERP framework designed focuses on features to be enhanced, improved and controlled so as to make ERP system efficient to provide optimum user satisfaction.



**Figure:** Major Success factors for efficient ERP implementation in TEIs

## Reference

Shivani Goel, Ravi Kiran and Deepak Garg, "A framework for efficient enterprise resource planning (ERP) implementation in technical educational institutions", African Journal of Business Management, Vol 5 Issue 34, pp. 13197-13204, Dec 2011.

## Molecular diversity and ligninolytic enzyme activities of morels (wild edible mushrooms) collected from Western Himalayas, India

True morels (*Morchella* spp.) belonging to ascomycetous fungi are highly prized for their edibility and appearance, which is similar to "a sponge on a stick". Due to their unique flavour and rich nutritional value, these morels have been used in soups and gravies, as a source of medicinal adaptogens, immunostimulants, and antitumour agents. In India, morels are commonly known by the name of "Guchhi" and these grow abundantly in Jammu and Kashmir, Himachal Pradesh and Uttaranchal during March to May and August to September. Based on the morphology, studies have revealed that there are three types of morels: yellow, black and half-free. Identification keys such as shape, size and colour change of ascocarp during developmental process may be highly polymorphic among species. Environmental and climatic factors along with the changes in the developmental process may induce the high degree of variability in the ascocarps. So rather than relying only on morphological features, molecular techniques are increasingly employed in fungal systematics, as they are highly reliable, fast and easily approachable. The molecular diversity of thirty-two different *Morchella* cultures/fruited bodies, collected from the Western Himalayan region was studied in this investigation. In the present study, sequence analysis revealed that in the Western Himalayan region of India, both yellow (*M. crassipes*, *M. spongiosa*) and black morels (*M. elata*, *M. angusticeps* and *M. gigas*) were prominent along with two *Verpa* species. Phylogenetic analysis by maximum parsimony, maximum likelihood and Bayesian inference revealed two different clades and a clear distinction between yellow and black morels.

In an attempt to cultivate these morels, effect of different carbon and nitrogen sources on sclerotia formation was investigated under in vitro conditions for black morel *Morchella elata* and yellow morel *Morchella crassipes*. The fungi were grown well with different carbon and nitrogen sources but the formation of sclerotia was influenced much by these nutritional parameters. Carbon sources such as ribose, cellobiose, galactose, xylose, sucrose and mannitol produced many large sized and cream coloured sclerotia in *M. crassipes* while in *M. elata*, small sized and brown pigmented sclerotia were formed in ribose, galactose, sorbose and mannitol. Among the nitrogen sources, sodium nitrate and yeast extract produced sclerotia in both the cultures that were smaller in size and lesser in number. Ligninolytic enzymes produced by these fungi when grown in presence of agricultural wastes and also different inducers were also studied.

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# Modeling The Spread of HIV in a Stage Structured Population: Effect of Awareness



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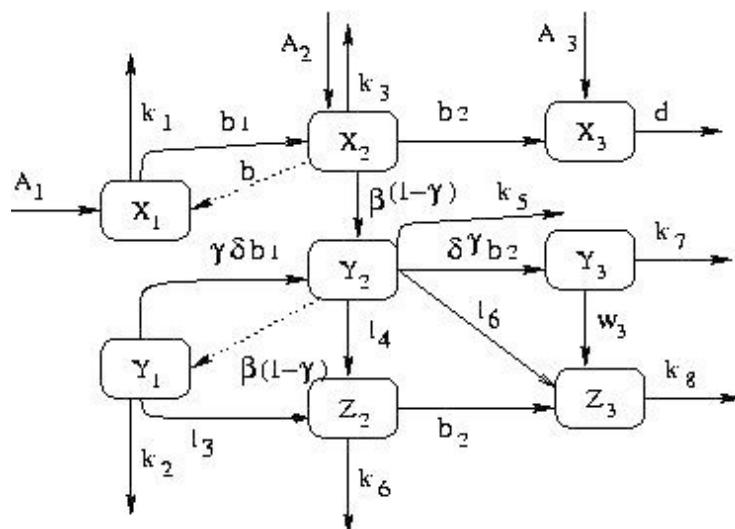
Human immunodeficiency virus (HIV) is a lenti-virus (a member of the retrovirus family) that causes acquired immunodeficiency syndrome (AIDS), a critical condition in humans in which progressive failure of the immune system allows life-threatening opportunistic infections. Over the past few years HIV has been spreading rapidly in the population. Almost, everyday there are thousands of new human cases of HIV infection being recorded in the world and these occur in almost every country of the world. However, the spread of HIV is relatively faster in the developing countries as compared to developed countries because developing countries have limited resources. In worldwide, 70% of HIV infections in the adults have been transmitted through heterosexual contact and vertical transmission accounts for more than 90% of global infection in infants and children.

In this paper, we proposed a nonlinear stage structured mathematical model to study the spread of HIV by considering transmission of disease by heterosexual contact and vertical transmission. This model is analyzed by considering the total population variable and dividing the whole population under consideration into three stages: children, adults and old. Also, it is assumed that the rates of recruitment are different in different groups of population. In this paper we proposed and analyzed a stage structured model for HIV and studied the effect of awareness. In the presented model, we get two equilibria: the disease free equilibrium point and the endemic equilibrium point. It is found that the disease free equilibrium is locally asymptotically stable when  $R_0 < 1$  and is unstable for  $R_0 > 1$ . In fact the equilibrium point  $E_0$  is globally stable under the condition  $R_0 < 1$ . The conditions for existence and local stability of the endemic equilibrium point have been obtained.

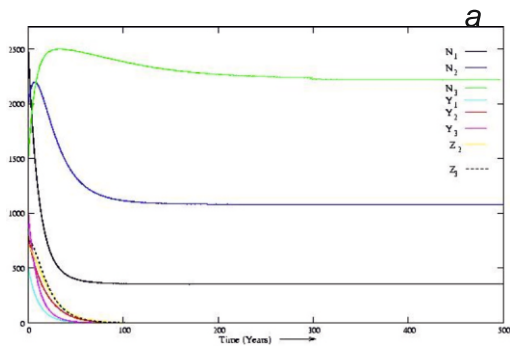
Numerical simulation has been performed for different set of parameters. Using the stability theory of differential equations and computer simulation, it has been shown that with the increase in the awareness of the disease in adult class the infection prevalence of HIV and AIDS can be reduced. The analysis shows that, the most effective way to lower the incidence level is by providing appropriate awareness about disease and its preventive measures. Cautiously, it can be concluded that the awareness is an effective way of reducing the infection prevalence of HIV/AIDS.



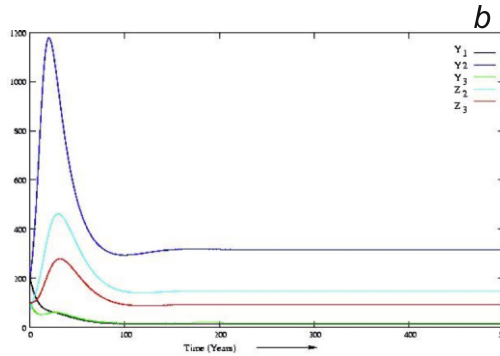
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**Figure** Transfer Diagram of Model



**Figure (a)** Stability of the disease free equilibrium point  $E_0$  for  $R_0 = 0.948483$



**Figure (b)** Stability of the endemic equilibrium point  $E_1$  for  $R_0 = 2.123477$

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1. Navjot Kaur, Mini Ghosh and Satinder Singh Bhatia, "Modeling The Spread of HIV in a Stage Structured Population: Effect of Awareness", International Journal of Biomathematics, Vol. 5, No. 2 (March 2012).



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## Role of important parameters in ring opening polymerization of polylactide

Different parameters, namely polymerization temperature, polymerization time, monomer/initiator ratio, nature of the initiator, amount of water or other impurities etc. are very significant for polymerization reactions either in bulk or solution. Monomer to initiator ratio has a very significant role in polymerization reactions and a value ranging from 50 to 5000 that has been reported by different researchers. Recrystallization of the monomer removes the meso compounds from the monomer, which absorbs the moisture and effects polymerization reaction. So, it is necessary to recrystallize the monomer with any anhydrous solvent like dry toluene, ethyl acetate etc. Prolonged reaction time cannot increase the polymer yield; it generally causes the decrease of molecular weight and broadening of molecular weight distribution of formed polymers. This is probably due to the transesterification side reaction in polymerization, intensifying at prolonged time periods. Several groups like hydroxyl and carboxylic acid affect the polymerization rate.

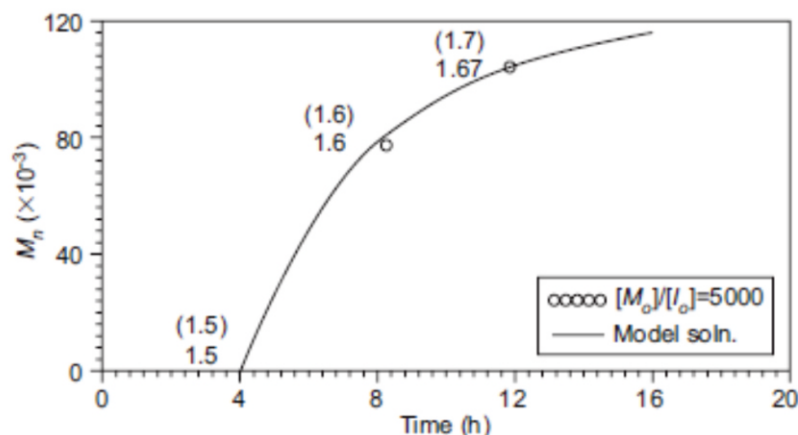
In most of the cases, the effect of polymerization temperature and time goes up to a certain value and after that polymer yield and molecular weight decreases. It also causes the broadening of molecular weight distribution. This is probably due to the transesterification side chain reaction. The average molecular weight decreases at very high monomer-to-initiator ratios. This may be due to the fact that with a fewer number of growing polymer chains, the presence of even a trace amount of chain terminating agent can limit the molecular weight. The presence of moisture also decreases the polymer yield, so it is very important to recrystallize the monomer before the start of polymerization, otherwise, low molecular weight product is obtained.

## Kinetic parameters estimation of ring-opening poly (lactic acid) polymerization by modeling and simulation

The modeling of ring-opening polymerization of lactide to poly(lactic acid) (PLA) has been carried out. Carothers first synthesized PLA in 1932. Since then, hundreds of research papers and patents have appeared in the literature. However, there is a lack of data concerning the rate constants for initiation, propagation and termination steps of PLA polymerization, except some data about the apparent rate constant. This work investigates, theoretically, the individual rate constants using a simple numerical technique. The progress of lactide polymerization can be modeled by assuming a ring opening reaction mechanism comprising chain initiation, chain propagation, and chain termination. The simulator developed, based on the solution of differential equations corresponding to the above-mentioned kinetic scheme, Generates a detailed molecular weight distribution that can be used to estimate average molecular weights (or average degree of polymerization) vs. polymerization time curves. These simulated curves, on matching with the reported experimental data (for different catalysts), yield the absolute values of rate constants. The values have been determined for zinc lactate. Rate constants could be determined by using the molecular weight and the polydispersity vs. polymerization data. This methodology offers greater opportunity for capturing high, non-equilibrium polymer yield through appropriately timed termination of the polymerization reaction.



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**Figure 1** A comparison of experimental (Schwach et al. [4]) and modeling results (number average molecular weight) for the polymerization of D,L-lactide, using zinc lactate catalyst. The solid lines are the solutions obtained from the model and points are the experimental values. The experimental polydispersity of selected points are noted in parentheses and the modeled polydispersity is shown below it.



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1. Rajeev Mehta, Vineet Kumar, Sidh Nath Upadhyay, Journal of Polymer Engineering, Volume 31, Issue 2-3, Pages 251-252, 2011.
2. Paramjit Kaur, Rajeev Mehta and Sidh Nath Upadhyay Role of important Parameters in Ring-opening polymerization of Polylactide, Journal of Polymer Engineering, 31(2-3), 243-249, 2011.

## Fusion reaction cross-sections using the Wong model within Skyrme energy density based semiclassical extended Thomas Fermi approach

First, the nuclear proximity potential, obtained by using the semiclassical extended Thomas Fermi (ETF) approach in Skyrme energy density formalism (SEDF), is shown to give more realistic barriers in frozen density approximation, as compared to the sudden approximation. Then, taking advantage of the fact that, in ETF method, different Skyrme forces give different barriers (height, position and curvature), we use the  $\chi$ -summed extended-Wong model of Gupta and collaborators (2009) under frozen densities approximation for calculating the cross-sections, where the Skyrme force is chosen with proper barrier characteristics, *not requiring* additional "barrier modification" effects (lowering or narrowing, etc.), for a best fit to data at sub-barrier energies. The method is applied to capture cross-section data from  $^{48}\text{Ca} + ^{238}\text{U}$ ,  $^{244}\text{Pu}$ , and  $^{248}\text{Cm}$  reactions and to fusion–evaporation cross-sections from  $^{58}\text{Ni} + ^{58}\text{Ni}$ ,  $^{64}\text{Ni} + ^{64}\text{Ni}$ , and  $^{64}\text{Ni} + ^{100}\text{Mo}$  reactions, with effects of deformations and orientations of nuclei included, wherever required. Interestingly, whereas the capture cross-sections in Ca-induced reactions could be fitted to any force, such as SIII, SV and GSK1, by allowing a small change of couple of units in deduced  $\chi_{\text{max}}$ -values at below-barrier energies, the near-barrier data point of  $^{48}\text{Ca} + ^{248}\text{Cm}$  reaction could not be fitted to  $\chi_{\text{max}}$ -values deduced for below barrier energies, calling for a check of data. On the other hand, the fusion–evaporation cross-sections in Ni-induced reactions at sub-barrier energies required different Skyrme forces, representing "modifications of the barrier", for the best fit to data at all incident center-of-mass energies  $E_{c.m.}$ 's, displaying a kind of fusion hindrance at sub-barrier energies. This barrier modification effect is taken into care here by using different Skyrme forces for reactions belonging to different regions of the periodic table. Note that more than one Skyrme force (with identical barrier characteristics) could equally well fit the same data.

## The decay of the compound nucleus $^{215}\text{Fr}^*$ formed in the $^{11}\text{B} + ^{204}\text{Pb}$ and $^{18}\text{O} + ^{197}\text{Au}$ reaction channels using the dynamical cluster-decay model

The decay of  $^{215}\text{Fr}$  nucleus, formed in  $^{11}\text{B} + ^{204}\text{Pb}$  and  $^{18}\text{O} + ^{197}\text{Au}$  reactions, is studied by using the dynamical cluster-decay model (DCM) with effects of deformations and orientations of nuclei included in it. The observed decay is mainly via fusion–fission, with data collected for both the fission excitation functions and fission fragment anisotropies. The chosen reaction channels have entrance channel mass asymmetries lying on either side of the Bussinaro–Gallone critical asymmetry parameter. In agreement with experimental data and conclusions based on the statistical code PACE2, for fission excitation functions, our DCM calculations with  $l_{\text{max}}$  value



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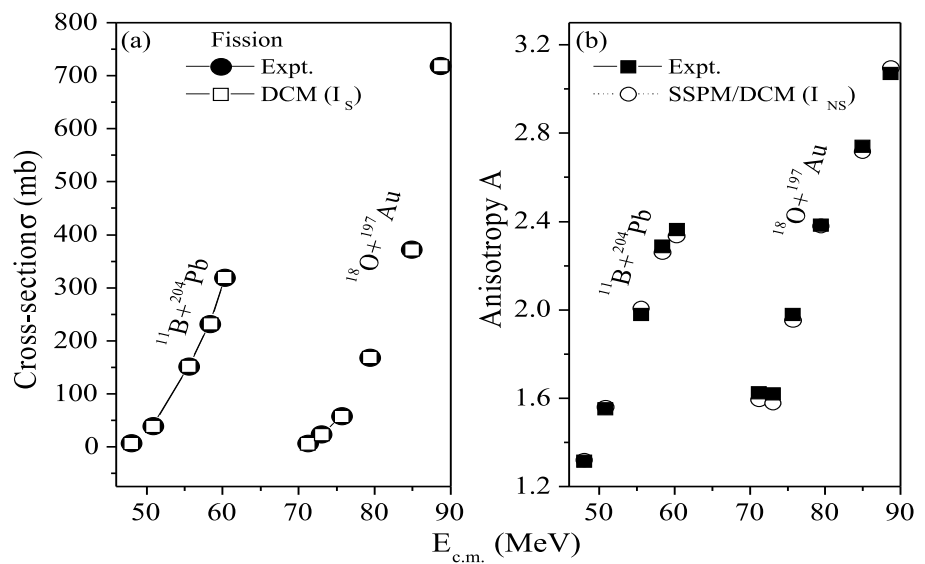
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used in accordance with the sticking moment of inertia also show no contribution of the quasi-fission component in fission cross-sections for both the reaction channels, measured at incident center-of-mass energy spread on either side of the Coulomb barrier. Due to deformation and orientation of nuclei, the fission mass distribution is asymmetric, and nearly independent of the entrance channel. Interestingly, for a best fit to data on fission cross-sections, an in-built 'barrier lowering' seems operative at sub-barrier energies for both the reactions under study. Also, the fission fragment anisotropies, calculated on DCM for the first time, using non-sticking moment of inertia are found consistent with experimental data for both the reaction channels, confirming beyond doubt the entrance channel's independence of the decay of  $^{215}\text{Fr}^*$



**Figure 1:** (a) The DCM calculated  $\sigma$  fission for the decay of CN  $^{215}\text{Fr}^*$  formed in  $^{11}\text{B}+^{204}\text{Pb}$  and  $^{18}\text{O}+^{197}\text{Au}$  reactions, using the moment of inertia  $I_S$ , at various  $E_{c.m.}$ 's, compared with experimental data (b) the same as for (a) but for the anisotropy  $A$ , using the INSLimit of moment of inertia.

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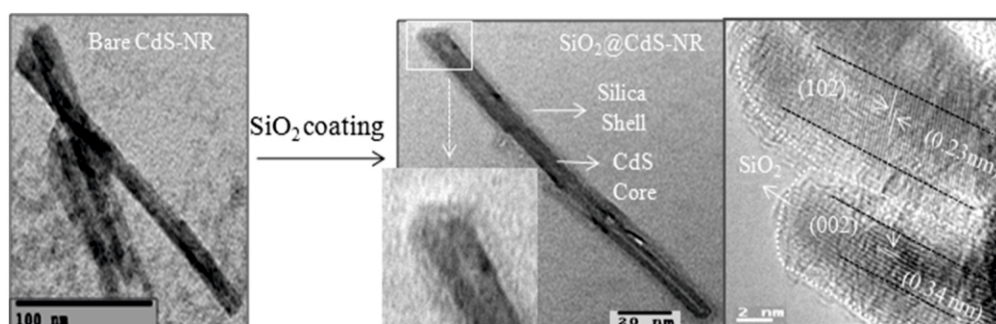
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**Letters** (also called *communications*, and not to be confused with *letters to the editor*) are short descriptions of important current research findings that are usually fast-tracked for immediate publication because they are considered urgent.



## The synthesis, structure, optical and photocatalytic properties of silica-coated cadmium sulfide nanocomposites of different shapes

CdS nanostructure undergoes photochemical dissolution, and hence, the photocatalytic activity deteriorates with light irradiation time. A thin layer of silica coating over CdS surface may prevent the photocorrosion and coalescence of quantum size CdS particles. Hence, we synthesized  $\text{SiO}_2@\text{CdS}$  nanocomposites of different shapes and characterized them by XRD, HRTEM, EDX, SAED, BET surface area measurement and absorption and emission study. The dispersion of spherical CdS (Cd-2.62 at% and S-2.33 at%) nanoparticles of cubic crystal structure into thick amorphous  $\text{SiO}_2$  (43.79 at%) matrix is demonstrated here. The fabrication of core (CdS)-shell ( $\text{SiO}_2$ ) structure ( $\text{SiO}_2@\text{CdS}$ ) consisting of CdS nanorods (Cd-19.79 at% and S-22.90 at%) core (length = 126 nm and width = 6 nm) having characteristic lattice fringes of hexagonal crystals and thin  $\text{SiO}_2$  (12.81 at%) shell (thickness = 1–1.4 nm) is successfully achieved for the first time. The surface area ( $21.2 \text{ m}^2/\text{g}$ ) of CdS nanorod (aspect ratio = 21) is found to increase ( $42.3 \text{ m}^2/\text{g}$ ) after  $\text{SiO}_2$  coating. The photoluminescence of CdS nanosphere (485 nm) and nanorods (501 nm) is highly quenched after  $\text{SiO}_2$  layer formation. The superior photocatalytic activity of  $\text{SiO}_2@\text{CdS}$  composites for the benzaldehyde oxidation under UV irradiation has been displayed. Figure 1 shows the TEM images of core (CdS)-shell ( $\text{SiO}_2$ ) morphology of silica coated CdS nanorod which displayed higher and stable photocatalytic activity under visible light irradiation as compared to bare CdS nanoparticles.



**Figure** TEM images of a thin layer (thickness 1-1.4 nm) of silica coated CdS nanorods.

## Size and shape dependent attachments of Au nanostructures to $\text{TiO}_2$ for optimum reactivity of Au- $\text{TiO}_2$ photocatalysis

This study demonstrated the effects of supported Au nanoparticles of various sizes and shapes on its co-catalytic activity imparted to  $\text{TiO}_2$  during photocatalytic oxidation of salicylic acid. The  $\text{TiO}_2$  photoactivity is remarkably improved with the decreasing size ( $9.5 \pm 0.06$  to  $3.5 \pm 0.25$  nm) and increasing surface to volume (S/V) ratio ( $0.629$  to  $1.95 \text{ nm}^{-1}$ ) of spherical Au co-



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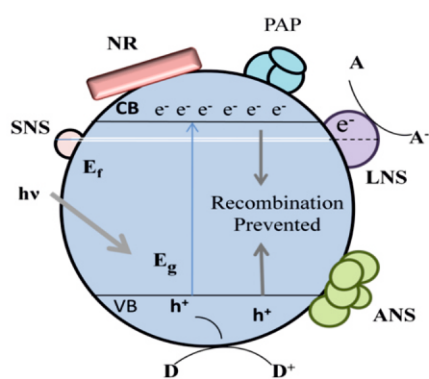


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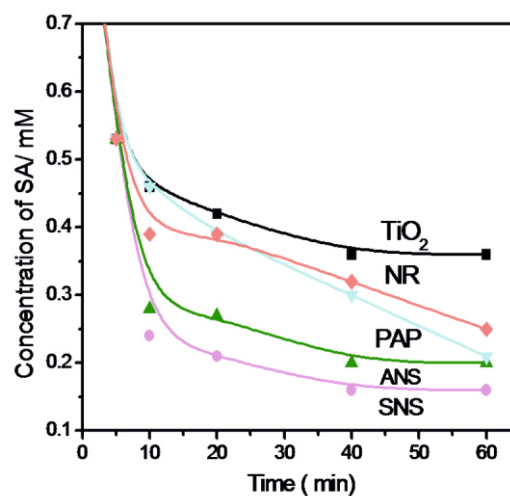


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catalysts loading. The amount of Au (0.02 wt%) nanostructures supported to TiO<sub>2</sub> for its optimum photoreactivity is found to be 100 times less than the conventional prerequisite of 1-2 wt% metal photodeposition. The Au nanorod (aspect ratio =  $2.8 \pm 0.12$  and  $S/V = 0.54 \text{ nm}^{-1}$ ) attachment to TiO<sub>2</sub> significantly decreased the photoactivity compared with the highly active quantum size ( $3.5 \pm 0.25 \text{ nm}$ ) Au co-catalysts loading. The interaction of Au nanoparticles of various morphology with TiO<sub>2</sub> induces the photoexcited charge transfer process in varied extent, leading to diverse photocatalytic activity. Zeta potential (surface charge and conductance) measurement of aqueous dispersion of TiO<sub>2</sub>, Au nanoparticles and salicylic acid was carried out to investigate the interaction among the various components in the photoreaction system. Figure shows below represent the co-catalytic activity of Au nanoparticles of different shapes and sizes attached to TiO<sub>2</sub> catalysts for its optimum photocatalytic activity.



**Scheme 1. Various morphology of Au nanoparticles-TiO<sub>2</sub> junctions.**



**Figure** Comparative photoactivity for the salicylic acid degradation by different Au (0.02 wt%)-TiO<sub>2</sub> photocatalysts under UV light irradiation. (Au nanostructure: NS-Nanosphere, SNS-small nanosphere NR-nanorod, LNS-large nanosphere, ANS-aggregated nanosphere and PAP-photodeposited aggregated particle)

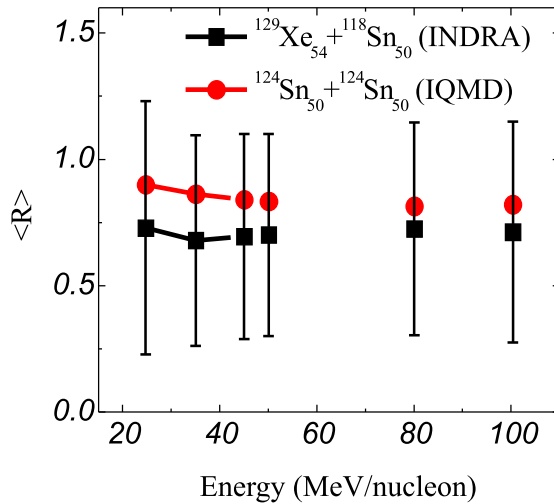
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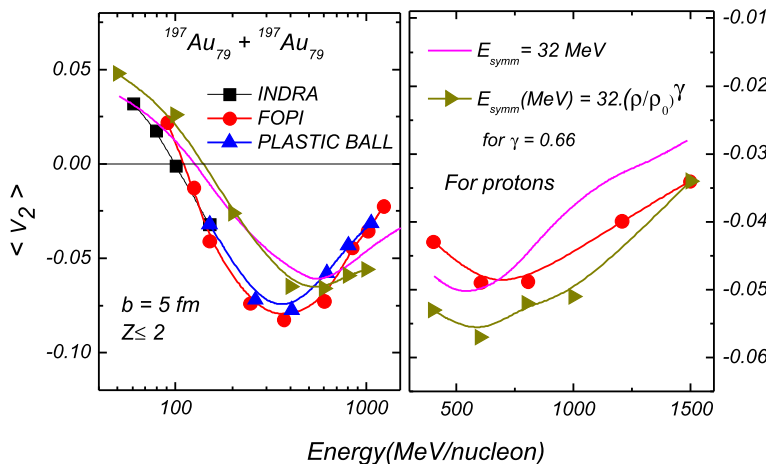
## Influence of charge asymmetry and isospin-dependent cross section on nuclear stopping

We study the effect of charge asymmetry and isospin-dependent cross section on nuclear stopping and multiplicity of free nucleons and light mass fragments, using the isospin-dependent quantum molecular dynamics model. Simulations were carried out for the reactions  $^{124}X_m + ^{124}X_{m'}$ , where  $m$  varies from 47 to 59 and for  $^{40}Y_n + ^{40}Y_{n'}$ , where  $n$  varies from 14 to 23. Our study shows that nuclear stopping depends strongly on the isospin of the cross-section and weakly on the charge asymmetry of the colliding nuclei. Theoretical results on the anisotropy ratio  $\langle R \rangle$  follow the same trend as recorded by INDRA collaboration.



## Influence of density-dependent symmetry energy on elliptical flow

The effect of density dependent symmetry energy on elliptical flow is studied using isospin-dependent quantum molecular dynamics model. We have used the reduced isospin-dependent cross-section with hard (H) equation of state to study the sensitivity of the elliptical flow to symmetry energy in the energy range 50 - 1000 MeV/nucleon. The elliptical flow becomes zero at a particular energy termed as transition energy. A systematic effort has been made to pin down the transition energy for the density dependent symmetry energy.



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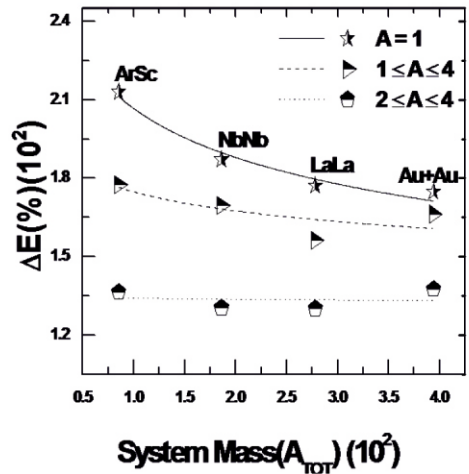
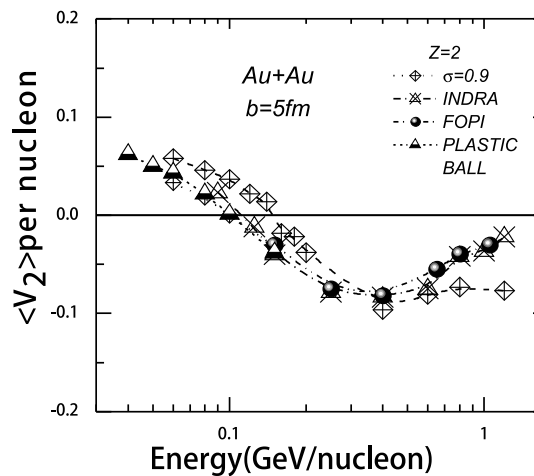
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## Correlation between balance energy and transition energy for symmetric colliding nuclei<sup>1</sup>

We study the correlation between balance energy and transition energy of fragments in heavy-ion collisions for different systems at incident energies between 40 and 1200 MeV/nucleon using an isospin-dependent quantum molecular dynamics model. With increasing incident energy, the elliptic flow shows a transition from positive (in-plane) to negative (out-of-plane) flow. This transition energy is found to depend on the size of fragment, composite mass of reacting system, and the impact parameter of the reaction. It has been observed that a reduced cross-section can explain the experimental data. There is a correlation between balance energy and transition energy as their difference decreases with an increase in the total mass of the colliding nuclei.



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**Research notes** are short descriptions of current research findings that are considered less urgent or important than *Letters*.



## Evaluation of clonal fidelity of in vitro raised plants of *Guadua angustifolia* Kunth using DNA-based markers

*Guadua angustifolia* Kunth is an important woody bamboo native to Colombia, Ecuador, and Venezuela. It is one of the 3 largest growing bamboo species and economically most important in the world. Due to its versatility, lightness, flexibility, endurance, hardness, strength, climatic adaptability, seismic-resistance, rapid growth and easy handling, it is widely employed in paper, charcoal and construction industries. Overexploitation of this bamboo has led to the rapid depletion of natural strands hence generating a grave concern about conservation as well as to develop propagation methodologies for new plantations and reestablishment of cleared strands. Limitations in traditional propagation methods such as the use of offsets, branch cuttings together with poor seed set and unpredictable and long flowering cycle (about 35 years) warrants an urgent need for an alternative approach for developing efficient and reproducible protocols for its mass propagation. Given the difficulties of conventional propagation techniques, in vitro propagation provides a promising alternative.

A protocol for efficient regeneration of plantlets using nodal explants from 4 year old potted plant was established. MS medium supplemented with BAP (2mg/l) effectively induced sprouting in 90% of the explants within 15 days of inoculation. After bud break, sprouted buds were excised from nodal explants after 3 weeks of growth on initiation medium and cultured on MS medium supplemented with different concentrations and combination of cytokinins. MS liquid medium supplemented with BAP (2 mg/l) and adenine sulphate (10 mg/l) produced maximum lateral shoots with an average shoot number of 18.2 and shoot length of 7.06 cm after 90 days of culture. Rooting was obtained simultaneously during shoot multiplication on the multiplication medium without addition of any auxin in 100% of the cultures. Well developed and rooted clumps of 5-6 shoots were selected for hardening. Plants were initially shifted to the plastic pots containing soil and were covered with jars for maintaining high humidity for 30 days. These were then shifted to a mixture of sand:soil:manure (1:1:1) and kept in a green house. They were regularly sprayed with Hoagland solution after seven days interval. Almost 100% of the plants survived during acclimatization.

Among the various methods of in vitro propagation, the enhanced axillary shoot proliferation is most reliable and least susceptible to genetic modifications. However, the possibility of somaclonal variations cannot be ruled out even with this method. Therefore, it is pertinent to screen the regenerants at regular intervals for the occurrence of any somaclonal variation. To test the clonal fidelity, the in vitro raised plants at various stages of subculture along with the hardened plants were chosen randomly. Random amplified polymorphic DNA (RAPD) and inter-simple sequence repeat (ISSR) markers were utilized to assure the genetic fidelity of in vitro raised clones. 30 RAPD and 27 ISSR primers were used for initial screening and 15 RAPD and 17 ISSR markers produced clear, reproducible and scorable bands. 15 RAPD primers produced 84 distinct bands with an average of 5.6 bands per primer. In addition, 17 ISSR



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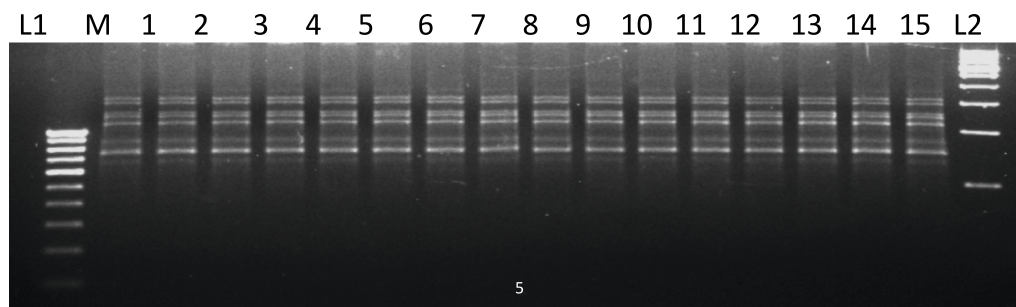
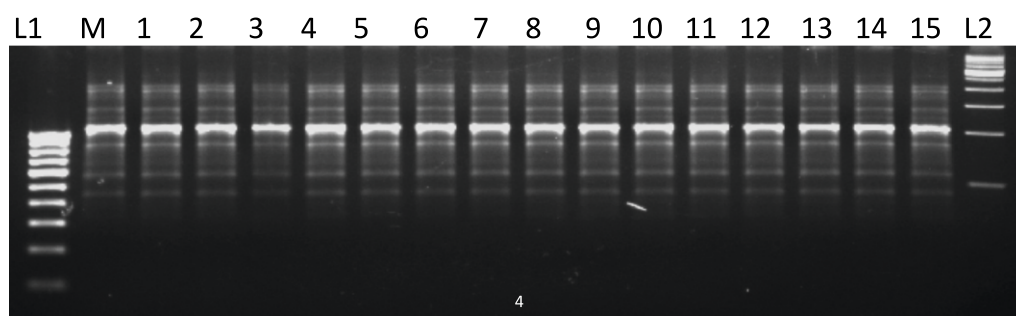
primers produced 61 distinct bands in the size range of 300 bp to 2500 bp. All banding profiles from micropropagated plants were monomorphic and similar to those of the mother plant, thus ascertaining the true to type nature of the in vitro raised plants.



**Figure 1-** Multiple shoot proliferation on MS medium supplemented with BAP (2mg/l) and adenine sulfate (10mg/l); **Figure 2-** Well developed rooted plant of *G. angustifolia*; **Figure 3-** Acclimatized plants of *G. angustifolia*



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**Figure 4-** Polymerase chain reaction (PCR) amplification products obtained with a random amplified polymorphic DNA (RAPD) primer OPT-13; **Figure 5-** ISSR products generated from 15 in vitro regenerated plants and mother plant of *G. angustifolia* amplified with primer UBC 808. Lane L1 represents 100 bp ladder, Lane M represents mother plant, Lane 1 to 15 represent in vitro raised clones of *Guadua angustifolia* and Lane L2 represents 500 bp ladder.

**Reference:-**

Harleen Kaur Nadha, Rahul Kumar, Ram Kumar Sharma, Manju Anand, Anil Sood. Evaluation of clonal fidelity of in vitro raised plants of *Guadua angustifolia* Kunth using DNA-based markers. *Journal of Medicinal Plant Research*, 5(23), 5636-5641 (2011)

## Antifungal activity of multifunctional Fe<sub>3</sub>O<sub>4</sub> – Ag nanocolloids

In recent years, rapid increase has been observed in the population of microbes that are resistant to conventionally used antibiotics. Antifungal drug therapy is no exception and now resistance to many of the antifungal agents in use has emerged. Therefore, there is an inevitable and urgent medical need for antibiotics with novel antimicrobial mechanisms. *Aspergillus glaucus* is the potential cause of fatal brain infections and hypersensitivity pneumonitis in immunocompromised patients and leads to death despite aggressive multidrug antifungal therapy. In the present article, we describe the antifungal activity of multifunctional core – shell Fe<sub>3</sub>O<sub>4</sub> – Ag nanocolloids against *A. glaucus* isolates. Controlled experiments are also carried out with Ag nanocolloids in order to understand the role of core (Fe<sub>3</sub>O<sub>4</sub>) in the antifungal action. The minimum inhibitory concentration (MIC) of nanocolloids is determined by the micro-dilution method. MIC of *A. glaucus* is 2000 mg/mL. The result is quite promising and requires further investigations in order to develop a treatment methodology against this death causing fungus in immunocompromised patients.



Photographic views of the antifungal tests of Fe<sub>3</sub>O<sub>4</sub>–Ag nanocolloids against *Aspergillus glaucus*. (A) control, i.e., medium + antifungal agent (Fe<sub>3</sub>O<sub>4</sub>-Ag); (B) zero concentration, i.e., medium + *Aspergillus glaucus* (C) below MIC: concentration of Fe<sub>3</sub>O<sub>4</sub>-Ag nanocolloids was 30% below MIC; (D) at MIC

## Nanoengineering of methylene blue loaded silica encapsulated magnetite nanospheres and nanocapsules for photodynamic therapy

Core–shell nanostructures have emerged as an important class of functional materials with potential applications in diverse fields, especially in health sciences. In this article, nanoengineering of novel magnetic colloidal dispersion containing surface modifiable silica with a core of single domain magnetite nanoparticles loaded with photosensitizer (PS) drug "Methylene blue" (MB) has been described. Magnetite core is produced by the well-established chemical coprecipitation technique and silica shell is formed over it by the modified hydrolysis and condensation of TEOS (tetraethyl orthosilicate). Conditions for reaction kinetics have been established to tailor the core–shell structures in the form of nanospheres and nanocapsules. MB is loaded into the nanostructures by demethylation reaction. The major conclusion drawn from this study is that the synthesis route yields stable, non-aggregated MB loaded



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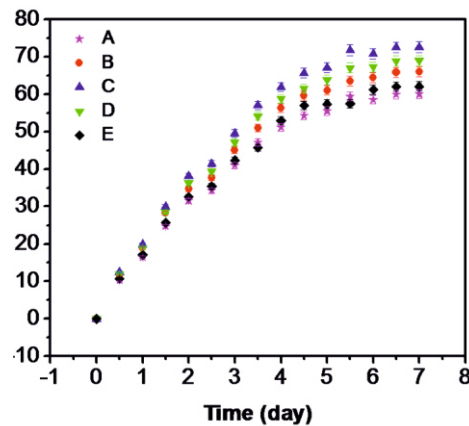


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superparamagnetic magnetite-silica nanostructures with tailored morphology, tunable loading, and excellent magnetic properties.



Drug release profile of MB loaded magnetite-silica nanospheres synthesized at different pH (A) 11 (B) 11.5 (C) 12 (D) 12.5 (E) 13

#### Reference:

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**Supplemental articles** contain a large volume of tabular data that is the result of current research and may be dozens or hundreds of pages with mostly numerical data. Some journals now only publish this data electronically on the internet.



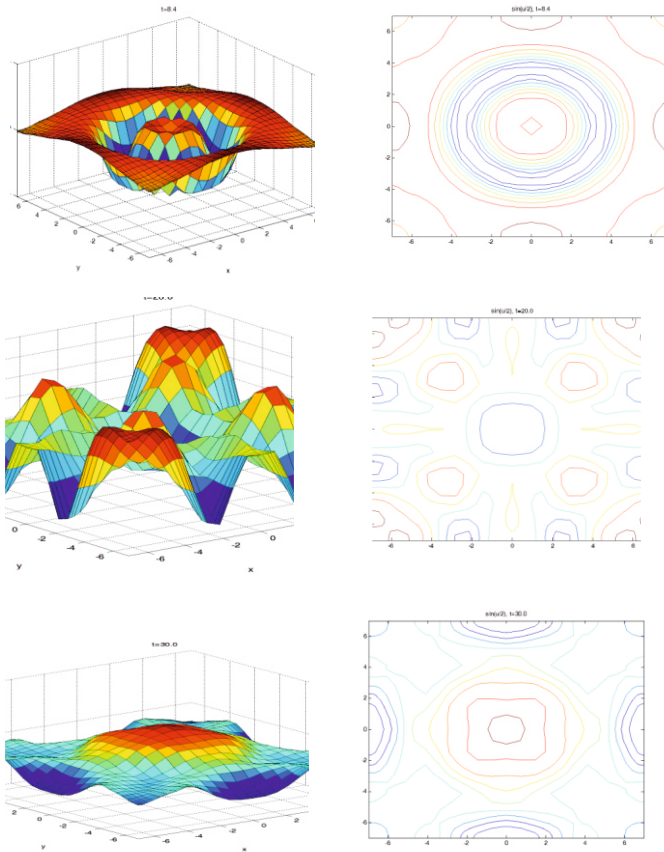
**Review articles** do not cover original research but rather accumulate the results of many different articles on a particular topic into a coherent narrative about the state of the art in that field. Review articles provide information about the topic and also provide journal references to the original research. Reviews may be entirely narrative, or may provide quantitative summary estimates resulting from the application of meta-analytical methods.





# Numerical simulation of two-dimensional sine-Gordon solitons by differential quadrature method

During the past few decades, the idea of using differential quadrature methods for numerical solutions of partial differential equations (PDEs) has received much attention throughout the scientific community. In this article, we proposed a numerical technique based on polynomial differential quadrature method (PDQM) to find the numerical solutions of two dimensional sine-Gordon equation with Neumann boundary conditions. The PDQM reduced the problem into a system of second order linear differential equations. Then, the obtained system is changed into a system of ordinary differential equations and lastly, RK4 method is used to solve the obtained system. Numerical results are obtained for various cases involving line and ring solitons. The numerical results are found to be in good agreement with the exact solutions and the numerical solutions that exist in literature. It is shown that the technique is easy to apply for multidimensional problems.



**Figure** Approximated solutions in form of Contour and 3 D plots of the two dimensional sine-Gordon equation.

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# Symmetries and exact solutions of the nondiagonal Einstein–Rosen metrics

We seek exact solutions of the nondiagonal Einstein–Rosen metrics. The method of Lie symmetry of differential equations is utilized to obtain new exact solutions of Einstein vacuum equations obtained from the nondiagonal Einstein–Rosen metric. Four cases arise depending on the nature of the Lie symmetry generator. In all cases, we find reductions in terms of ordinary differential equations and exact solutions of the nonlinear system of partial differential equations (PDEs) are derived. For this purpose, first we check the Painlevé property and then corresponding to the nonlinear system of PDEs, symmetries and exact solutions are obtained.

## Einstein vacuum equations

$$2(x+y)uu_{xy} - 2(x+y)(u_x u_y - v_x v_y) + u(u_x + u_y) = 0, \tag{2.8}$$

$$2(x+y)uv_{xy} - 2(x+y)(v_x u_y + u_x v_y) + u(v_x + v_y) = 0,$$

Table 1. Similarity reductions of system (2.8) to ODEs.

Essential fields	Similarity variable ( $\zeta$ )	Similarity solution ( $u, v$ )	Reduced ODEs
$V_1$	$x+y$	$u = F(\zeta), v = G(\zeta)$	$2\zeta FF'' - 2\zeta(F'^2 - G'^2) + 2FF' = 0,$ $2\zeta FG'' - 4\zeta(F'G') + 2FG' = 0$
$V_2$	$\frac{x}{y}$	$u = F(\zeta), v = G(\zeta)$	$2(\zeta+1)F(-\zeta F'' - F')$ $-2(\zeta+1)(-\zeta F'^2 + \zeta G'^2) + F(F' - \zeta F') = 0,$ $2(\zeta+1)F(-\zeta G'' - G')$ $+4(\zeta+1)\zeta F'G' + F(G' - \zeta G') = 0$
$V_3 + \alpha V_2$	$\frac{x}{y}$	$u = F(\zeta), v = \log(y^{1/\alpha} G(\zeta))$	$2(\zeta+1)F(-\zeta F'' - F')$ $-2(\zeta+1)(-\zeta F'^2 - \frac{G'}{\alpha G} + \zeta G'^2)$ $+F(F' - \zeta F') = 0,$ $2(\zeta+1)F(\frac{\zeta G'^2}{G} - \zeta G'' - G')$ $-2(\zeta+1)(-2\zeta F'G' - \frac{FG'}{\alpha})$ $+F(G' + \frac{G}{\alpha} - \zeta G') = 0$
$V_4 + \beta V_2$	$\frac{x}{y}$	$u = y^{1/\beta} F(\zeta), v = y^{1/\beta} G(\zeta)$	$2(\zeta+1)F(-\zeta F'' - F' + \frac{F'}{\beta})$ $-2(\zeta+1)(-\zeta F'^2 - \frac{GG'}{\beta} + \zeta G'^2 - \zeta F'^2)$ $+F(F' - \zeta F' + \frac{F'}{\beta}) = 0,$ $2(\zeta+1)F(\frac{G'}{\beta} - \zeta G'' - G')$ $-2(\zeta+1)(-2\zeta F'G' + \frac{FG'}{\beta} + \frac{FG'}{\beta})$ $+F(G' + \frac{G}{\beta} - \zeta G') = 0$



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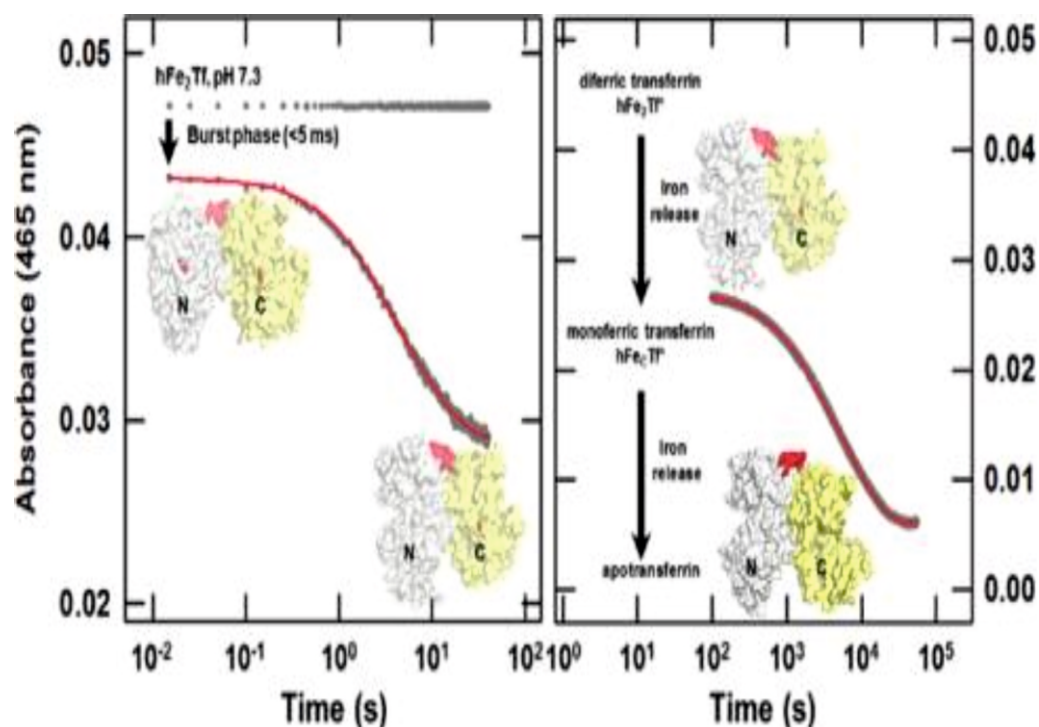


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**Reference:** Nisha Goyal, R. K. Gupta, *Physica Scripta* 85 (2012) 015004 (6pp)

## Protonation and Anion Binding Control the Kinetics of Iron Release from Human Transferrin

Iron release in vitro from human serum diferric transferrin (hFe<sub>2</sub>Tf) in acidic media ( $4.2 \leq \text{pH} \leq 5.4$ ) in the presence of non-synergistic anions occurs in at least five kinetic steps. Step 1 (most rapid) involves proton assisted release of carbonate from the protein. In subsequent steps, iron release from both the N- and C-terminal lobes is controlled by slow proton transfers and anion binding. In Step 2, the N-terminal lobe takes up one proton with kinetic linkage to the binding of one anion. In Step 3, iron release from the anion-linked N-terminal lobe is controlled by slow uptake of two protons with rate-constant,  $k_{2N}$  of  $2.6(6) \times 10^7$ ,  $6.1(6) \times 10^7$ , and  $9(1) \times 10^7 \text{ M}^{-2}\text{s}^{-1}$  in the presence of  $\text{Cl}^-$ ,  $\text{NO}_3^-$ , and  $\text{SO}_4^{2-}$ , respectively. In Step 4, the C-terminal lobe takes up one proton with kinetic linkage to the binding of one anion. In Step 5, iron release from the anion-linked C-terminal lobe is controlled by slow uptake of two protons with rate-constant,  $k_{2C}$  of  $8.4(2) \times 10^4$ ,  $4.4(6) \times 10^5$ , and  $8.1(2) \times 10^5 \text{ M}^{-2}\text{s}^{-1}$  in the presence of  $\text{Cl}^-$ ,  $\text{NO}_3^-$ , and  $\text{SO}_4^{2-}$ , respectively.



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### Reference:

**Rajesh Kumar, and A. Grant Mauk,** "Protonation and Anion Binding Control the Kinetics of Iron Release from Human Transferrin" *Journal of Physical Chemistry B (American Chemical Society)*, 116, 3795-3807, 2012.

# Research Profile

## *Department of Biotechnology and Environmental Sciences*

The Department of Biotechnology and Environmental Sciences (DBTES) came into existence in 2002 when erstwhile School of Biotechnology and School of Environmental Sciences & Technology merged together with the mission of defining and establishing a new discipline fusing biotechnology with environmental engineering, with the goals: to advance fundamental understanding of different operating principles of biological systems; to develop, through research and education, biology-based technologies for wide range of applications to address the needs of the society; to research and develop engineered processes and technologies instrumental for protection as well as remediation of the environment. The innovative educational programs followed in the department are designed to achieve these objectives through integration of life sciences with quantitative, systems-oriented engineering analysis and synthesis approach, offering research opportunities through undergraduate, postgraduate and doctoral programs.

### Some of the main research areas of interest of the department include

- **Agro & Food Biotechnology** Food processing & preservation, tissue culture & plant biotechnology, sustainable agriculture
- **Industrial Biotechnology** Synthesis of useful chemicals utilizing microbes, microbial concrete, bioactive molecules from herbs and microbes
- **Medical Biotechnology** Cancer biology, immunology, genetic and epigenetic gene regulation, natural product based drug discovery, genetic engineering
- **Environmental Biotechnology** Bioremediation of contaminated sites, detoxification of toxic metals, metal bio-transformations, synthesis of biopolymers for water treatment
- **Environmental Engineering** Trace contaminant removal from water and wastewater, microbial treatment of municipal and industrial wastewater, environmental catalysis, advanced oxidation processes, air quality, and air pollution control technologies

The department has been attracting a number of sponsored research grants from various agencies such as DST, DBT, NRB, DRDO, AICTE, CSIR, BRNS, AERB. In the year 2011-2012, the department received research funding of more than 25 million rupees.

The department is also doing industrial consultancy in the field of environmental management and impact assessment studies. The departmental faculty keep visiting foreign countries to present their research work or to do collaborative research work or as visiting professors.

In the last three years, the department has published about 100 research papers - over 70 of them of international repute. The department has supervised 25 PhD students who have found academic as well as industrial positions both in India and abroad. Currently, 45 research scholars are working towards their PhD degrees.

### The diverse areas of research work being pursued include, but not limited to

- Inhibition of starch granule based proteins in potato and related genetic engineering
- Selenium mobilization, its bio-accessibility and utilization in fortification in food grains and cereals
- Use of calcifying bacteria for cementation leading to better building materials





- Development of quaternized bio-polymeric flocculants for enhanced kill of pathogens in water and wastewater
- Bio-conversion waste biomass for ethanol production
- Microbial and fungal treatment in different building material for enhancement of property of concrete
- Photo-catalytic, biological and advanced oxidation processes for removal of pesticides, industrial dyes, and other organic compounds from water and wastewater
- Bio-sensor development, leaching studies involving water treatment residuals, heavy-metal contaminated wastewater, etc
- Different types of drug design against antibiotic resistant species
- Water and watershed management studies
- Microbial solubilization of phosphate-bearing rocks.



The department has state-of-the-art research facilities including TIFAC-CORE, which also has tie-up with various industries such as PepsiCo, McCain Foods, Ballarpur Industries, NALCO. The department also has the facilities of STEP (Science & Technology Entrepreneur Park) - a joint venture with NSTEDB and DST - for nurturing innovations in industrial, agricultural and food biotechnology to convert them into commercial ventures. STEP

has collaborations with Punjab Council for Science & Technology (PCST), CIPHET, ICRISAT and American Soy Association.

For other details of DBTES including academic programs visit [www.thapar.edu](http://www.thapar.edu) or email your query to [hbtesd@thapar.edu](mailto:hbtesd@thapar.edu)

**Articles** are usually between five and twenty pages and are complete descriptions of current original research findings, but there are considerable variations between scientific fields and journals – 80-page articles are not rare in mathematics or theoretical computer science.



## **Thapar University - proud past promising future**

Thapar University (formerly known as Thapar Institute of Engineering and Technology) founded by Late Lala Karam Chand Thapar in 1956 is a premier educational and research institute located in the 250-acre campus, in the historic city of Patiala. TU became 'Deemed University' in December 1985, and, is, today recognized among the leading private engineering institutions of the country and the best of its kind in the north-western region of India; it runs undergraduate, postgraduate, and PhD programs in all the disciplines. As of today, the institute has produced over 17,000 alumni.

The institute is running undergraduate (BE), postgraduate (MTech, ME, MSc, MCA, MBA), and doctoral programs in almost all disciplines. From the next academic year, the following new programs are being added: Dual BSc-MSc (Physics), (Chemistry), (Mathematics and Computing), and (Biotechnology); BCA-MCA; MSc (Environmental Science); MCom; ME (Information Security), and (Wireless Communication); MTech (Biotechnology); BE (Mechatronics).

At TU, an aptitude for learning and growth is well reflected through a vibrant student life. TU provides modern, spacious, and architecturally striking hostels as well as excellent sports facilities. The students are encouraged to participate in multifarious extra-curricular and co-curricular activities, such as movie making, fine arts, photography, dance, music, literary, drama on one side and helping the needy including the children of the unprivileged and underprivileged class on the other. The students are also provided opportunities to express their views on a plethora of academic and non-academic issues through University magazines and TnI – a student newspaper. In fact, TU understands that the educational innovations certainly do not come about automatically. It is the environment which influences and changes the standards of learning.



**Nava Nalanda Library, TU**