PLENARY SECTION

Computer science for biomedical science: biochip design and drug repurposing

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ABSTRACT

In this talk, we focus on the applications of computer science in biology and biomedical technology research. Two approaches will be discussed.

Firstly, we consider a SERS based biochip design development, in lab fabrication and experimental results and consequently, a system development of experimental data analysis for the diagnosis of COVID-19 infection. The biosensor under consideration detects SARS-CoV-2 proteins rapidly with a high sensitivity, specificity and accuracy.

Secondly, we briefly discuss a drug repurposing study for treatment of a neglected disease of echinococcosis. The graph and machine learning based algorithms have been occupied in the drug-target-disease interaction network construction and analysis. The computation for drug efficacy and side effects has also been carried out.

Keywords: *Biomedical technology, biochip design, COVID-19, SARS-CoV-2.*

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Build up a resource-recycling society developing the phosphorus recovery process from sewage sludge ash and relating technology

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ABSTRACT
In November 2022, the Earth's inhabitants reached 8 billion. The economic system of mass production, consumption, and disposal, in which living resources are gathered from nature, processed, used, and then disposed of, is no longer viable. The earth's resources are no longer infinite for human beings, but finite. We now have no choice but to adjust our use of resources while keeping an eye on the total resources of the earth and the amount that can be used. Until now, the main themes have been the treatment of wastewater/groundwater, and the depletion of fossil energy due to its massive use and the global warming problem resulting from the mass using of fossil energy. From now on, the problem of food shortage is expected to become more serious, and we need to prepare countermeasures against it before the problem occurs.
Fertilizer is the most important factor in food production, and the three major components of fertilizer are N, P, and K. Among them, N has been freed from the problem of scarcity by the Haber-Bosch method. In other words, it has become an unlimited resource. The most depletion concern is P, which is projected to run out in 150 years. Phosphorus resources are also a strategic resource, with about 80% unevenly distributed among the five countries. In countries that do not have P resources, P resources need to be circulated for use.
Brown coal is one candidate for solving problem of fossil fuel depletion because of a great deal of resources. Moreover, a detailed understanding of the chemical reaction mechanism and fundamental understanding of kinetics of coal utilization processes such as pyrolysis, gasification and combustion.
Hazardous chemical removal from wastewater and groundwater as a result of industrial and consumer activities has become a more severe and concerning issue. Specifically, removing arsenic in groundwater is critical in many areas, however there are not efficient adsorbent materials.

Keywords: *Resource-Recycling Society, Phosphorus Recovery Process, Sewage Sludge Ash, Fertilizer, groundwater, adsorbent, Brown coal.*

Quivers: Representations, Bundles, Applications

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ABSTRACT

Quivers or directed graphs and their representations were used to describe representations of finite dimensional algebras. However, they also appear in many applications, such as control theory, data analysis, and, more recently, neural networks.

In algebraic geometry, quiver representations have been generalized to quiver bundles. In the talk, I will give a brief overview over quivers and their representations. Then, I will sketch the applications mentioned above, in particular, a joint project with Marco Armenta on network moduli. In the final section, I will report on recent results of mine from concerning quiver bundles.

Keywords: *Quiver, representation, moduli space, persistence, control theory, neural network.*

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Towards nanomagnetic materials design

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ABSTRACT

Since neodymium–iron–boron ($Nd_2Fe_{14}B$) permanent magnet was developed in 1982, a permanent magnet with higher performance has not been reported yet. Ever since, search for permanent magnet materials that do not contain rare-earth elements, but compatible to ferrites in price, is underway. In the first half of this talk, we will review the properties that make a material good permanent magnet, including saturation magnetization, uniaxial magnetocrystalline anisotropy, maximum energy density product, Curie temperature, and thermodynamic stability and discuss our approach to designing new permanent magnets free or reduced content of rare-earth elements while retaining a comparable performance with $Nd_2Fe_{14}B$. In addition, preliminary results of our *ab initio* calculations for the selected Fe–Sm–N, Fe-Co--P, and Fe–Ni–Ga alloys, will be presented. Our experimental attempts at fabricating and characterizing select alloys will be briefly discussed.

On the other hand, two-dimensional (2D) class of nanomaterials has attracted tremendous interest from both academia and industry due to their wealth of remarkable properties. The production of high quality 2D magnetic materials is still challenging and the opportunities they offer are still poorly understood. In particular, first-principles materials design and prediction of novel 2D nanomagnetic structures with desirable/tailoring-on-demand functional properties and utilization in a diverse spectrum of applications through efficient synthetic routes are the most crucial and desirable step. In the second half of this talk, we will present our recent first-principles prediction on the possibility of achieving scaled preparations of multilayer graphene or hexagonal boron nitride (h-BN) on metal substrates that can lead to a fabrication route of very large area ultrathin sp^3-bonded carbon or BN films, representing an entirely new 2D nanomaterial. We will also discuss towards novel approaches for manipulating magnetism, emphasizing on magnetization switching, and electronic structures of the other 2D nanostructures including transition metal dichalcogenides (TMDs) by an external stimulus, that are, various doping effects, strain effect, or applying an electric field.

Keywords: *Permanent magnet, magnetization, magnetocrystalline.*

Determination of causes of groundwater pollution in major cities of southern India - a case study through major ions and trace element analysis

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ABSTRACT

Management of ground water resource is a challenging task and requires a structured approach starting from monitoring of water levels and quality to analyzing hazards to groundwater regime, assessing the risk they may cause for a specific supply, setting priorities in addressing these and developing management strategies for their control. During recent years much of the emphasis in ground water has shifted from problem of ground water supply to considerations of ground water quality, from researchers studying groundwater contamination in various part of developing countries like India, China, Pakistan, Turkey, Srilanga and Nigeria. From the drinking water quality status various major cities of Sothern India cities like Bangalore, Chennai, Hyderabad and Thiruvananthapuram are chosen for identification of pollution sources over the last 2 decades. The major objective of this study is to bring out the sources and scale of groundwater contamination and the consequences for human health through water higher concentrations than the maximum permissible limits of major ions and trace elements. From the study it is inferred that the groundwater pollution is mostly caused by anthropogenic activity in the city of Chennai and Hyderabad, the geo-genic source of rock-water interaction act important role in groundwater pollution in the cities Bangalore and Thiruvananthapuram.

Keywords: *Groundwater Regime, Sothern Indian Cities, Anthropogenic Activity, Geo-genic Source, and Rock-water Interaction.*

Convergence of discrete exterior calculus

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ABSTRACT
Discrete exterior calculus (DEC) is a framework for constructing discrete versions of exterior differential calculus objects, and is widely used in computer graphics, computational topology, and discretizations of the Hodge-Laplace operator and other related partial differential equations. However, a rigorous convergence analysis of DEC has always been lacking. We develop a general framework for analyzing issues such as convergence of DEC without relying on theories of other discretization methods, and demonstrate its usefulness by establishing convergence results for DEC for the scalar Poisson problem in arbitrary dimensions. This method is closely related to the lattice gauge theory discretization of the classical Yang-Mills equations, and therefore might shed some light on quantum gauge field theories in the future.

Keywords: *exterior calculus, discretization, convergence analysis*

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Exploring two-dimensional materials for emerging photovoltaic cells

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ABSTRACT

Energy is currently one of the most pressing issues in the world. Over the years, the world's energy consumption has dramatically increased because of the rapidly growing global population and the development of modern technologies. The US Department of Energy predicts that the world's energy demands will double by 2050 and triple by 2100. Although today's energy requirements are principally met by burning fossil fuels, continued increases in the fuel price must be taken into account. More importantly, potential damage to the environment, caused by the fuel-burning process, has become a serious problem.

The fact that only one-thousandth of the Sun's energy incident on the Earth is equal to the entire world's current energy needs means direct conversion of this energy into electricity – photovoltaic (PV) energy – is now a mainstream renewable energy source. PV devices, or solar cells, have undergone considerable development over the past two decades: i) first generation silicon (Si) solar cells; ii) second generation solar cells based on semiconductor thin films; and iii) most recently, third generation (emerging) solar cells. While the first two generations are well established, their manufacture is inherently complex and expensive.

Emerging solar cells including perovskite solar cells, dye-sensitised solar cells, organic solar cells and silicon-based heterojunction solar cells have attracted much attention due to their low-cost, high efficiency, ease of fabrication and tailorable design. Despite their great promises, these solar cells do have some disadvantages such as use of expensive electrode materials, the high temperature required during manufacturing and poor operational stabilities. The high degree of tunability in the properties of unique two-dimensional (2D) nanomaterials such as graphene, black phosphorus and metal carbide (MXene) offers an abundance of opportunities for next-generation solar cells. In this talk, I will present our recent contributions to this cutting-edge research area and also highlight the future promises in this area.

Keywords: *Energy, photovoltaic, solar cells, nanomaterials, 2D materials.*