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ISSUES 11 (JANUARY - APRIL 2023)

Welcome to the Newsletter e-Science Putra. This issue presents the research activities from January to April 2023 which highlight the latest research findings by the selected faculty members.

HIGHLIGHTS

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SYNERGISTIC POLYHERBAL COMBINATIONS: A HOLISTIC APPROACH TOWARDS DIABETES MELLITUS

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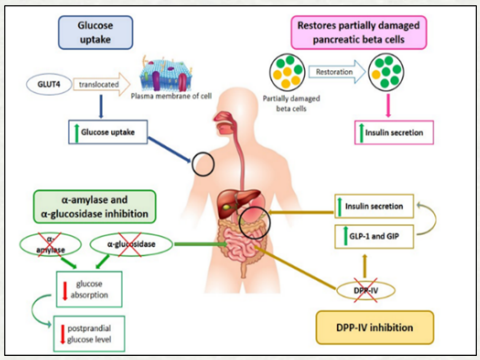
Type 2 Diabetes mellitus (DM) accounts for 90% of most diabetes cases globally. Diabetes mellitus is infamously known as the 'mother of all diseases' due to its increased risk of other comorbidities such as heart disease, high blood pressure, stroke, and kidney failure. As the burden of diabetes increases drastically, numerous drugs are invented continuously to combat this disease. Unfortunately, these drugs apart from failing to restore the normal glycemic level, also causes serious side-effects to the consumers. Therefore, there is a dire need to discover an effective, economical, safe and wholesome antidiabetic remedy from nature (Perumal et al., 2022). Ayurvedic treatment approaches combine more than a single plant for desirable therapeutic efficacies. Formulations of combined herbs with synergistic impact have been noted to have minimal adverse effects while maintaining pharmaceutical efficacy (Puspa et al., 2021).

In our research group, combinatorial herbs study is central for evolving botanicals, nutraceuticals and phytopharmaceuticals. One success story has been the polyherbal combination of M. charantia and T. officinale (PCMT) has proven to effectively improve antidiabetic activity compared to single extracts (Perumal et al., 2022) . The effect of the polyherbal combination heavily depends on the intricate interaction between the phytochemical components that results in a reduction or enhancement of a specific bioactivity (Gupta et al. 2017).

PCMT has shown efficacious blood glucose lowering effects via several metabolic pathways:



- Inhibition of dipeptidyl peptidase IV (DPP-IV) and recovery of partially damaged pancreatic β-cells, hence increasing insulin secretion.
- Inhibition of α-amylase and α-glucosidase enzymes which retarded the breakdown of starch to glucose and slowing down the absorption of glucose in the GI tract.
- Insulin-like action by promoting the uptake of glucose into muscle cells.

Owing to its multiple-dimensional antidiabetic mechanism of action, PCMT can be utilized as a safe, non-toxic, cost-effective potential combinatorial therapy for Type 2 DM with further pharmacokinetic and pharmacodynamic studies.

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EXPLORING PIEZOELECTRIC PROPERTIES OF ZNO NANOWIRES: SYNTHESIS AND CHARACTERIZATION USING CHEMICAL BATH DEPOSITION AND PIEZORESPONSE FORCE MICROSCOPY

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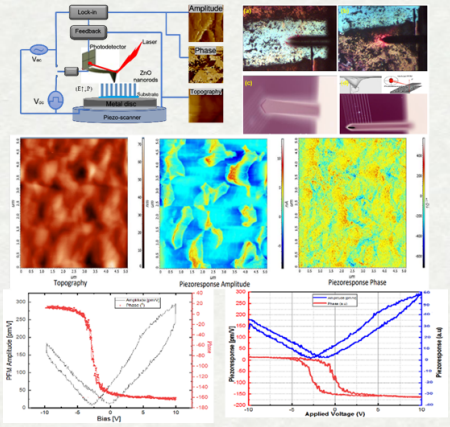
Energy harvesting devices convert ambient mechanical energy into electrical energy, making them a promising renewable energy source. This technology relies on the converse piezoelectric effect, where induced polarization generates a potential difference due to an electric field. To enhance the piezoelectric response, controlling the growth orientation and density of nanostructures is important. ZnO nanorods or nanowires (NWs/NRs), one-dimensional nanostructured semiconductor materials, have shown promise in a range of applications, including piezoelectric transducers, photovoltaic solar cells, gas sensors, biosensors, transistors, optoelectronics, and nanogenerator technologies. Dye-sensitized solar cells (DSSCs) are a type of low-cost, highly transparent sunlight converter that has tunable colors and has the unique property of harvesting scattered photons. The use of sputtered ZnO seed layers before nanorod growth leads to better alignment and enhanced energy-harvesting abilities. Highly oriented ZnO nanorod arrays are required for high-performance piezoelectric devices, and chemical bath deposition is a fine technique for the deposition of high-quality nanostructures. The substrate's surface plays a crucial role in the crystal orientation and growth of the nanorods, and flexible substrates enhance the device's flexibility, stretchability, and effective area for energy harvesting. As research continues, it is expected that new and innovative applications of ZnO nanorods in energy harvesting devices will emerge, contributing to sustainable energy solutions.

The studies investigated the piezoelectric properties of zinc oxide nanorods (ZnO NRs) grown on various substrates through a chemical bath deposition (CBD) approach. The aligned nanorods with high aspect ratios were observed through field-emission scanning electron microscopy (FESEM). Piezoresponse force microscopy (PFM) was utilized to examine the piezoelectricity of the samples, and the results showed that all grown ZnO NRs on Si, glass, and ITO substrates exhibited piezoelectric deformation. The piezoelectromechanical coupling coefficients were calculated to be 9.13 pm/V, 4.74 pm/V, and 8.42 pm/V for ZnO NRs on Si, glass, and ITO, respectively. Meanwhile, another study examined ZnO NRs grown on bare sputtered silicon and patterned interdigitated electrodes (IDE) using various techniques, including FESEM, XRD,FTIR, and AFM/PFM. The results indicated that the nanostructures possessed a hexagonal wurtzite crystal structure and had piezoelectric properties. The coupling between the IDE and the piezoelectric ZnO nanostructures increased the deflection sensitivity, and PFM measurements demonstrated the ferroelectric-like behavior of the samples. The attained piezoelectric coefficient values suggest that PFM measurements can be employed as a routine test to assess the multifunction of the patterned microelectrode for actuation, signal control, resonators, and piezoelectric nanogenerators. These studies provide significant insights into the fabrication and integration processes of piezoelectric-based ZnO nanogenerators.

In conclusion, the use of ZnO NWs/NRs in energy harvesting devices has shown great promise due to their unique properties such as high aspect ratio, good molecular absorption and electron transport properties, and excellent piezoelectric performance. The growth orientation and density of the nanorods can be controlled to enhance their piezoelectric response, and the use of flexible substrates can further improve the device's performance. Moreover, the low-cost and simple preparation method of chemical bath deposition make ZnO nanorods an attractive material for large-scale production. As research in this field continues, it is expected that new and innovative applications of ZnO nanorods in energy harvesting devices will emerge, contributing to the development of sustainable energy solutions.



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ACCURATE ESTIMATION OF LATTICE CONSTANT OF PYROCHLORE COMPOUND BASED ON MACHINE LEARNING MODEL

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Pyrochlore compound ($A_2B_2X_7$) is one of the precious crystal materials that are important for energy innovation. It is applicable as ionic conductors for solid state batteries, environment catalyst for clean energy production and as bioanode in fuel cell of microbial. Accurate determination of lattice constant would help in materials characterization. Example of lattice constant location of $Lu_2V_2O_7$ pyrochlore on the cubic structure is shown on Figure 1. The accurate knowledge of the lattice parameter would give information about the compound thermal properties, strain state and defect in the structure. Due to that, it is important for precise lattice constant value to be determined. Most of techniques to determine the lattice parameter is by using X-Ray Diffraction which is tedious and costly. To overcome the problem, we proposed an accurate machine learning algorithm to model the pyrochlore compound lattice value.

In our research [1], we proposed an optimized Machine Learning (ML) model based on Particle Swarm Optimization paired with Support Vector Regression (SVR) algorithm. Our input data of 220 dataset to predict the lattice constant are based on ionic radii (rA, rB and rX) and electronegativities (xA, xB and xX) values of each cation (A and B) and anion (X). We validate our results using multiple fold technique and found that 15-fold method achieve the best results as shown in Figure 2. Predicted value using kernel SVR function of Radial Basis Function outperformed the others as the average value of Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Correlation Coefficient (CC) is evaluated at 0.0122, 0.0099, and 0.9990, respectively. We checked our results with previously reported findings using other ML model such as Bayesian SVR [2], Artificial Neural Network [2], and statistical algorithm using linear model [3] to confirm the superiority of our techniques. The RMSE and CC improve 64% and 1% respectively compared to the second-best model. Through this analysis, the modelling based on ML technique can provide a highly accurate prediction in accessing the pyrochlore compounds crystal structure properties which means it could replace the traditional measurement technique effectively.

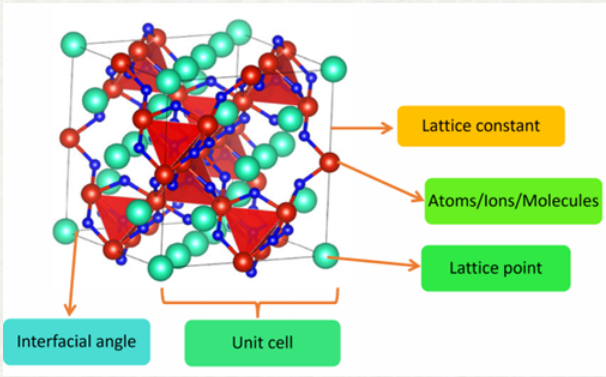

Figure 1: Lattice constant and other parameters for cubic structure of Lu2V2O7 pyrochlore compound.

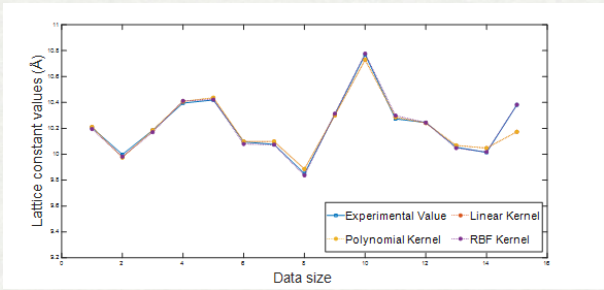

Figure 2: Comparison of predicted PSO-SVR model with experimental values using 15-fold validation technique.

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EXPLORING THE POTENTIAL OF BENZIMIDAZOLE-QUINAZOLINE COMPOUNDS AS DRUG CANDIDATE

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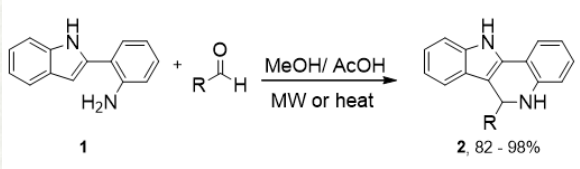
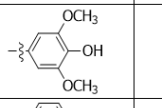
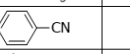
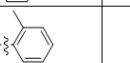
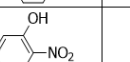
Benzimidazole-quinazoline compounds are tetracyclic molecules consist of benzimidazole and quinazoline ring that are fused together. Separately, both benzimidazole and quinazoline compounds have been reported to possess interesting biological activities such as antibacterial, anticancer, antioxidant and antiviral. Therefore, it is expected that benzimidazole-quinazoline compounds would have equally interesting properties. However, reports on this type of compounds in the literature is quite scarce. Thus, this system would be a good candidate to explore in development of new drugs.

Accordingly, several benzimidazole-quinazoline compounds were synthesized and their antioxidant and antimicrobial properties were evaluated. Condensation reaction of 2-(2-aminophenyl)-1H-benzimidazole (**1**) with various aldehydes, Scheme 1, proceeded to give benzimidazole-quinazolines **2**, via in situ cyclization using conventional and microwave heating method in 82 – 98% yield. Two antioxidant assays, 2,2-diphenyl-1-picryl-hydrazyl-hydrate (DPPH) and 2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonate) (ABTS), were conducted which were followed by antimicrobial assays. Only benzimidazole-quinazoline **2a**, showed excellent scavenging activity for both DPPH and ABTS assays while the other compounds only showed excellent scavenging activity for ABTS, Table 1. The excellent ABTS scavenging activity can be attributed to ability of aromatic system with electron donating group to stabilize radical. Meanwhile, it was difficult for the bulky benzimidazole-quinazoline compounds to access the sterically hindered DPPH radical leading to poor activity. However, there is no correlation of antioxidant activity towards microbial activity with benzimidazole-quinazoline **2d** exhibited the best antibacterial activity against *Staphylococcus aureus* (23 mm) and *Bacillus subtilis* (13 mm) with inhibition zone closer to the positive standard, tetracycline (29 and 21 mm respectively). All compounds showed poor activity towards gram negative bacteria and fungus. Interestingly, these benzimidazole-quinazolines also exhibited interesting photoactivity in absorption and emission spectrum. We are currently exploring the potential of these type of compounds not only as drug candidate but also as organic dyes.



Scheme 1: General scheme for synthesis of benzimidazole-quinazoline compounds.

2	R group	Scavenging activity/ mg trolox equivalent		Diameter of inhibition zone/ mm	
		DPPH	ABTS	*S. aureus* ATCC 43300	*B. Subtilis* UPMC 1175
a		752	782	13	10
b		8.49	809	7	-
c		22.48	923	7	-
d		67.65	597	23	13
e	Pentyl	21.52	670	14	8
Tetracycline (+ve control)		-	-	29	21

- means no inhibition zone observed.

Table 1: Antioxidant and antibacterial activity of selected benzimidazole-quinazolines.

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A BRIEF OVERVIEW ON GROUPS AND GRAPHS

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Group is one of algebraic structures which contains of a set together with its operation and it must satisfy four properties which are closure, associativity, a unique identity for all group elements and having unique inverse for each of the group element. Representing groups as graphs has been widely studied by mathematicians in order to have a different view on the group elements which are assumed to be vertices of the graph. The connectivity of the graph, the diameter bound, and the structure of sub-orbits are among the main aspects researchers in this field will focus on, for instance in [1].

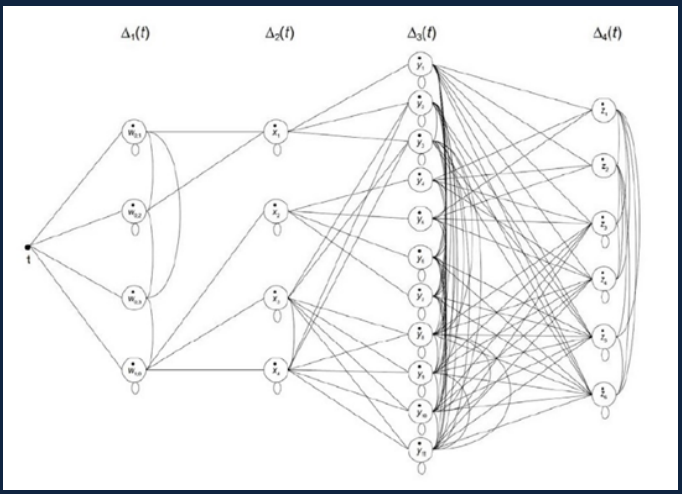

Figure 1: Commuting Graph of Symmetric Group of Degree 9, Sym(9).

Figure 1 shows a graph called commuting graph which is defined as a graph whose vertex set is a subset of the group with two distinct elements and , are joined by an edge whenever they commute in the group (). In [3], we consider the elements of order three in Symmetric Group of degree 9, Sym(9) to be the vertices. Clearly that the graph in Figure 1 is connected of diameter 4.

When graphs are disconnected, we can highlight on the structure, the number and the size or diameter of each component. The commuting graph of Symmetric Group of Degree 6, Sym(6) is found to be disconnected [2] resulting four components each of size 4. Evidently, each component is connected and isomorphic to a complete graph of order 4, as shown in Figure 2.

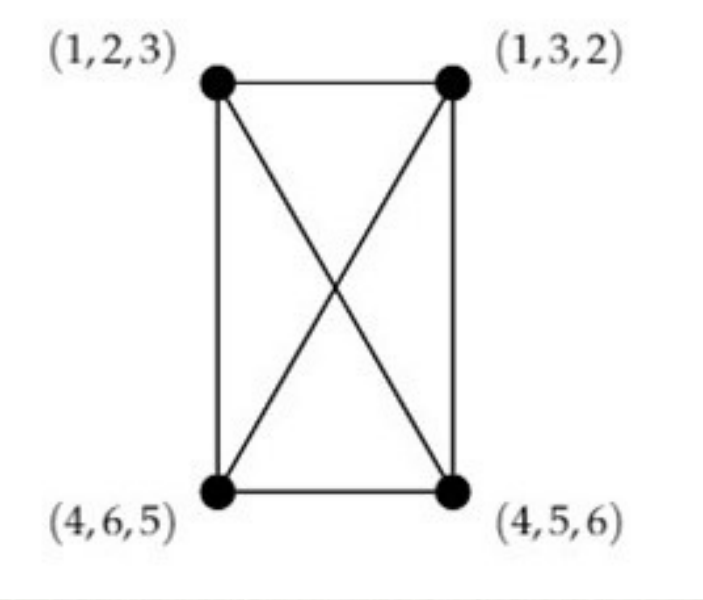

Figure 2: A Component in the Commuting Graph of Symmetric Group of Degree 6, Sym(6).

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Science is much more than just a body of KNOWLEDGE.
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