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**( 24 & 25 October, 2020 )**



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**INTERNATIONAL  
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ON  
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INNOVATION**

*(ICSETI – 2020)*

**24 & 25 October, 2020**

*Conference Proceedings Issue - 19*

*The Managing Editor:*

*Dr. Chirag M. Patel*

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Department, Kryvyi Rih National University, Ukraine  
and**

**Research Culture Society**

***International Conference***  
***On***  
**Science, Engineering & Technological  
Innovation**

**24 & 25 October, 2020**

**( Conference Proceedings – Special Issue )**

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ACST department trains specialists in computer science, automation and computer-integrated technologies. The main educational and scientific areas are: information support for decision making, , development and implementation of process automation and mechatronics systems.

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## **Objectives of the International Conference :**

Our main objective is to promote scientific and educational activities towards the advancement of common citizen’s life by improving the theory and practice of various disciplines of science and engineering. The aim of the conference is to provide an interaction stage for researchers and practitioners from academia and industries to deal with state-of-the-art advancement in their respective fields.



## KRIVYI RIH NATIONAL UNIVERSITY

**Prof. Natalia Morkun**

Head of Department of Automation,  
Computer Sciences and Technologies

e-mail: nmorkun@knu.edu.ua



### MESSAGE

Dear Colleagues!!!

I am proud to be the part of Organizational Committee of two-day International online “International Conference on Science, Engineering & Technological Innovation-2020”, jointly organized by Research Culture Society and Department of Automation, Computer Sciences and Technologies, Kriviy Rih National University (24 & 25 October, 2020).

We have an exciting program at this conference that will allow participants to reflect upon and celebrate their accomplishments, renew friendships and extend networks, and jointly explore current and future research directions. I hope that all participants will have a productive and fun-filled time at this online conference.

I sincerely hope that this conference will deliberate and discuss all the different facets of this exciting topic and come up with recommendations that will lead to a better world.

I wish the conference great success.

Prof. Natalia Morkun

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# CRISPR/Cas-9 Genetic Editing of 'Neu' gene in Breast Cancer Prognosis

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## **Abstract:**

**Introduction:** Breakthrough research in this field has earned *Jennifer Doudna* and *Emmanuelle Charpentier* with Noble prize in Chemistry for the year 2020. Their findings in 2012 that CRISPR/Cas9 could be programmed with RNA to edit the genomic DNA brought a significant milestone in the advancement of molecular biological research. Briefly, CRISPR/Cas9 is a bacterial defensive mechanism that exhibits the cutting of the genomic DNA at its desired location resulting in to the exit of the old ones with the induction of a new set of genes. Fidelity or accuracy or precision of the genetic cut depends on the target and the protospacer adjacent motif (PAM) sequence. The target sequence is 20 bases long which belong to a particular CRISPR locus on a crRNA array. Cas9 protein selects the correct location of base pair bonding with in the target sequence. The PAM sequence (5'-NGG-3') on the host genome is recognized by Cas9. Assembling the sequence related to PAM, target sequence into plasmid and transfecting the plasmid into a cell shows that Cas9 with the help of crRNA was able to detect the correct sequence with in a host cell resulting to a single or double stranded break at the appropriate location in the DNA thereby addressing the issue of genetic cut and working as a molecular scissor. We orchestrated this tool in achieving the information related to the generation of PAM sequence and the off target sites related to Neu genes responsible for breast cancer prognosis. To achieve the same we analyzed the set of the said genes on the preformed online software tool available like that of ccTop, and CRISTA in order to generate the best possible target sequence along with their appropriate guide RNA's. Furthermore, approach has also been done to establish the protein characteristics related to generation of hydropathy index, the alpha helix, beta-turns, helix wheel, and the transmembrane tendency. **Experimental Design:** The amino acid sequence of the Neu protein with its accession number was obtained from Expassy. The FASTA file of the nucleotide sequence of each amino acid was scanned batch mode in CRISTA and CCTop computational tools respectively. **Result:** We have identified the top 4 best gRNA sequences based on the highest CRISTA scores range 0.98 to 0.99. Furthermore, we used CCTop to break down the entire sequence into several target sequences and also to find out a guideRNA corresponding to each target sequence and accordingly we have identified the 4 best target and guide RNA sequences with highest efficacy score. **Conclusion:** Our manuscript is aimed at showcasing the best target sequence and guideRNA sequence complimentary to the target sequence utilizing the model software like that of CRISTA

and CCTop. In addition we also demonstrated the chemical properties of the protein in term of its hydropathy index, alpha helix, helix wheel and transmembrane tendency.

**Key words:** *CRISPR/Cas9; gRNA; molecular scissor; Neu gene; & CRISTA and CCTop computational tool.*

## 1. Introduction:

The clustered regularly interspaced short palindromic repeats (CRISPR)–CRISPR-associated protein 9 (Cas9) system is basically a bacterial defense mechanism against phage infection and has been intentionally used as a powerful RNA-guided DNA targeting platform for genome editing, transcriptional perturbation, epigenetic modulation, and genome imaging. This technology allows precisely to manipulate any genomic sequence specified by a short stretch of guide RNA, allowing elucidation of gene function involved in disease development and progressions, correction of disease-causing mutations, and inactivation of activated oncogenes or activation of deactivated cancer suppressor genes when utilizing a fusion protein of nuclease-deficient Cas9 and effector domain [1, 2, 3, 4]. Moreover, this programmable endonuclease technology enables researchers to examine the function of multiple genes at once by simultaneously targeting multiple genomic loci in a single experiment [5], which markedly accelerates our understanding of pathological processes that involve large sets of genes or mutations, such as tumor development. Using single-guide RNA (sgRNA) libraries, CRISPR based genome-wide screens can be leveraged to identify drug-target or disease-resistance genes, such as novel tumor suppressors or oncogenes, and to quickly assess drug targets [6, 7].

CRISPR/Cas9 endnuclease system is currently targeted as a molecular surgery to achieve success in cancer treatment. Mostly canacers are associated with the genetic alteration and mismatch cell cycle check points. Genetic system of human body are controlled by different checkpoints in the cell cycle. The tumor suppressor gene and proteins play a pivotal role in controlling the cell cycle. But mutation in any of the checkpoints or the tunor suppressor gene may change the scenario and may cause topsytruvy situation to a individual life causing the clinical manifestation leading to cancer. Thus in one words the cancer is a genetic alteration. In such condition the CRISPR/Cas9 technology can help in genetic editing and thereby shall be able to remove the mutated base pair with correct basepair. Briefly, Cas9 locates specific 20-base-pair (bp) target sequences within the genomes that are millions to billions of base pairs long and subsequently induces sequence-specific double-stranded DNA (dsDNA) cleavage. In this manuscript we are highlighting the genetic changes associated with the Neu oncogene enhancement, also known as HER-2 or Herceptin, a transmembrane protein. Studies revealed amplification of Neu gene as much as in 15-40% of primary breast carcinomas. Amplification leads to higher rates of neu-mRNA and protein synthesis. Furthermore as Neu gene encodes a transmembrane protein known as Herceptin, we also envisaged the charcterstic properties of the Herceptin protein so as to get the holistic picture of the gene as well as the protein associated with breast carcinoma. Our main approach is to highlight the CRISPR/Cas9 technology as a novel genetic cutting tool that may be employed in editing the target region of the Neu gene and at the same time, to give a overall view of the physical properties associated with the protein encoded by the Neu gene that is the Herceptin protein.

Inspite of its full potential, this genetic cutting tool has its own demerits to the point that it can not be used in full therapeutic measures since it is indeed a matter of further investigation regarding the precision and accuracy of cutting the target sequence and not generating the *off targets*, which may cause genetic damage instead of its achieving the goal. Even though of its demerits it is now the buzz of frontier research and had opened a new dimension in the field of cancer biology or onco research in the name of a new discipline termed as CRISPR biology. This manuscript stand over the others since it highlight the latest tool ever developed in the treatment of any form of cancer and here to specify is the breast cancer.

## 2. Research Objective :

Our research is focused in elucidating the target sequence associated with the neu gene responsible for the clinical manifestation of breast cancer or mammary carcinoma, that may be possible recognized by the PAM sequence corresponding to the target sequence and employing the computational tool we have focused to elucidate the corresponding PAM and target sequence related to the Neu gene . At the same time we also elucidated the protein properties in terms of its hydropathy index, protscale graphs, helix loop wheel related to the Herceptin protein. Our manuscript gives the necessary information regarding further work in synthesizing the software based generated PAM sequence and transplanting the same in the plasmid vector and to check out the interference of the generated PAM sequence with the single guide RNA for target identification and finally cessation of the target sequence and establishing the cut sequence with modified sequence which shall normalize the function of the neu gene or rather deactivate the over expression of the neu gene and thereby would diminish the cancer prognosis.

## 3. Research method:

The research method or the experimental set up for this manuscript is divided in to two parts. Part-A mainly emphasizes the protein properties elucidated as protscale graphs related to hydropathy index, secondary structure of protein, and elucidating the transmembrane tendency as well as featuring the helix loop wheel. Part-B mainly emphasises the computational tool based approach undertaken to identify the target sequence, PAM sequence and SgRNA obtained from different online computational tool like that of ccTOP and CRISTA

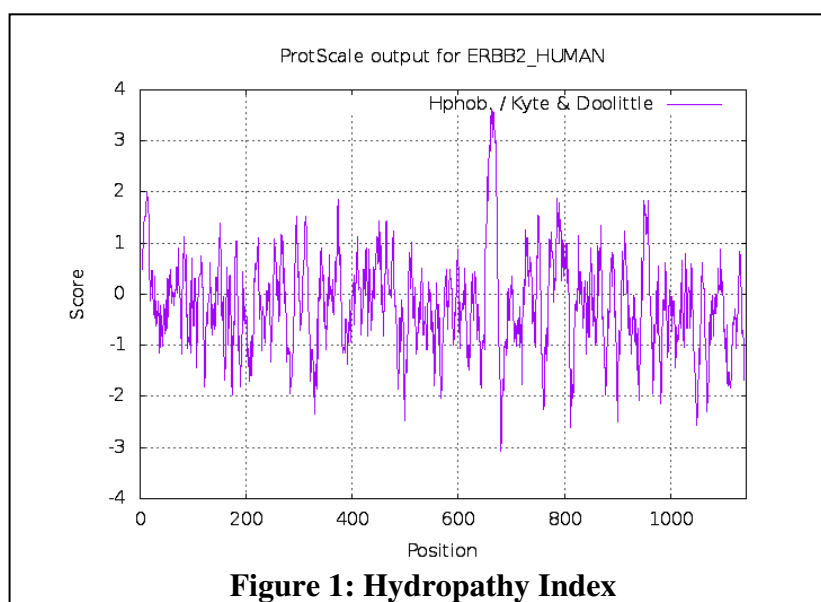
### Part-A : Elucidation of Protein Properties

#### 3.1 Elucidation of ProtScale Graphs

In order to properly understand and work with the Herceptin protein, we first examined and analyzed the chemical properties of the protein starting from its accession number, proteomics, properties such as hydropathy index, structural composition[8] through beta turns, and alpha-helix and its transmembrane tendencies.

##### 3.1.1 Hydropathy Index

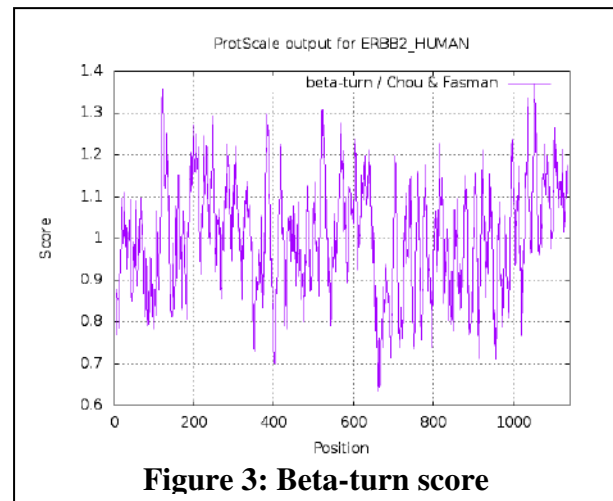
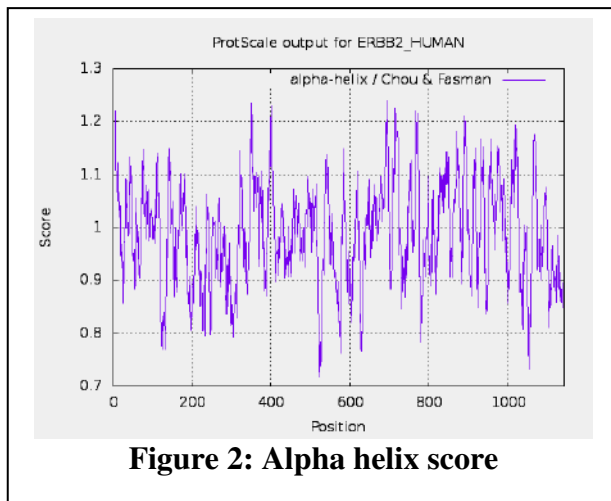
An amino acid's hydropathy index is a number reflecting the sidechain's hydrophobic or hydrophilic properties[9]. The greater the number, the higher is the hydrophobic character of the amino acid. The most hydrophobic amino acids are considered to be Isoleucine and Valine. Arginine and lysine are the most hydrophilic ones. It is very important in the composition of proteins; hydrophobic amino acids appear to be central (in terms of the 3-dimensional form of the



protein[10]) while hydrophilic amino acids are more generally located on the protein surfaces. We have identified the amino acid sequences that show hydrophobic properties and it has been represented in **Figure 1**.

### 3.1.2 Secondary structure of the protein

We have studied the alpha helix and beta sheets regions of the amino acid sequence. In an  $\alpha$  helix, one amino acid's carbonyl ( $C = O$ )[11] is hydrogen-bonded to the amino H ( $N-H$ ) of an amino acid that is 4 down the chain. This bonding pattern pulls the polypeptide chain into a curled ribbon-like helical structure, with 3.6 amino acids in each turn of the helix as shown in **Figures 2** and **3**. Furthermore, we have also found the helix wheel of the amino acid sequence using the

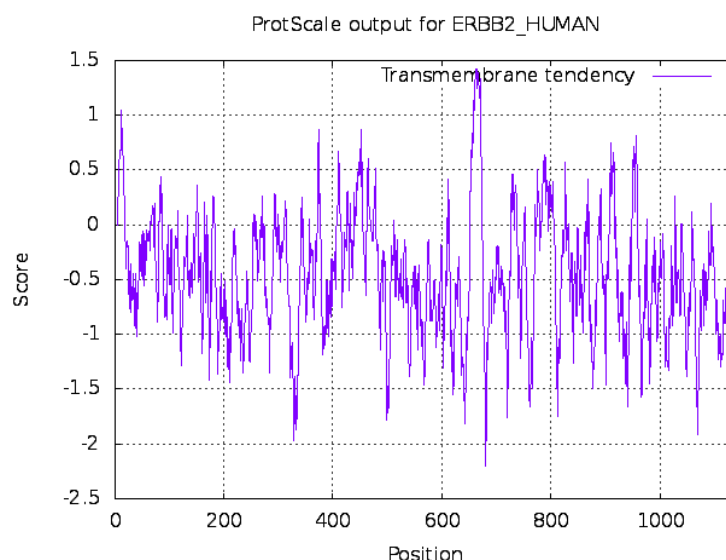


Helixator of TCDB[12] and shown it in **Figure 5**.

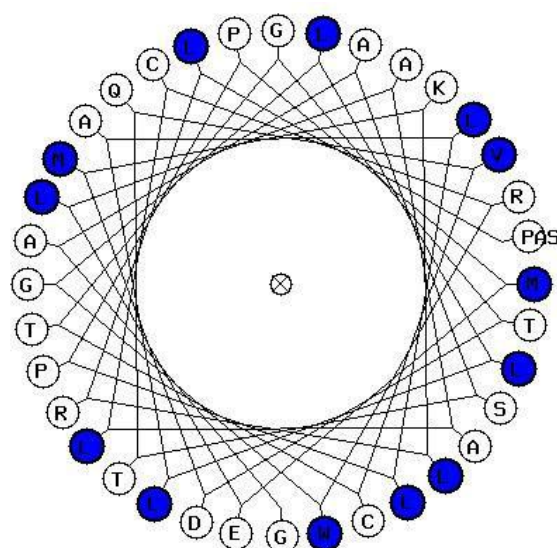
The amino acid R groups stick outwards from the  $\alpha$  helix, where they can interact freely and as for the beta-sheets, two or more segments of a polypeptide chain line up next to each other in a  $\beta$  plated sheet, forming a glass-like arrangement that is bound together by hydrogen bonds. The backbone of carbonyl and amino groups are held together by the formation of hydrogen bonds and the alkyl groups tend to extend above and below the planar sheet. We have used ProtScale to identify the secondary structure of the amino acids.

### 3.1.3 Transmembrane Tendency:

*An integral type of membrane protein that has the ability to span the entire cell membrane is known as a transmembrane protein (TP). Many transmembrane proteins act as gatewayss to allow the conveyance of specific substances across the membrane. To move a substance through the membrane they frequently undergo significant conformation changes[13]. Typically they're strongly hydrophobic, accumulate and precipitate in the mud. For extraction, they need detergents or non-polar solvents, although some of them (beta-barrels) can also be removed using denaturing agents. We have analyzed the transmembrane tendency through the hydropathy index and used protscale to plot the graph in **Figure 4**.*



**Figure 4: Transmembrane Tendency**



**Figure 5: Helix Wheel**

### **Part-B : Computation tool based approach to identify target sequence for CRISPR**

At first, we worked out the amino acid sequence of the Neu protein with its accession number from Expassy after which we individually looked at the nucleotide sequence of each amino acid and converted that into a FASTA file. Now this FASTA file was scanned in batch mode in two different software – CRISTA and CCTop and the following factors were common for both the software before analysis. *Genome* – Homo sapiens – *Ensembl GRCh38 (Genome Reference Consortium Human Build 38. Nuclease* – *SpCas9* – *Streptococcus pyogenes*.

### **3.2 COMPUTATIONAL TOOL BASED APPROACH**

The negative marks are a prime explanation representing the wastefulness of CRISPR in its space. Be that as it may, with present-day computational instruments, the system of activity of CRISPR was improved as well as its plausible results were likewise anticipated all the more precisely. The calculation is based on information that has been extracted through various sources and the amalgamation of all this information can be utilized by the AI to predict cleavage efficiencies. The essential bad mark of Cas-9 is that it divides askew DNA thus to counter that,



analysts began executing AI calculations utilizing computational instruments to develop a progressively exact cleavage result and disposing of the off-target bad marks. They would break down a portion of the most important and reliable CRISPR AI systems that are eligible for usage and assess their validity by looking at their yields for our desired outcomes. Of the well-known analytical methods, CRISTA[14] and CCTop[15] are considered as the most innovative solutions because of its willingness to take into account DNA bulges, which are sometimes ignored by other devices. This has had a significant impact on improving accuracy because DNA bulges are very common phenomena that tend to hinder the desired result of our DNA manipulation.

#### 4. Result:

##### 4.1 CRISTA Output

The output from CRISTA, in the form of guideRNA followed by its complementary target sequence and each of the sequences, are categorized based on the score of CRISTA. The CRISTA[16] scoring is based on factors like DNA bulges, loops, the efficacy, off-target cleavage activity, and the final product is presented in the form of the highest CRISTA score sequence to lowest. The output consists of sgRNA, target DNA, the strand, the start site, end position, and the CRISTA score. We have identified the top 4 gRNA based on the highest CRISTA scores ranging between 0.99 to 0.98 as shown in Table 1.

	sgRNA	DNA site	strand	start position	end position	CRISTA score
1	AAACCCGGAATATCTGGGCCNGG	AAACCCGGAATATCTGGGCCCTGG	+	3732	3754	0.99
2	GCGTATAGCCTGACCCTGCANGG	GCGTATAGCCTGACCCTGCAGGG	+	1318	1340	0.99
3	GACCTGCTTTGGCCCGGAAGNGG	GACCTGCTTTGGCCCGGAAGCGG	+	1722	1744	0.98
4	CCGGAATATCTGACCCCGCANGG	CCGGAATATCTGACCCCGCAGGG	+	3580	3602	0.98

**Table 1:** Table shows the sequence related to the Single guide RNA and corresponding score

##### 4.2 CCTop Output

As for CCTop, it's not yet known to take into account the bulges and loops totally while analyzing the sequence, however, the output presented by CCTop is more detailed and organized when it comes to actual experimentation. The output is given by breaking down the entire sequence into several target sequences and suggesting a guideRNA corresponding to that. It is sorted according to the target sequence and the varying efficacy score that depends on their off-target activity and is presented with its oligo-pair extension coordinates, PAM, gene name of the corresponding sequence, and the gene id giving a higher control to the experimentation carrier.[17]. We have

<b>T102 out of 596</b> <a href="#">&lt;Previous</a> <a href="#">Next&gt;</a> Sequence: GTTCGGCATCGCGCCGCTCGGG Efficacy score by CRISPRater: <b>0.90 HIGH</b> Oligo pair with 5' extension fwd: TAGGTTTCGGCATCGCGCCGCTCG rev: AAACCGAGCGCGCGCATGCCGAA Oligo pair with 5' substitution fwd: TAGGTCGGCATCGCGCCGCTCG rev: AAACCGAGCGCGCGCATGCCGA							
Coordinates	strand	MM	target_seq	PAM	distance	gene name	gene id
<a href="#">chr3:123291256-123291278</a>	+	4	GCTCATCA[TTGCGCCGCTCG]	CGG	0	E ADCY5	<a href="#">ENSG00000173175</a>
<a href="#">chr19:1067075-1067097</a>	-	4	GCTCGGAG[CCGCGCCGCTCG]	CGG	69	I HMHA1	<a href="#">ENSG00000180448</a>
<a href="#">chr16:31459563-31459585</a>	+	3	GTTCGTC[TCGCGCAGCTCG]	CGG	0	E RP11-452L6.5	<a href="#">ENSG00000260267</a>
<a href="#">chr20:17531128-17531150</a>	+	4	GCCCGGCA[TTGCGCTGCTCG]	AGG	0	E BFSP1	<a href="#">ENSG00000125864</a>
<a href="#">chr17:81961072-81961094</a>	+	4	GCTCGGCG[TCGAGGCGCTCG]	GGG	0	E NOTUM	<a href="#">ENSG00000185269</a>
<a href="#">chr10:79347803-79347825</a>	-	4	GCCCGGCA[CCGCGCCGCTCG]	GGG	60	I PPIF	<a href="#">ENSG00000108179</a>
<a href="#">chr5:32312954-32312976</a>	-	4	GGGCGGCA[TCGCGCGCTCG]	CGG	0	E MTMR12	<a href="#">ENSG00000150712</a>
<a href="#">chr12:123533380-123533402</a>	-	4	GTACGACA[TCGCGTCGCTTG]	TGG	0	E RILPL1	<a href="#">ENSG00000188026</a>

**Figure 6: Efficacy score of 0.90**

identified the 4 best target sequences and guides based on the highest efficacy score as shown below as showcased in Figures 6, 7, 8, and 9.



T412 out of 596

[<Previous Next>](#)

Sequence: AAAGTGAAGTGCTGGGCAGCGG

Efficacy score by CRISPRater: 0.89 HIGH

Oligo pair with 5' extension fwd: TAGgAAAGTGAAGTGCTGGGCAG rev: AAACCTGCCAGCACTTTCACTTT

Oligo pair with 5' substitution fwd: TAGgAGTGAAGTGCTGGGCAG rev: AAACCTGCCAGCACTTTCACT

Top 20 offtarget sites out of 52 (including on target; for full list see xls file)

Coordinates	strand	MM	target_seq	PAM	distance	gene name	gene id
<a href="#">chr9:89411853-89411875</a>	+	3	AAAGCCGA[AGTGCTGGGCAG]	TGG	5927	SEMA4D	<a href="#">ENSG00000187764</a>
<a href="#">chr5:148915261-148915283</a>	+	4	AGATTGTC[AGTGCTGGGCAG]	AGG	8356	SH3TC2	<a href="#">ENSG00000169247</a>
<a href="#">chr6:117660295-117660317</a>	+	4	AAATTGTC[AGTGCTGGGCAG]	GGG	15185	NUS1	<a href="#">ENSG00000153989</a>
<a href="#">chr16:5223208-5223230</a>	+	3	GAAGTGAG[ATTGCTGGGCAG]	AGG	2614	RP11-382N13.2	<a href="#">ENSG00000261811</a>
<a href="#">chr22:44918793-44918815</a>	+	4	GAGAGAG[GCTGCTGGGCAG]	AGG	1583	PHF21B	<a href="#">ENSG00000056487</a>
<a href="#">chr10:127692917-127692939</a>	+	4	AACCTGGA[AGTCTGGGCAG]	AGG	41623	RP11-288A5.2	<a href="#">ENSG00000279725</a>
<a href="#">chr9:82430965-82430987</a>	+	4	ACAGTGCA[GGGCTGGGCAG]	AGG	902	RP11-15B24.3	<a href="#">ENSG00000228123</a>
<a href="#">chr16:71492905-71492927</a>	+	4	CAGGGGAA[AGTGCAGGCAG]	AGG	2027	ZNF19	<a href="#">ENSG00000157429</a>

Figure 7: Efficacy score of 0.89

T480 out of 596

[<Previous Next>](#)

Sequence: TCGGGCGCGCGCCCGCTGCGG

Efficacy score by CRISPRater: 0.89 HIGH

Oligo pair with 5' extension fwd: TAGgTCGGGCGCGCGCCCGCTG rev: AAACAGGGCGCGCGCGCGCA

Oligo pair with 5' substitution fwd: TAGgCGGCGCGCGCCCGCTG rev: AAACAGGGCGCGCGCGCGG

Top 20 offtarget sites out of 52 (including on target; for full list see xls file)

Coordinates	strand	MM	target_seq	PAM	distance	gene name	gene id
<a href="#">chr17:79815350-79815372</a>	+	4	CCCGGCC[CGTGCCCGCTG]	GGG	8080	RP11-353N14.2	<a href="#">ENSG00000262772</a>
<a href="#">chr16:527684-527706</a>	+	3	GTCGGCGC[CGCGCAGCCCTG]	TGG	11	CAPN15	<a href="#">ENSG00000103326</a>
<a href="#">chr11:30894368-30894390</a>	+	4	TGCCGCTA[CTCGCCCGCTG]	AGG	0	DCDC1	<a href="#">ENSG00000170959</a>
<a href="#">chr10:63521928-63521950</a>	+	4	CGCAGCGC[GGCAGCCCGCTG]	CGG	78	JMJD1C	<a href="#">ENSG00000171988</a>
<a href="#">chr9:136203155-136203177</a>	+	4	TGCGCCCG[CGGCGCCCGCTG]	GGG	0	LHX3	<a href="#">ENSG00000107187</a>
<a href="#">chr22:50058533-50058555</a>	+	2	TGCGGCC[CGCGCCCGCTG]	TGG	836	MLC1	<a href="#">ENSG00000100427</a>
<a href="#">chr3:51956245-51956267</a>	+	4	TGCGCGGT[CGCGCTGCCCTG]	AGG	0	GPR62	<a href="#">ENSG00000180929</a>
<a href="#">chr2:95649314-95649336</a>	+	4	TGCTTCCC[CGCGCTGCCCTG]	TGG	7334	AC009237.16	<a href="#">ENSG00000236750</a>

Figure 8: Efficacy score of 0.89

T498 out of 596

[<Previous Next>](#)

Sequence: GCCGGGCGCGCCCGGCAGCGG

Efficacy score by CRISPRater: 0.89 HIGH

Oligo pair with 5' extension fwd: TAGGCCGGGCGCGCCCGGCAG rev: AAACCTGCCGGCGCGCGCCCGG

Oligo pair with 5' substitution fwd: TAGGCGGGCGCGCCCGGCAG rev: AAACCTGCCGGCGCGCGCCCGG

Top 20 offtarget sites out of 52 (including on target; for full list see xls file)

Coordinates	strand	MM	target_seq	PAM	distance	gene name	gene id
<a href="#">chr18:35581722-35581744</a>	+	2	GCCGGGG[AGCCGCCGGCAG]	TGG	0	GALNT1	<a href="#">ENSG00000141429</a>
<a href="#">chr12:121467015-121467037</a>	+	3	CCCGGCC[CCCGCCGGCAG]	CGG	121	KDM2B	<a href="#">ENSG00000089094</a>
<a href="#">chr2:60881732-60881754</a>	+	4	ACTGGGG[CCCGCCGGCAG]	AGG	0	REL	<a href="#">ENSG00000162924</a>
<a href="#">chr17:51120680-51120702</a>	+	3	GCCCGGG[CGTCGCCGGCAG]	AGG	0	SPAG9	<a href="#">ENSG00000008294</a>
<a href="#">chr3:126380922-126380944</a>	+	3	GCTGGGT[CGTCGCCGGCAG]	AGG	12088	CCDC37-AS1	<a href="#">ENSG00000249833</a>
<a href="#">chrX:49250256-49250278</a>	+	4	GCCGTAGG[AGCCGCCGGCAG]	AGG	0	CCDC22	<a href="#">ENSG00000101997</a>
<a href="#">chr4:2250558-2250580</a>	+	4	GCGGGCC[AGCCGCCGGCAG]	TGG	0	MXD4	<a href="#">ENSG00000123933</a>
<a href="#">chr4:1172555-1172577</a>	+	4	AGCGGAG[CGCGCCGGCAG]	CGG	0	SPON2	<a href="#">ENSG00000159674</a>
<a href="#">chr19:41883360-41883382</a>	+	4	GCTGGGG[CGTCGCCGGCAG]	CGG	71	ARHGEF1	<a href="#">ENSG00000076928</a>
<a href="#">chr16:5239696-5239718</a>	+	4	TGCGGGG[AGCGCCGGCAG]	AGG	84	RP11-420N3.3	<a href="#">ENSG00000279877</a>

Figure 9: Efficacy score of 0.89

## 5. Discussion and Analysis:

The manuscript aims at deciphering the latest molecular biology technique in terms of CRISPR/Cas-9 genetic alteration or modification or edition related to Neu gene. At the same time, it also envisages the protein characteristics related to the Herceptin protein, a biomarker in breast cancer prognosis. Herceptin is a protein, overexpression relates to the breast carcinoma and has got clinical implication in diagnosing the breast carcinoma other than histochemical or histopathological or histoimmunological techniques. The Herceptin protein is encoded by the gene termed as “Neu” gene whose over expression translates it into herceptin protein. We tried to explore the concept of CRISPR/Cas-9 system to decipher the genetic alteration of the neu gene using computational tool like that of CRISTA and ccTOP to generate the target sequence as well as the PAM for each sequence of the Neu gene. Our result in terms of Herceptin protein characteristic like that of hydropathy index, transmembrane tendency, alpha helix and beta turn, and helix wheel envisages that the protein is a transmembrane spanning between the inner and outer domain of the membrane as evident from the **Figures 1, 2, 3, 4, and 5**. The hydropathy index indicates that the most of the amino acid composition of the herceptin protein is hydrophobic in nature. We have also studied the alpha helix and beta sheets regions of the amino acid sequence as the secondary structure of the protein. In an  $\alpha$  helix, one amino acid's carbonyl ( $C=O$ ) [11] is hydrogen-bonded to the amino H ( $N-H$ ) of an amino acid that is 4 down the chain. This bonding pattern pulls the polypeptide chain into a curled ribbon-like helical structure with 3.6 amino acids in each turn of the helix. Furthermore, we attempted to elucidate the single guide RNA sequence corresponding to the target sequence as referred to here as the DNA site sequence as evident from **Table 1**. For each SgRNA sequence we attempted to elucidate the possible target sequence and PAM sequence generated from the two computational tool (**CRISTA** and **ccTOP**) with highest efficacy score as shown in the **Figure(s) 6, 7, 8, and 9**. The sequence reflected in the manuscript is needed to be processed in the wet lab by transfecting the designed SgRNA sequence into plasmid and validating the same for precision and accuracy cutting or edition of the said target sequence as recognized by the corresponding PAM sequence.

## 6. Future directions:

Our aim in this manuscript was to study the structure and the properties of the herceptin protein encoded by Neu gene as well as to generate the target sequence with appropriate guideRNAs for genetic alteration or cutting or modification employing CRISPR/Cas9 genetic tool. The technique got more relevance and importance after being awarded with Noble prize by the investigators. Future research is needed to achieve the precision and accuracy of identifying the target location among the million base pair of a gene and cutting the exact target sequence and not generating the offtarget sequence is a million dollar question that needs to be answered or investigated further to achieve its full potential in using as a therapeutic measures against all form of cancer and genetic disorders. It is well known fact that DNA bulges after certain base pairs that may get unrecognized by the Cas-9 system and therefore may generate offtarget sequence which shall be more detrimental rather than to be useful.

## 7. Conclusion:

Our paper identifies the best sequences of the Neu gene that can be targeted with the highest efficacy and lowest off-target cleavage with the CRISPR system and potentially pave way for higher oncological research for humans welfare [18]. We have tried to contribute to the existing knowledge of science using some computational tools to aid the advances with limited resources since we are unable to visit our labs during this pandemic. We aspire to keep working using computational tools and work on the demerits of existing technology to make it desk to bed readily.

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**International E-Conference on  
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**Automation, Computer Science and Technology Department,  
Kryvyi Rih National University, Ukraine and 'Research Culture Society'.**

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**EFFECT OF PARTICULATE MATTER (PM) ON AN ECOSYSTEM  
INCLUDING CLIMATE, PLANTS AND HUMAN HEALTH**

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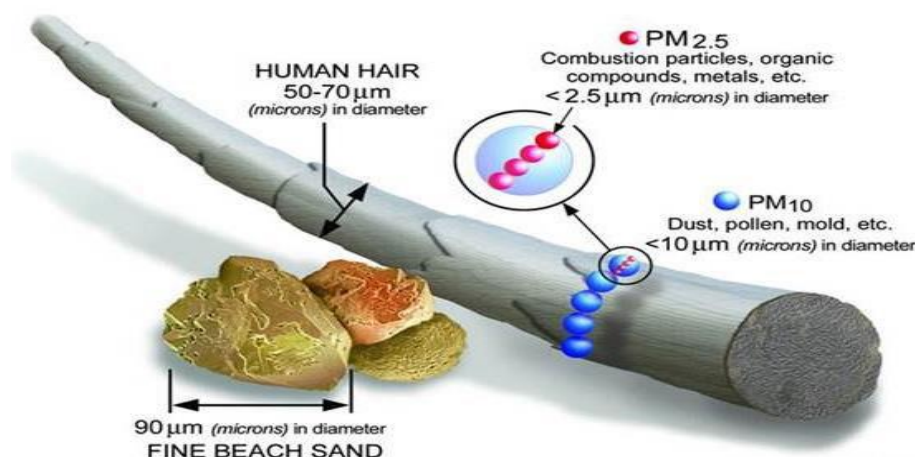
**Abstract :** *Particulate issue (PM) is an unpredictable blend of strong and fluid particles that are suspended in air. These particles regularly comprise of a blend of inorganic and natural synthetics, including carbon, sulfates, nitrates, metals, acids. Exploration recommends that molecule size is a significant factor that impacts how particles store in the respiratory plot and influence human wellbeing. Coarse particles are saved solely in the nose and throat; though, fine and ultrafine particles by and large can infiltrate to profound zones of the lung. Fine and ultrafine particles are available in more noteworthy numbers and have more prominent surface region than bigger particles of a similar mass, and they are commonly viewed as more harmful. Most nations add to airborne particulate issue contamination in different nations. In the recent years particulate issue has received media consideration, consequential to the revelation of thousands of individuals kicking the bucket youthful of particulate issue presented wellbeing impacts. This incorporates both present moment and long haul impacts. Particulate issue doesn't just motivation wellbeing impacts; it likewise assumes a function in the green house impact and an unnatural weather change as a result of its commitment to cloud arrangement.*

*The work revealed in this paper is essential for an a lot bigger exploration venture on airborne particulate issue. These particulates have now gotten a matter of genuine worry in the worldwide climate, since not exclusively would they be able to have generous negative consequences for human wellbeing however they can likewise impact precipitation levels, the world's atmosphere and the biological system. Besides, the testimony of these particles on vegetated surfaces can unfavorably influence plant and creature life. The size, compound structure, and cause of these particulates shift enormously. The impacts of these particles have been thoroughly examined and explored in this paper with their related natural effect.*

## **1. Introduction:**

Particulate matter is additionally referred to as atmospheric aerosol particles, particulates, or suspended particulate (SPM). At the foremost basic level, particulate may be a collective term that encompasses a mix of the many fine solid and liquid particles, suspended within the earth's atmosphere. These particles may include dust, fly ash, soot, smoke, aerosols, fumes, mists and condensing vapours which will be suspended within the air for extended periods of your time. Within the previous couple of years, particulate has received considerable media attention largely thanks to the increased number of deaths due to particulate related health diseases. Environmental degradation has also been attributed to airborne particulate, especially in developing countries where the concentration of those particulates are very high thanks to construction/industrial activities. The damage from these particulates in developing countries is estimated at billions of dollars. Particulate has also drawn significant attention from the scientific community due to it's apparent role/contribution in cloud formation and global climate change and is currently a topic of in depth research.

These sources include windblown dust and wildfires. Secondary PM sources directly emit air contaminants into the atmosphere that form or help form particulate. Hence, these pollutants are essentially considered precursors to PM formation. These secondary pollutants include SO<sub>x</sub>, NO<sub>x</sub>, VOCs, and ammonia. There are many various sorts of particulate, which can be distinguished into separate groups, supported their size; Total suspended particles, which include all particles of whatever size; PM<sub>10</sub> which are particles that are but 10 µm (10 microns) in diameter; PM<sub>2.5</sub> that are but 2.5 µm in diameter. the foremost dangerous among the category of particulate are fine particles that are but 2.5 µm in diameter. These particles can penetrate very deeply into the system a respiratorium and obtain deposited within the lungs as sediments or enter the bloodstream.



## DEPOSITION PROCESSES:

Particulate matter can collect or deposit themselves on solid surfaces, via two sub-processes: dry and wet deposition. the previous includes deposition by impaction, interception, gravitational sedimentation, turbulence and other pro-cesses like thermophoresis, electrophoresis etc while within the latter condition, atmospheric hydrometeors (rain drops, snow etc.) scavenge aerosol particles. This essentially means wet deposition is gravitational, Brownian and/or turbulent coagulation with water droplets. These deposition can induce great changes within the ecosystem. subsequent section discusses the varied effects of particulate on plants, climate, human health and ecosystem generally.

## CLIMATE EFFECTS:

The change within the earth's climate is driven by certain perturbations within the earth's energy balance. These perturbations are collectively mentioned as "climate forcing", and are the topic of considerable research for predicting future change within the earth's climate. Variations in climate forcing are defined or determined by physical influences on the atmosphere like orbital and axial changes also as by the presence of certain agents like greenhouse gases and aerosol particles, which are capable of altering the earth's energy balance. This successively brings about changes within the earth's global temperature and thereby changes within the climate. The contribution of particulate during this change is extremely substantial. particulate can affect the climate either directly i.e. through the method of scattering and absorption of the radiation, or indirectly i.e. through the formation of cloud condensation nuclei (CCN). The direct contribution of particulate is thanks to the presence of sulphate aerosols, fuel soots and emissions from biomass burning within the earth's atmosphere.

Certain pollutants, among which elementary carbon appears to be the dominant factor aside from ozone, can induce rise in temperature through the method of warmth absorption. as an example, black carbon, a particulate pollutant produced from combustion contributes to the warming of the world. On the opposite hand, some components of particulate like SO<sub>2</sub> cools the earth's atmosphere.

### ***1.(a) Scattering and absorption of light due to aerosol particles***

The scattering of sunshine may be a general physical process and is defined because the redistribution of sunshine in non parallel directions when it interacts with small particles of matter. Light scattering of aerosol particles can happen thanks to the presence of a good sort of aerosol types, among which the carbon and sulphate containing particles is believed to be the foremost efficient. Scattering thanks to aerosol mode particles (particles whose diameter are of an equivalent order because the wavelength of the incident light) produces a negative forcing (cooling effect) because the scattered light from these particles falls predominantly into the region of Mie scattering which is characterised by up-scattered light that's reflected back to space (i.e. the scattered light doesn't reach the earth's surface).

### ***1. (b) Formation of cloud condensation nuclei by aerosol particles***

Many different sorts of aerosol particles can act as cloud condensation nuclei (CCN) around which the cloud drop-lets are formed. The relative ability of those different sort of aerosol particles to supply cloud droplets differ according to their size and composition. the entire number and therefore the sorts of CCNs formed can directly influence the quantity of precipitation, lifetime and therefore the radiative properties of the cloud, and hence directly affect global climate change .

## **2. EFFECT ON HUMAN HEALTH:**

Particulate matter is, at the present , being extensively researched due to its visible and indisputable effect on human health, although it truly drew increased attention from scientists at the start of the 80s. Many scientific studies have since than been published that shows that an immediate link are often established between exposure to particle pollution (both short term and prolonged exposure) and health risks, including premature death. Such studies indicate that fine particles are largely liable for the observed health problems in humans and correlate exposure to fine particles to increased instances of asthma, decreased lung functioning ability in children, increased hospital admissions. The heavy metal constituents of particulate is additionally a matter of important consideration. There are many substantial evidences that shows that heavy metals adsorbed to atmospheric particulate is what confers toxicity to PM. These heavy metals have complex pollution features. Fine particles can contain heavy metals like arsenic, cadmium, selenium etc. Many studies on these heavy metal constituents of PM have reported that exposure to high concentration of heavy metals can have adverse effects on the human health. additionally, these metals can get deposited to plant leaves, soil, water bodies etc via wet and dry deposition. These may then get collected within the plant's body through biochemical processes and humans may accumulate these metals through consumption of the contaminated plant.

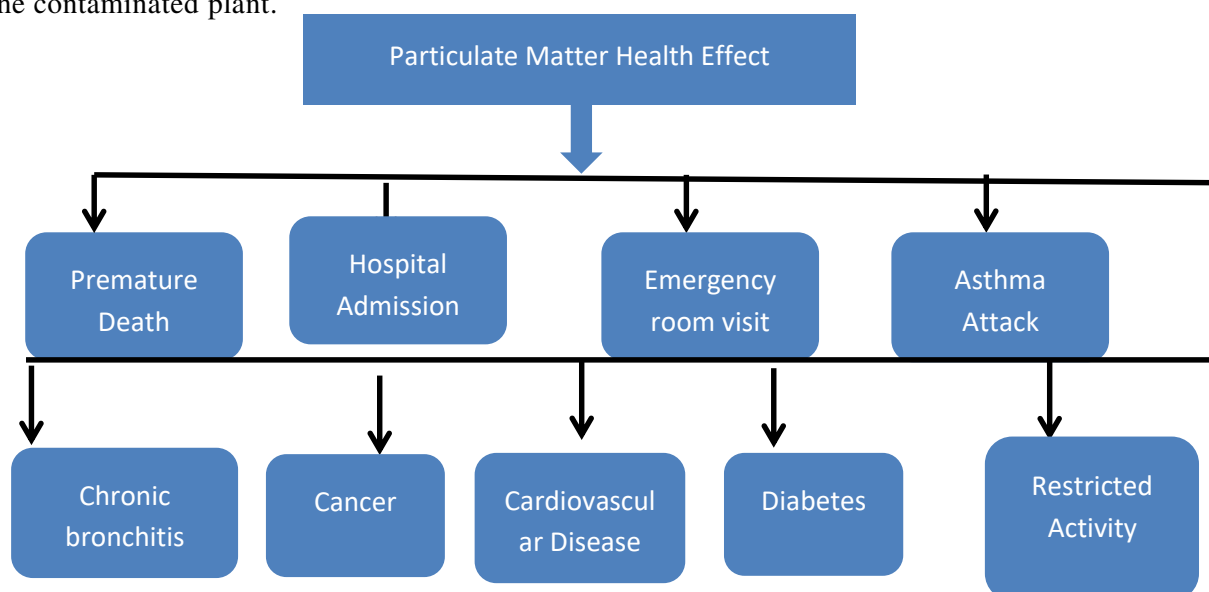
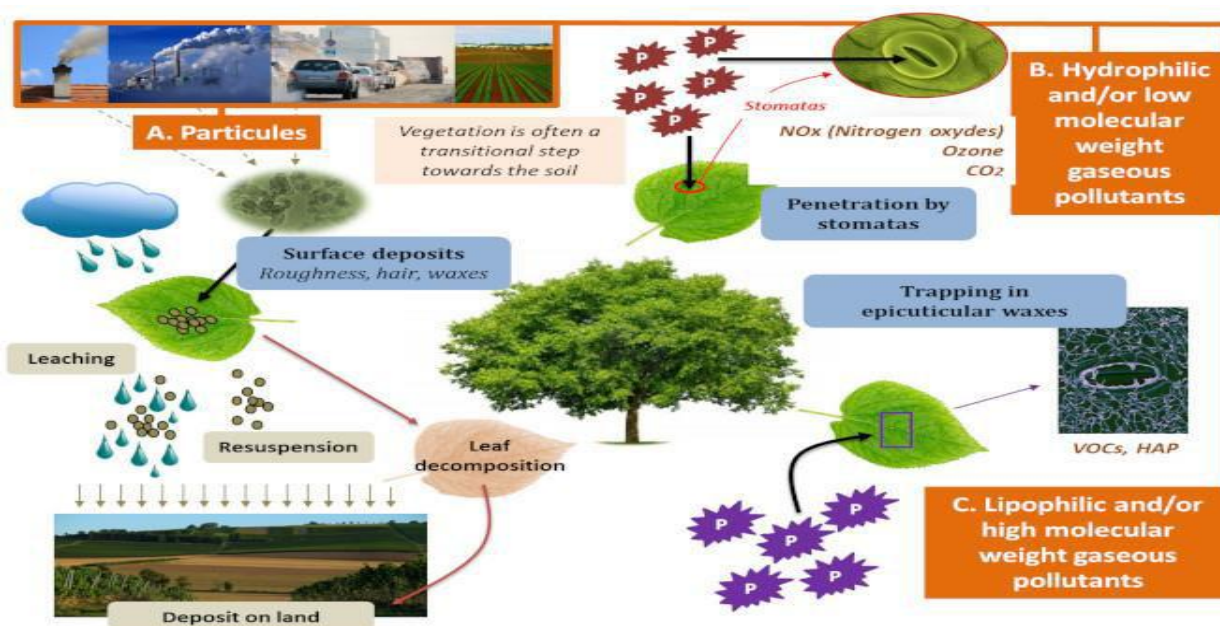


Table 2 discusses some heavy metals and their associated effects on human health.

POLLUTANT	SOURCE	EFFECT ON HUMAN HEALTH	MINIMUM PERMISSIBLE LEVEL
ARSENIC	Chemical pesticides, electronic wastes, smelting etc.	Inflammation of the respiratory organs; bronchitis, dermatitis, inflammation of liver, anaemia, cardiovascular diseases	0.0003 mg/kg/day of oral exposure
LEAD	Emissions from vehicles and industries, paint, mining, burning of plastic etc.	Irritation of the gastro-intestinal tract, kidney and liver damage	Less than 10 micrograms per decilitre of blood
ZINC	Oil and petroleum refineries, plumbing, metal plating etc.	Irritation of the eye, suppression of iron and copper absorption	0.002-0.005 mg/kg/day
MERCURY	Electronic wastes, dental and pharmaceuticals wastes etc.	Poor coordination, skin rashes, anxiety and memory problems, decreased intelligence	Less than 10 micrograms per decilitre of blood
CADMIUM	Pesticides, chemical fertilisers, welding, nuclear power plants etc.	Gastrointestinal damage, kidney damage, has carcinogenic properties	Less than 1 microgram per decilitre of blood

Table 2: Effects of heavy metal constituents of PM on human health



### 3. EFFECT ON PLANTS:

When plants are exposed to a good range of pollutant concentration, the pollutants may trigger various phytotoxic responses in plants, counting on the characteristic features of the particulate mixture that's being deposited. generally , plants are capable of filtering coarse particles at a way faster rate than fine particles. Particulate deposition on plants may contains (i) nitrate and sulfate and (2) trace elements and heavy metals. The acid-forming sulfate and nitrate particles are comparatively more soluble and more reactive than mineral dusts. particulate with pH values of  $\geq 9$  may prove toxic to the leaf tissues on which they're deposited. they will also adversely affect the plants indirectly through modification of the soil pH.





Plants provide a huge leaf area for absorption and accumulation of dust particles. Dust deposited on the surface of the leaves can greatly modify the optical properties of photosynthetic tissues, and therefore the amount of sunshine that's available for photosynthesis. This happens because the dust particles are finely arranged or targeting the leaf surface, thus effectively shading or shielding the leaves from photosynthetically active radiation (PAR).

#### 4. EFFECT ON ECOSYSTEM:

Ecological responses to particulate stress varies widely. Succession in unpolluted environment is taken into account favour-able while those places where particulate pollution is high hinders the expansion of organisms and plants. These par-ticulates interferes with the traditional physiology and biochemistry of the plants and animals and subsequently affects the organic phenomenon , nutrient cycling and energy flow. Furthermore, particulate from anthropogenic sources may affect the environment and therefore the organisms so harshly that it becomes impossible for them to recuperate from the damage and propel them towards further degradation. Chronic pollutant injuries to a forest ecosystem may end in the permanent loss of susceptible species of plants, and even animals. Dust coating may prompt abrasion and radiative heating, and should greatly reduce the photosynthetically active radiation reaching the plant tissues.

#### 5. CONCLUSION:

It is clear that particulate has important and predictable effects on plants, climate, human health and therefore the ecosystem. Industrialisation, increase and associated increase in energy demands have resulted during a profound increase of those fine particles. The elevated levels of those particles within the earth's atmosphere can't only threaten the health of citizenry , plants and animals but also adversely affect the ecosystem balance. Hence, there's utmost got to study, visualise and identify new strategies which will minimise the presence of those particles within the environment.

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**Automation, Computer Science and Technology Department,  
Kryvyi Rih National University, Ukraine and 'Research Culture Society'.**

## **Evaluation of Phosphorus Recovery from Decentralized Sewage Treatment systems**

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**Abstract:** *Developing countries have low sanitation facilities with only 32.7% population having access to sewerage network out of which only 20-25% is treated. While 100% collection efficiency is not feasible in near future, decentralized systems are being promoted to improve local sanitation facilities and achieve SDGs 3, 6 and 11. These systems are often less diluted than centralized systems in terms of nutrient concentration and thus possess a huge potential for nutrient recovery. Alongside, scientific reports have established that phosphate rock (P) reserves are diminishing which may impact food security and vulnerability of marginalised farmers in developing countries. Recovering P from waste will help in addressing P vulnerability issues and develop an alternative source of P fertilizer. Most of the technologies that have been developed to recover P are designed for centralized treatment systems. In this study, waste in decentralized wastewater treatment system is studied attempted for the first time to assess their feasibility of P recovery. Partial anaerobic digestion in systems like septic tanks convert organic P to orthophosphate allowing it to be recovered as struvite. Thus, feasibility and efficiency of recovering P from septic tank effluent was evaluated. The impact of this recovery process on pH and reduction of pollutants like BOD, COD, TSS in septic tank treated effluent was also analyzed. P recovery efficiency of almost 90% was achieved leading to 65 g P from a litre of septic tank effluent. The concentration of BOD, COD, TSS and P decreased by approximately 20%, 47%, 27% and 90% respectively while the pH decreased from 9 to 8.74. Overall, recovery of P was associated with simultaneous improvement in the effluent wastewater generated. Thus, the study showed that decentralized systems are a suitable source to develop a local P fertilizer while also reducing the pollutant concentration in wastewater.*

### **1. Introduction:**

With the growing realization of health issues, improvement in provision of basic sanitation facilities is one of the emerging challenges in developing countries. Sustainable development goal (SDG) 6 also emphasizes on the availability and management of clean water and sanitation for all (United Nations, 2015). Present situation in developing countries reveal low sanitation facilities with only 38% of urban population having access to the sewerage network, 47% of population is connected to onsite decentralized systems while 6% connected to pit latrines (Weitz et al., 2016). The share of onsite system of treatment is expected to increase with the introduction of sanitation drive in a missionary mode in developing countries like India, Nepal where decentralized systems like septic tanks and pits still remained the mainstay methods for faecal sludge management (Ministry of Housing and Urban Affairs, 2017; National Planning Commission, 2011). However, these systems treat wastewater partially and are the major source of water pollution in rivers and lakes.

Phosphorus (P) being a valuable nutrient is pre-requisite for agricultural productivity. With the exponential rise in population, the demand for food and consequently fertilizer production will also rise. Scientific evidence has warned about the alarming rate of phosphate rock reserves depletion worldwide

which could pose a threat to food security directly or indirectly (Cooper et al., 2011). Further, the distribution of these reserves in the world (about 70,000 million tonnes as reported in 2018) – is concentrated in selected countries namely Morocco and Western Sahara, China, Algeria, Brazil, and South Africa (Jasinski, 2018). Developing countries are the most vulnerable to the skewed distribution and depletion of phosphate with the possibility of spike of international price of P (Boer et al., 2019). Establishment of water-energy-nutrient nexus can serve the dual purpose of nutrient recovery as well as maintaining sanitation. Current waste water treatment practices aim at removal of P to meet the discharge standards. Thus, a transition from nutrient removal to nutrient recovery would be required to achieve this water-energy-nutrient nexus.

Developed countries with efficient waste water collection and treatment systems have been able to achieve this transition by adopting various new technologies for P recovery. Most of these recovery technologies are based on precipitation of phosphoric minerals (Cieřlik & Konieczka, 2017) and produce high quality products like HAP (Hydroxy apatite), Struvite, K-Struvite, calcined phosphates and phosphoric acid which find application in agriculture or in fertilizer manufacture industry. Technological variations are based on the method as well source employed for P recovery; for example, crystallization and precipitation method is mostly used for sources like sludge liquor or sludge supernatant (employed in technologies such as Ostara Pearl (USA), Phospaq(UK)), while chemical leaching is used to recover P from sewage sludge as adopted in Seaborne (Germany) technology (Nakagawa & Ohta, 2018; Sartorius et al., 2012). Egle et al., 2015 concluded a recovery efficiency ranging from 80-90% from such technologies.

In addition to centralized sources of P recovery, water-nutrient-energy nexus can also be achieved by recovering P from decentralized streams like urine, slaughter house, dairy wastewater, fertilizer wastewater. Source separated urine does not get diluted with water and thus has a high concentration of P which be recovered. Studies on P recovery from source separated urine or black water reported an efficiency of 90-95% (Ronteltap, 2009; Zeeman & Kujawa-Roeleveld, 2011). Similarly, high nutrient concentration along with calcium content in dairy waste water can be used to recover P as HAP or struvite as reported by Harris et al., 2008; Lavanya & Sri Krishnapurumal Thanga, 2020. Another such decentralized source is septic tanks that are used to reduce BOD and TSS in sewage for its land-based disposal. Partial anaerobic digestion in septic tanks generates an effluent enriched with  $\text{NH}_4\text{-N}$ , orthophosphate phosphorus (Withers et al., 2011). Using decentralized sources has twin benefits of achieving sanitation goals as well as developing a local source of P fertilizer. Although developing countries are dominated by large number of septic tanks, P recovery from septic tank effluent has not received much attention.

In light of this background the present study assesses the feasibility of recovering P from septic tank effluent and also the associated impact on the resultant wastewater characteristics like Biological oxygen demand (BOD), Chemical oxygen demand (COD), Total suspended solids (TSS) and pH. This is based on the assumption that recovery process might also result in improvement of quality of wastewater before it is discharged onto land or water bodies. Thus, this study is carried out with the objective of treating septic tank wastewater to reduce its contribution towards water bodies pollution while also develop a local P fertilizer source.

## 2. Methodology:

Experiments were carried out to assess the potential of recovering P from septic tank effluent. Corresponding effect of this recovery on pH and concentration of major water pollutants namely BOD, COD and TSS was evaluated to assess the percentage reduction in pollution. Three replications for each pollutant were performed based on which mean values were calculated. Percentage reduction in each of the above pollutants was calculated by dividing the difference between the pollutant concentration before and after P recovery process by the initial pollutant concentration.

### 2.1) Collection and characterization of wastewater

Samples of septic tank effluent were collected from the outlet of a septic tank located in Delhi, India. The samples collected were kept in an icebox and brought to laboratory. The wastewater was then characterized for pH, 5-day BOD, TSS, COD and Orthophosphate levels before and after P recovery process. Method of analysis as given in Standard Methods (APHA, 2017) were used where, orthophosphate was measured by Vanadate-molybdate method at a wavelength of 470 nm.

### 2.2) P recovery setup

Lab scale P recovery experiments were carried out using jar test apparatus. One litre volume of sample used for the experiments were dosed with appropriate amount of  $\text{NH}_4\text{Cl}$  and  $\text{MgCl}_2$  to maintain N/P

ratio at 5 and Mg/P ratio of 2 respectively. Presence of excess ammonia is important for recovering P in the form of struvite and also for maintaining the pH of the solution. Conditions for recovery process were set at pH 9, Mg:P of 2:1, time duration of 60 minutes and speed of jar test apparatus at 140 rpm. pH is increased from its initial value to pH 9 by adding 1M NaOH drop wise to initiate precipitation and obtain maximum recovery efficiency as proved in other studies (Peng et al., 2018). At the end of P recovery experiment after 60 min, the resultant precipitate was allowed to settle down leaving a clear supernatant and characterized for the parameters mentioned above.

### 3. Results and discussion:

#### 3.1) Characteristics of effluent sample collected

Characteristics of the septic tank effluent before and after P recovery are given in Table 1. Initial average Mg/P ratio was 1.25 while Ca/Mg ratio was 0.88. For precipitation of P as struvite calcium interference is a significant factor. This interference can be reduced by adding Mg as  $MgCl_2$  to the working solution thereby increasing the Mg/P ratio. The initial pH of the solution i.e. 6.3 has to be adjusted towards the alkaline side to initiate the precipitation reaction. P recovery potential and effect of recovery process on the concentrations of BOD, COD and TSS is shown in Table 2. These observations are further described in sections 3.2- 3.5.

Table 1 Initial characteristics of septic tank effluent

Parameter	Mean value <sup>1</sup> (standard deviation)
pH	6.3(3.00)
Dissolved P	72.2(1.78)
Magnesium	70.8(6.99)
Calcium	107.1(9.73)
Biological oxygen demand	191.7(7.61)
Chemical oxygen demand	486.1(7.02)
NH <sub>4</sub> -N	100.8(9.31)
Total suspended solids	74.2(3.45)

<sup>1</sup> all values in mg/l except for pH

Table 2 Impact of P recovery on wastewater pollutant concentrations (average of three experimental runs)

Wastewater pollutant	Average concentration (mg/l)
Initial P	72.2
Final P	7.2
Initial BOD	191.7
Final BOD	153.0
Initial TSS	74.2
Final TSS	53.6
Initial COD	486.1
Final COD	253.9

#### 3.2) Impact of P recovery on pH of septic tank effluent

Struvite precipitates in the presence of magnesium ( $Mg^{+2}$ ), ammonium ( $NH_4^+$ ), and phosphate ( $PO_4^{-3}$ ) according to the equation (1) when the thermodynamic solubility product,  $K_s$ , is exceeded:

$$Mg^{+2} + PO_4^{-3} + NH_4^+ + 6H_2O \rightarrow MgNH_4PO_4 \cdot 6H_2O \quad \dots 1$$

With the onset of precipitation at pH 9.2, a decline in the pH of the solution was observed. This is because the dominant form of P in crystallization process changes from  $PO_4^{3-}$  to  $HPO_4^{2-}$  thereby generating protons as showed in equation (2) which decrease the pH (Liu et al., 2013). Thus, drop in pH is characteristic of struvite formation within the system and the pH of the resultant solution was in the range 8.74– 8.90. However, there is an increase in the pH of the effluent with respect to the original pH of the effluent.

$$Mg^{+2} + HPO_4^{-2} + NH_4^+ + 6H_2O \rightarrow MgNH_4PO_4 \cdot 6H_2O + H^+ \quad \dots 2$$



### 3.3) Impact on TSS concentrations of septic tank effluent

The TSS of septic tank effluent after P recovery decreased by an average of 27%. Suspended solids being negatively charged absorb  $\text{NH}_4^+$  and  $\text{Mg}^{+2}$  at alkaline pH (Fang et al., 2015). Also, during flocculation TSS can adhere to surface of struvite crystals (Ping et al., 2016). The above two processes resulted in precipitation of the suspended solids leaving behind a clear solution with low TSS concentration.

### 3.4) Impact of P recovery on BOD and COD concentration of septic tank effluent

Mixing of septic tank effluent dissolved oxygen in the solution which favoured aerobic bacteria to break down the organic compounds to carbon dioxide. This resulted in 20% and 47 % reduction in BOD and COD respectively. This break down also converted organic P to inorganic P (orthophosphate form) making it available for recovery. A sharp decline in BOD concentration was not observed because major portion of organic content is settled down in the septic tank itself from where the effluent sample was collected.

### 3.5) Estimation of P recovery from septic tank effluent

Following the precipitation reaction under the optimal conditions of pH 9, Mg/P ratio of 2, Ca/Mg <1, phosphorus concentration fell sharply from 72.2 mg/l to 7.27 mg/l. On an average 90% of phosphorus was recovered in the form of struvite and calcium phosphates amounting to 65g of P recoverable from a litre of septic tank effluent. The decrease in P concentration would significantly reduce its contribution downstream of the process that is towards land pollution caused by disposal of the resultant wastewater. It must be noted that the P recovery efficiency is dependent on the operating conditions of pH, Mg and Ca concentrations (Huang, 2003) and thus may vary with changes in these factors.

## 4. Conclusion :

Decentralized systems such as septic tanks are a suitable source to recover P as struvite. Anaerobic digestion in the septic tanks converts the P from its organic to inorganic form so that it can be recovered. Under optimum conditions of pH 9, Mg/P ratio of 2; about 90% of the P present in the septic tank effluent was recovered. Around 65 g per litre of effluent was obtained. A drop in the pH of the solution during the recovery process was indicative of the fact that struvite was formed. The final pH of the resultant effluent was in the range of 8.74 – 8.90. Further, the P recovery process was associated with mild reductions in BOD (21%), COD (47%) and TSS (27%). Recovery of P from septic tank effluent will have small but positive implications downstream of the process due to reduction in the pollution strength of the disposed effluent wastewater. Parallely, it also exhibits the potential to develop a P fertilizer source at the local level.

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## **Mathematical applications in day to day human life.**

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**Abstract:** *This article throws light upon the applications of Mathematics in our day to day life. Applied Mathematics is a branch of mathematics that deals with the applications of Mathematics in various fields. We make use of mathematics in multiple ways in our day to day life. Right from the moment we rise from our sleep and till we go to bed, we are confronted with many mathematical operations knowingly or unknowingly. Mathematics is a science of number which deals with Calculation. Multiplication, division and all the logical terms topics and branches like Algebra, generalization, geometry trigonometry and abstractive.*

*Mathematics in the broadest sense is just a formal science but traditionally mathematics means more arithmetic, algebra, geometry, and analysis which are roughly speaking, the study of quantity, structure, space and change. Mathematics is incredibly important in our lives and without realizing it we use mathematical concept as well as the skills from doing math problem every math. The laws of and without a good understanding of them one can encounter signification difficulties in life.*

*Today's students are expected to learn about and use information and communication technology (ICT) in mathematics to prepare them for their future, the work force and the challenges of everyday life. However, international studies show that secondary mathematics teachers are still not effectively integrating computer technology in their classroom. Computers offer powerful opportunities for pupils to explore mathematical ideas, to generalize, explain results and analyze situations, and to receive fast and reliable, and non-judgmental, feedback. Their use needs careful planning – not just of the organization of hardware and appropriate software but also of activities that allow for off-computer mathematical thinking as well as on-computer exploration. Mathematics is related to science infect mathematics is considered to be the of all the sciences knowledge of mathematics is necessary in order...*

**Key words:** *Mathematics, daily, operations, Calculate, life, technology.*

### **1. Introduction:**

- 1) Mathematics that we attain in our daily lives.
- 2) Mathematics that we need in our daily lives.

Mathematics is an application of matter and contributes to all of our methodical and systematic behaviours. It is mathematics for instance, that has brought order to the communities across this planet and prevented chaos and catastrophes many of our inherited human qualities are natured and developed by mathematics theories. Like our spatial awareness, our problem solving skill, our power to reason ( which involves calculated thinking ) and even our creativity and communication.



“ Day to day “or “daily” can also be used as an adverb, meaning every day. Daily life and every day life both might identify something that occurs every day, something regular. Everyday life could also be interpreted as something that is commonplace, usual or well known (to the pupils), and not necessarily something that occurs every day. Everyday life could also identify something that is suitable for, or used on, ordinary days, and herein is a connection to the complex and somewhat dangerous term of usefulness. We suggest that daily life could therefore be a more limited term than every life. In this paper, we mainly use the term day to day life. Another important, and related, term is “real life/world”.

## 2. Brief Story of mathematics:

Since Mathematics is abroad application of matter rather than a discovery, We cannot credit one person with the invention of mathematics itself; however, We can take a look back at when mathematics started to play a role in the life of human.

Unsurprisingly, evidences show that this was pretty much the beginning of as we know it! Even those living in Prehistoric times had some understanding of mathematics concepts, records of which were found on many items, like bones, and wall carving marking would have shown that they used rational thinking when learning how to solve simple mathematics problem like adding thing up on a surface area.

The Ishango bone is about 20,000 years old and has a series of notches carved into it in three columns. Patterns in these numbers in these numbers many show that they were made by someone who understood addition, subtraction, multiplication, division and prime number.

People understood geometry and algebra by about 2000BCE. Around this time, both the Babylonian and Ancient Egyptians were aware of the number  $\pi$  (pi) the ratio of a circle's circumference of its diameter. By about 1500 BCE the Babylonian were also aware of Pythagoras theorem, which show how the lengths of the sides of right angle triangles are related.

Keplers was also inspired by Pythagoras, and believed that the motion of the planets produces music. He used mathematics to show that the planet orbit the Sun in ellipse and by 1619, he was able to determine the time it takes each planet to orbit and their relative distance  $s$  from Sun. In 1687. Newton published his law of universal gravitation, this was ground breaking because it showed, not just that abstract mathematics principle, such as the newly invented calculus, could be applied to what we observe in nature, but that the responsible for the movement of the planets are also responsible for the movement of objects on earth. Newton also believed that the universal could be understood as a mathematical object, and described GOD as “skilled in mechanics and geometry” Newton's contemporary, Leibniz, discovered another link between mathematics and nature when he first considered the idea of fractals.

20<sup>th</sup> century mathematics, such as French mathematic Gaston Julia and Polish French American mathematician Benoit Mandelbrot, were inspired by Leibniz to create complicated fractals to their own.

By this time, quantum mechanics, and German Swiss American physicist Albert Einstein' theories of special and general relativity, had shown that nature obeys the law of mathematics, even when this contradicts our common sense understanding of the world.

## 3. What is mathematics?

We cannot answer this question at the spur of the moment .Most of the times many elucidations, explanations give an incomplete answer to this question.

Mathematics is the branch of science, which deals with numbers and their operations. It comprises calculations, computations, and solutions to the problems, drawing, maps, and pie charts etc. The Dictionary meaning of the word mathematics says that “It is the science of Numbers and space or Mathematics is the science of Measurements, quantity and magnitude”. It is exact, precise, systematic and logical subject.

Mathematics reveals hidden patterns that help us to understand the world around us. Now such more than Arithmetic and Geometry, Mathematics today is a discipline with diverse branches that deal with data, measurement and observation from science, with reference, deduction and proof and with Mathematical models of natural Phenomenon of Human behaviour and of social system.

#### **4. Importance of Mathematics in day to day life.:**

Mathematics is fundamentally important in an all pervasive ways, both at the workplace and for the individual citizen. Importance of Mathematics can be well understood by the definition given by Galileo Galilee .He defined Mathematics as, “ a language in which God has written the world.”. The literal meaning of Mathematics is “things which can be counted.” In our day to day life mathematics plays a vital and multiple role. Basically humans need every time the simple operations like addition, subtraction, multiplication, division, percentage etc. At Psychological level, mathematics helps people in developing an analytical talent of the Students and also helps in better organisation of Ideas. And an accurate expression of thoughts. Mathematics helps boosting our recreational activities. The activities like solving puzzles, computer games, chess, video games, cricket, hockey, kabadi, and basket ball etc. In such activities mathematical talents like reasoning, logical thinking, and aptitude are fully developed. We need to study Mathematics in the fields like Physics, chemistry, life sciences, Economics, Commerce and Trade, Social sciences, Architect, designing ,tailoring, carpentering, beauticians, sport person, Farming Conductor, drivers, cashiers, shopkeepers, musicians. Magicians etc.

Thing that you would not expect to bear any relation to mathematics do in fact come down to an under lying need for mathematics and the structure if bring to our day to day lives. Mathematics, everywhere when you consider the education and professional worlds. Whether you aspire to study sociology, psychology, physics, biology or even economics mathematics is held in high regard, and you will be called on solve various mathematics problems as part of your work. Since times immemorial people have been using mathematics and defining it in many ways. It is used in diverse fields of life such as natural science, engineering, arts, economics. In leading discoveries, applied mathematics has played a significant role. Some new disciplines also emerged out of this.

#### **5. There are many fields in which we can use Mathematics. For ex.**

1. Medical science 2.budget. 3. Shopping. 4. Construction or civil works 5.Grocery.6.coocking.
7. Visiting of Foreign countries. 8. Computing or calculating.

In the present era, teachers of mathematics have to teach mathematics through real concept and social life of a student. Our day to day life is full with mathematical applications. Whoever he/she may be either a cook, farmer, carpenter or a mechanic, shopkeeper or a doctor, an engineer or a scientist, musician everyone needs mathematics. Only human beings can apply Mathematics for day to day purposes knowingly or unknowingly everyone uses Mathematics. For ex. When we get up in the morning we see the time on watch, when we take brush to clean our mouth we see the dates of manufacturing and expiry. When we go in market we use simple mathematical operations for calculating. We thereby maintain a balance between our budget and purchase. We lend money or borrow money at that times we need to know the rules of simple and compound interest. When we go into the bank we come across different mathematical terms in the form of accountancy. In the previous days people did not make use of calculators because of its high prices.

But now a days its use has become a common factor.

The teachers in the present era should be able to teach their students mathematical concepts related or applicable to the day to day life such as :

1. Student should be able to use their knowledge of data analysis and mathematical modelling to understand social problems and workplace problems.
2. Should also use mathematics for explaining complex applications in the outside world.
3. Student should also recognise and use connections among mathematical ideas.

Mathematics provides an effective way of building mental discipline and encourage logical and mental rigor in addition mathematical knowledge plays a crucial role in understanding the content of other school subjects such as science, social studies and even, music and art.

### **Mathematics and Geometry in Our House**

Imagine that we plan to build our own house. We would first calculate volumes and dimensions, and gradually bring our designs to life plans. After completing construction, we would need to furnish the space. Here is how to carry out our project using geometry.

### **Mathematics in Health**

Human life in its earliest developmental stage can be seen in –utero using ultrasound. When the foetus is only slightly bigger than a bean, it can be visualised, and its heartbeat heard. Mathematics then comes into play in a child's health record, showing their estimated growth curve in relation to weight and height.

### **Mathematics in medicine**

Medicine has become increasingly reliant on mathematics in recent years, different equation and statistics have long played a role recent medical advances have involved the use of mathematics in new and exciting ways such as the role geometry and topology in:

- Modelling potential drug targets:
- Predicating cardiac defibrillation:
- Comparing human brains:
- Screening treatment for harmful side effects.

Professional in the medical field use math to determine proper doses for patients medicine read result from CAT scans, MRIs and X-rays and to evaluate body other in the medical industry use mathematics on a daily basis in hospital and office and when performing research, math plays a crucial role in health, as it allows for the safe ensure appropriate treatment and diagnoses.

### **6. Mathematics is used for many day to day activities as follows:**

- Awareness of time, reading clock, watch, planning one's routine.
- Cost accounting.
- Awareness of environment, nature, preservation of the same.
- Practical knowledge of ratio and proportion in domestic life also.
- Water use of conservation.
- Measurement of length, skill in transformation of cloth into clothes and other ideas indicated.
- Practical study of commercial Mathematics can be used as project at various levels
- This study is interesting in itself with shades of time and work, time and distance with more in depth analysis as below.

Fees, salary got calculated suitably for the person, post, work ethics, work involvement daily, weekly monthly compared with the international or

National or state standardization involves a good deal of mathematics though it may require some units of management and accounting which can be done effectively by a student of mathematics.

- Entertainment industry gaining ground in the economy also needs mathematics knowledge.
- Solving puzzles, riddles, construction of magic squares in general, data magic squares studied by Ramanujan, construction of problem of this type are all possible if, taste in mathematics is cultivated and practised.

### **7. Mathematics in a present world:**

The need to understand and be able to use mathematics in day to day life and in workplace has never been greater and will continue to increase. Knowing mathematics can be personally satisfying and empowering. The underpinning of every life are increasingly mathematical and technological. For instance, making purchasing decisions, choosing insurance or health plans, voting knowledgeably all call for quantitative sophistication.

Mathematics is one of the greatest cultural and intellectual achievements of human kind, citizen should have an appreciation and understanding of that achievement, including its aesthetic and even recreational aspects. Just as the level of mathematics needed for intelligent citizen has increased dramatically, so too has the level of mathematical thinking and problem solving needed in the workplace, in professional areas ranging from health care to graphic design.

In this changing world, those who understand and can do mathematical calculations will have significantly enhanced opportunities and options for shaping their futures. Mathematical competence opens doors to productive futures. A lack of mathematics competence keeps those doors closed. Generally it is an assumption that mathematics is only for the select few. On the contrary, every one needs to understand mathematics. All students should have the opportunity and the support necessary to learn significant mathematics with depth and understanding. There is no conflict between equity and excellence. Principles and standards call for a common foundation of mathematics to be learned by all students.

A society or a human society is a group of people related to each other through persistent relation, a large social grouping sharing the same geographical or virtual territory, subject to the same political, authority and dominant cultural expectations. More broadly, a society may be described as an economic, social, industrial infrastructure, made up of a varied collection of individuals.

Mathematics occupies a crucial and unique role in the human societies and represents a strategic key in the development of the whole mankind. The ability to compute, related to the power of technology and to the ability of social organisation and geometrical understanding of space time, that is the physical world and its natural patterns, show the role of mathematics in the development of a society. The society consists of its members, who make government and organize the natural resources to develop infrastructure. The human beings are the one who develop the society. Therefore; we will discuss the role mathematics in the development of an individual as well as the development of the society.

### **The most common jobs for mathematics graduates**

- Accountant
- Actuary
- Investment manager.
- Investment banker
- Retail banker
- Statistician
- Data analyst
- Data scientists
- Researcher (math)
- Teacher (math)
- Meteorologist
- Computer engineer

If you're seeking a career in finance, then some level of math qualification is required, but you may not necessarily need a degree. Aside from the financial sector, there are industries such as engineering and information technology that can benefit from someone who is good with numbers. For example, roles like defence and intelligence officer, statistician, operation researcher, academic mathematician, teacher of mathematics in a primary or secondary school or positions within the law, media, business or public sectors.

Some of your typical employers might be, the government, educational establishments, IT companies, a pharmaceuticals company, engineering companies, insurance companies, and banking and accountancy firms

### **Practically every career uses mathematics in some way**

Obviously, mathematicians and scientists rely on mathematical principles to do the most basic aspect of their work, such as test hypotheses. While scientific careers famously involve math, they are not the only careers to do so. Even operating a cash register requires that one understands basic arithmetic. People working in a factory must be able to do mental arithmetic to keep track of the parts on the assembly line and must, in some cases, manipulate fabrication software utilizing geometry properties (such as the dimension of a part) in order to build their products. Really, any job requires math because you pay check and balance your budget.

### **8. Mathematics is a universal language:**

Sure, it's mostly equation, numbers, and some Greek letters, but mathematics is understood the same virtually all over the world (and who knows, maybe all over the universe)! A mathematics equation does not need to be translated to another language to be understood by someone on the other side of the planet. A mathematical law does not change because someone has a different religion than you or speaks a different language from you.  $4 + 4 = 8$  in every single place on planet Earth. Pretty cool! The universality of math is one of the many things that makes it such a power tool and, indeed, essential life skill.

In summary, mathematics is not only important for success in life, it is around us. The laws of mathematics are evident throughout the world, including in nature, and the problem solving skills obtained from completing mathematics homework can help us tackle problems in other areas of life. While many may complain that mathematics is boring or complicated, the truth is that a life devoid of mathematics means that we go around experiencing the world on a much less interesting level than we could.

### **9. Impact of ICT on teaching –learning Mathematics:**

Modern technology can provide student with a new means experience mathematical concept. it is essential for everyone involved in teaching community to understand if these means affect and how they affect what student learn. Education need to know the realities and the possibilities for learning in the era of ICT .Because ICT can help them to (i) practice and consolidate number skill (ii) explore, describe and explain number patterns ; (iii) take their first steps in mathematics modelling by exploring interpreting and explaining patterns in data (iv) experiment with and discuss patterns in number and shape and space

### **10. The main uses of ICT in mathematics are:**

- The use of calculators for calculating purposes.
- Small programs, such as number games or investigations in a particular context;
- Programming languages, such as Logo or Basic, and the programming capabilities of graphical calculators;
- General-purpose software, particularly spreadsheets, but also databases;
- Content-free mathematics software, such as graph plotters, dynamic geometry software and data handling packages; tailored to the needs of individual pupils;
- Graphical calculators and data-loggers;
- CD-ROMs and the Internet.

They can successfully impart education characterized imparting instructions. collaborative learning ,multidisciplinary problem solving and promoting critical thinking skill as highlighted by National Curriculum framework (NCF 2005).



## 11. Conclusion:

- Mathematics in everyday life refers to the curriculum area with this same name, and to the connection with mathematics and everyday life
- Real life refers to the physical world outside the classroom
- Real life Daily life Everyday life
- Realistic Everyday mathematics School mathematics Outside world Real world
- Everyday life mainly refers to the same as real life, and we thereby do not distinguish between real-life connections' and connections between mathematics and everyday life or similar.
- Everyday mathematics" both refers to a curriculum, but also to a distinction between mathematics that is attained in everyday life and mathematics that is needed in everyday

Mathematics is used in our day to day life in multiple ways. Human beings cannot walk a single step without the use of mathematics. Mathematics has made human life easier to live. Mathematics helps the man to give exact interpretation to his ideas and conclusion. It is the numerical and calculation part of man's life and knowledge. It plays a predominant role on our every life and it has become an indispensable factor for the progress of our present day world. Moreover Mathematics makes man very accurate and precise with the use of devices like computer and calculators. It saves time and energy on a large scale..It develops strong will power ,patience, precision analytical, logical talent of the individual boosting the faculty of discovery and invention to a greater level.

Teacher can use Mathematical free software on internet for teaching. The use of ICT in Education, especially in difficult mathematics can make the teaching process more effective as well as enhance the students' capabilities in understanding basic concepts. Nevertheless, implementing its use in teaching is not without problems as numerous barriers may arise. The survey among the students and teachers will be conducted and a conclusion will be drawn.

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## **Hirshfeld Surface Analysis as a “Novel Tool” for Studying Intermolecular Interactions in Cu Catecholase Complexes: A Guiding Tool for Future Application (s)**

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### **Abstract:**

The present research reports the study of intermolecular secondary interactions in terms of hydrogen bonds or such interactions using a Cu (II) catechol system. The present group has initially reported and studied such Cu (II) for understanding the spin exchange coupling among paramagnetic Cu (II) centers. In light of such outcomes, such compounds are expected to have other applications viz. catalysis, drug delivery etc. However, the researchers are in search of a theoretical tool that would facilitate an initial screening for such proposed application and validation. Hirshfeld analyses is undertaken as such a tool to reveals some important secondary interactions within the complexes which initiates a train of thought for the possibility of utilising these complexes as potential drug carriers and for other relevant application. Selective compositions of same family of Cu (II) complex are examined for Hirshfeld surface analyses, wherein significant variability in the interactions can be observed by variable functionalization. Such, variability in terms of secondary interactions can be well implemented in guiding the functionality and application of such compounds.

**Keywords:** Hirshfeld Analyses, Cu (II) Catecholase, Secondary Interaction, Functionalization

### **1. Introduction & Literature Study:**

The chemical design of dinuclear Copper complexes has drawn immense attention from chemists because type III copper proteins, such as catechol oxidase, tyrosinase and methane monooxygenase, contain dinuclear copper centres in their active sites<sup>1</sup> and a detailed study of their magnetic property can help understand the factors that influence the spin-exchange coupling between the paramagnetic Copper (II) centres. By putting bio mimicking Cu Catecholase systems in focus of understanding the spin exchange coupling between paramagnetic Cu (II) centres [5]. S. Dasgupta et al have studied the making of such complexes, the coordination parameters like denticity, ligand associations, chelation etc. to design such antiferromagnetically coupled multi bridged Cu (II) Catecholase systems [6]. This is done by varying the “auxiliary” part of the complexes attached to the ligand backbone which is not necessarily a part of the complexation sphere. In another study, they explained the influence of solvent over the nuclearity of Cu (II) attained in the final product and its consequent effect over the Catecholase activity [6]. Another study conducted using Ni complexes which showed effective binding of such complexes with DNA, BSA, HSA in its octahedral conformation [7]. These studies show a potential for these systems to be used as potential drug delivery agents for which a clear understanding of their surrounding chemical environment needs to be analysed. In order to attain a deeper insight into the different interactions within the complexes whether intra

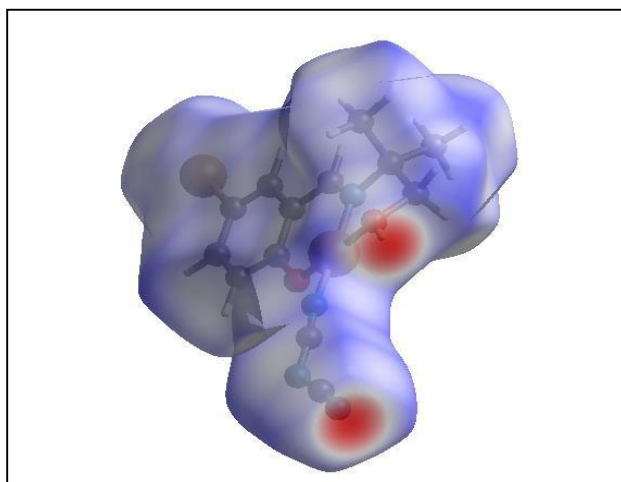


or inter, the utilisation of Hirshfeld surface analysis using Crystal Explorer 17.5 has been implemented. The analysis reveals some important secondary interactions within the complexes which initiates a train of thought for the possibility of utilising these complexes as potential drug carriers and for other relevant application.

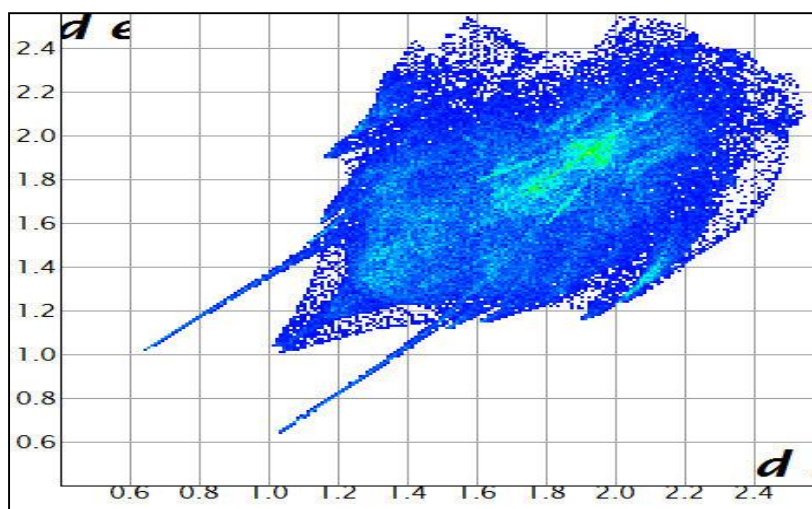
The widespread presence of NH and OH groups in proteins and nucleic acids have the potential to explain the different catalytic process, ligand binding, interaction with water solvent and other such parameters on bifurcation of strong and weak hydrogen bonding interactions [1]. Hydrogen bonding interactions involve a “donor-acceptor” mechanism of pairing that helps in eliminating to an extent the influence of aqueous solvent [2]. It is evident as such that a detailed study of these weak secondary interactions can give us a significant amount of data for coming to a conclusion of whether or not a system under study can be used as a drug carrier owing to the intra or intermolecular hydrogen bonding present within the system, which in turn can bind to proteins provided all other criteria and requirements are met. This viewpoint has been utilised in our study with the objective of choosing a “novel” methodology to study the secondary interactions present in three bio mimicking Cu Catecholase systems previously synthesized by S. Dasgupta et al. [3] which show structural and functional probability of a “drug carrier”, a major topic of research for our future analyses.

## 2. Discussion:

A very innovative and head on approach in studying and analysing crystal structures is done via the study of “Hirschfeld surfaces” using software called the “Crystal Explorer.” The key feature of this approach includes “the stockholder partitioning technique”, visual pattern recognition technique using “colour coded surfaces” for easy comprehension, and “complementary 2D mapping.” Speaking in layman’s terms, for proper visualisation of the scenario, a 3D surface is generated around a single asymmetric unit of the molecule under consideration [Fig 1]. The surface that is generated surrounds the asymmetric unit completely. The crystal under consideration is divided into regions based on different electron densities integrate to give us the entire 3D picture. In reality, these surfaces generated are triangular and the distances between molecules are calculated by using a line passing through the “centroid” of these triangular surfaces. The properties to be ascertained are considered by taking an average of the properties of the vertices of each triangle and thus it is evident that integration of properties plays an important role in this method [4]. Thus, various inter-molecular as well as intra-molecular interactions can be studied and analysed using this novel approach. Thus the distance to the nearest atom either interior or exterior to the surface can be obtained, types of interactions including the strength of such interactions can be obtained giving us enough information about certain properties of the crystals which in turn can help us to compare, categorise and if possible tune properties of crystals using the data obtained from such studies. For this particular review, we are going to focus mainly on the qualitative aspect of the analysis and leave aside the quantitative part for some other day. Our focus in this review is not in the construction of the Crystal Explorer 17.5 software (used to study Hirshfeld surfaces) itself but rather its application to the crystal systems under consideration. The surface as we have mentioned earlier is “colour coded” to indicate



**Figure 1.** Hirshfeld surface generated over a Schiff Base (the transparent surface generated shows the “ball and stick” molecule enclosed within) interactions based on the inter-nuclear distances and consequently strengths of these close contact points.

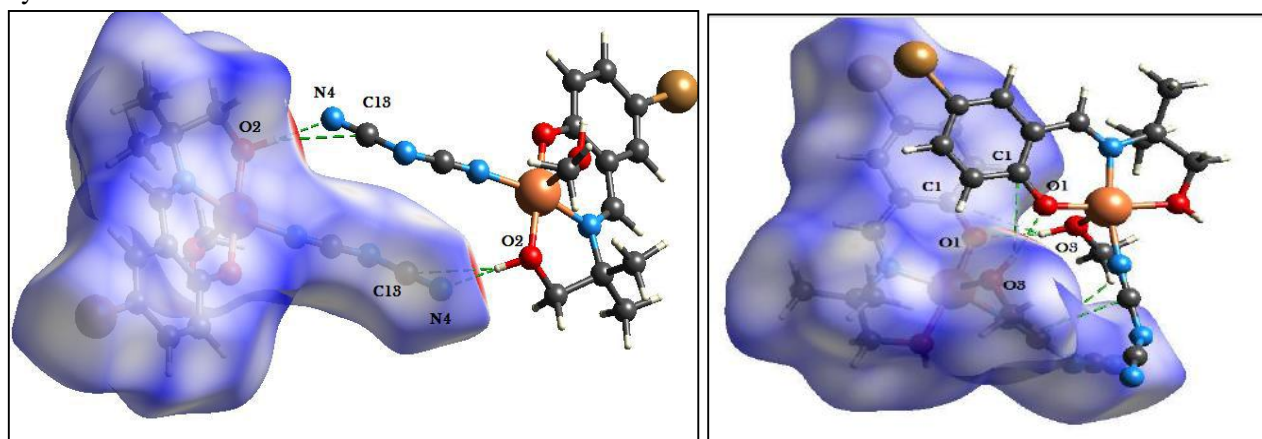


**Figure 2.** Corresponding 2D fingerprint plot

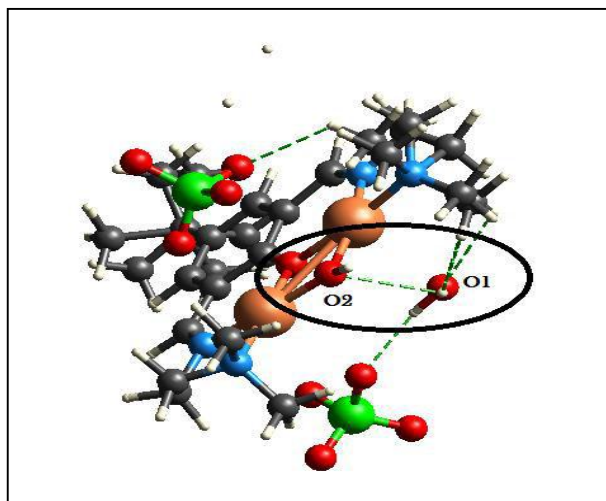
Atoms that are in close proximity compared to the other atoms present in the system give rise to a flat region on the Hirshfeld surface that is prominently red in colour. On one hand  $d_e$  is the distance between the Hirshfeld surface to the nearest nucleus in another molecule giving us an idea about the inter-molecular interactions), on the other hand  $d_i$  indicates distance from the surface to the nearest atom within the molecule itself. Thus we can say that each point on the surface has a well-defined ( $d_i$ ,  $d_e$ ) pair [4]. Where intermolecular contacts between atoms are closer than the sum of their van der Waals radii, these contacts will be highlighted in red on the  $d_{\text{norm}}$  surface, longer contacts are blue, and contacts around the sum of van der Waals radii are white [Fig 2]. The 2D fingerprint plot basically uses the  $d_i$  and  $d_e$  values by considering each ( $d_i$ ,  $d_e$ ) pair. Data is generally taken in the range of 0 to 3 Å and the area of each triangle in that range is added to the data. The axes  $d_e$  vs.  $d_i$  of the 2D plot gives a summary for the fraction of surface area covered by each of these interactions.

### 3. Results and Findings:

For instance, if we look at Complex 1 [ $\text{C}_{14}\text{H}_{17}\text{BrCuN}_4\text{O}_3$ ], two nearest neighbour short contact interaction between O and C were obtained, which otherwise goes unnoticed. The  $\text{C}_{13}$  of the dca extension showed a close contact interaction with the alcoholic  $\text{O}_2$ . Additionally, The  $\text{C}_1$  attached to  $\text{O}_1$  (phenolate) showed a another close contact interaction with  $\text{O}_3$  (methanolic). [Fig 3(a), 3(b)] Again, in complex 2 [ $\text{C}_{13}\text{H}_{13}\text{BrCuN}_4\text{O}_2$ ], using this technique, the already existing interactions were confirmed without attainment of any additional information. In complex 3 [ $\text{C}_{20}\text{H}_{36}\text{Cl}_2\text{Cu}_2\text{N}_4\text{O}_{11}$ ], we obtained a O-H...O type of Hydrogen bonding [ Fig 4]. This knowledge of the electronic environment of such complexes unlocks information and possibility of their further study and manipulation to design efficient drug delivery agents in the biological systems.



**Figure 3(a)** nearest neighbour short contact interaction between O and C ( $\text{C}_{13}$ ,  $\text{O}_2$ ) and (b) Hydrogen bonding observation: O...H-O ( $\text{O}_1$  acceptor,  $\text{O}_3$  donor) and nearest neighbour short contact interaction between O and C ( $\text{C}_1$ ,  $\text{O}_3$ )



**Figure 4.** The OH group shared by both the Cu atoms show a Hydrogen bond with the OH<sub>2</sub> group via an O-H...O type of linkage (O1 donor, O2 acceptor)

### Conclusions:

In a nutshell, the present study focuses the study on Hirshfeld Surface analyses of Cu (II) compounds. Study is focussed on three compounds of same family based on the variability of functionalization. Theoretically, it is established that, for a same family of Cu (II) system, the extend of secondary interactions and other type of binding are significantly different. Such finding enables an insight for an initial screening for effective application in un-attempted ventures not discussed or reported till date.

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An Insight towards Ionic and Electronic Conductivities for  
La-Sr-Co-Fe-O & Ba-Sr-Co-Fe-O -based Perovskites through  
"ab initio first principle" for Application in Ceramic Fuel  
and Electrolyser Cell Air Electrodes

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**Abstract:** Solid oxide cell (SOC) is considered as the most efficient energy conversion devices in renewable energy sector. It has the capability to get operated in dual modes viz. fuel cell and electrolyser cell thereby leading to maximum efficiency and minimum energy loss. The primary challenges in this arena is the choice of materials, compatibilities among the components, cyclability and long-term endurance at the high operating temperature. The present study intends to study the functionalization of cathode i.e. the air electrode since it suffers from delamination due to the localized strains within the electrolyte/electrode functional layer (LSM-YSZ) and electrode current collection layer for the cells using LSM as air electrode have been widely reported. The present group has already reported the synthesis and application of MIECs,  $\text{La}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_3$  (LSCF) and  $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_3$  (BSCF) based oxides as cathode in SOFC. The primary objective of the present study is to undertake the ab initio first principle studies to determine the density of states for pristine perovskites like  $\text{SrFeO}_3$ ,  $\text{BaFeO}_3$ ,  $\text{BaCoO}_3$  etc. The results are analysed in terms of density of states and orbital splitting guided by Linear combination of atomic orbital (LACO) theory. It is also observed from impedance studies that,  $R_0$  of LSCF is much smaller than that of BSCF in both operating temperature regime. This should be attributed to the presence of aliovalent substitution of  $\text{Sr}^{2+}$  in the A site of  $\text{La}^{3+}$  creating sufficient metal ion pairs of  $\text{Co}^{3+} / \text{Co}^{4+}$  and thus optimizing the disproportionation reactions of  $\text{Co}^{3+}$  rather than BSCF.

**Keywords:** Solid oxide cells; LCAO, Density of states; Cathode electrode, Impedance spectroscopy.

## 1. Introduction & Literature Study:

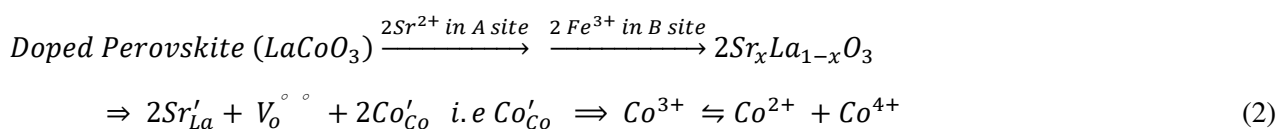
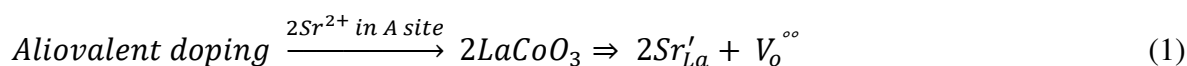
Solid oxide Cell (SOC) is considered as one of the most efficient energy conversation devices which can play the most vital part for a socio-economic development in near future [1-2]. Power generation technologies have significant potential to discover a future of sustainable energy without the emission of



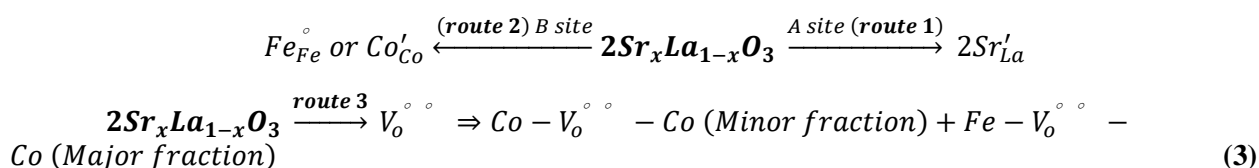
greenhouse gases by the utilization of renewable energy sources. In advanced energy conversion devices using Solid Oxide Cells (SOC's) play an important role both in Fuel Cell (SOFC) and Electrolyser Cell (SOEC). Fuels are fed to the fuel electrode in SOFC mode and in SOEC mode the reverse operation of the cell is done by connecting an external power supply across the cell to convert high temperature steam to hydrogen. Primarily, SOC's consist of a dense electrolyte conventionally yttria stabilized zirconia (YSZ), bridged between two porous electrodes Strontium doped Lanthanum Manganite (LSM) as air electrode and Nickel (Ni)-YSZ cermet as fuel electrode. The primary shortcomings associated with such Soc's are long term stability of the cell/stack, catalytic degradation of the electrodes, polarization losses and microstructural flaws. In the past few decades tremendous efforts have been devoted towards the development of the air electrode to suppress the delamination and degradation issues. Apart from the problems associated with all cell components, degradation in performance including delamination of the air electrode due to the localized strains within the electrolyte/electrode functional layer (LSM-YSZ) and electrode current collection layer for the cells using LSM as air electrode have been widely reported. The several shortcomings viz. degradation in cell performance arising out of the conventional air electrode are being addressed by employing newer functional perovskite based multicomponent mixed ionic and electronic conducting (MIEC) oxides with lower polarization losses. Significant studies are ongoing using  $\text{La}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_3$  (LSCF),  $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_3$  (BSCF),  $\text{Ba}_{1-x}\text{Co}_x\text{Fe}_y\text{Nb}_{1-y}\text{O}_3$  (BCFN),  $\text{Nd}_{0.6}\text{Sr}_{0.4}\text{CoO}_3$  (NSC) etc. where the oxygen reduction and evaluation reactions are regulated by oxygen diffusion and surface exchange [3-4]. Among the MIECs,  $\text{La}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_3$  (LSCF) and  $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_3$  (BSCF) based oxides have been widely reported as an efficient air electrode for SOC because of the extended triple phase boundary (TPB) for oxygen reduction or evaluation reaction through the bulk path [5-6]. However, these concepts are not well studied and established through direct measurement techniques viz. Impedance spectra, AC frequency perturbation or advanced Butler Volmer studies.

## 2. Objective, Results & Discussion :

Therefore, the primary objective of the present study is to undertake the ab initio first principle studies to determine the density of states for pristine perovskites like  $\text{SrFeO}_3$ ,  $\text{BaFeO}_3$ ,  $\text{BaCoO}_3$  etc. The results are analysed in terms of density of states and orbital splitting guided by Linear combination of atomic orbital (LACO) theory. Non-symmetry in the doped system restricts orbital splitting. The primary driving force for difference in functionality in LSCF and BSCF is based on charge compensation and hole creation due to aliovalent ( $\text{Sr}^{2+}$  in  $\text{La}^{3+}$ ) and isovalent ( $\text{Sr}^{2+}$  in  $\text{Ba}^{2+}$ ) substitutions.



Using Eq. 2, two simultaneous reactions can be highlighted as:

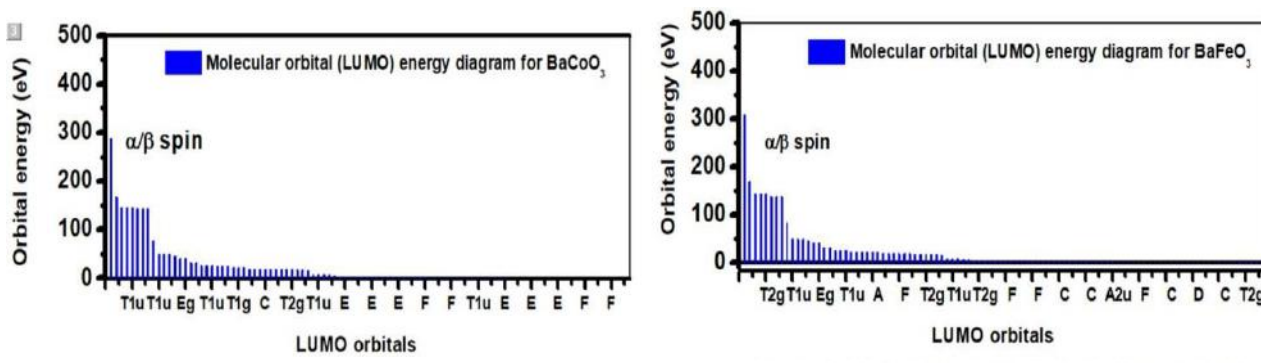


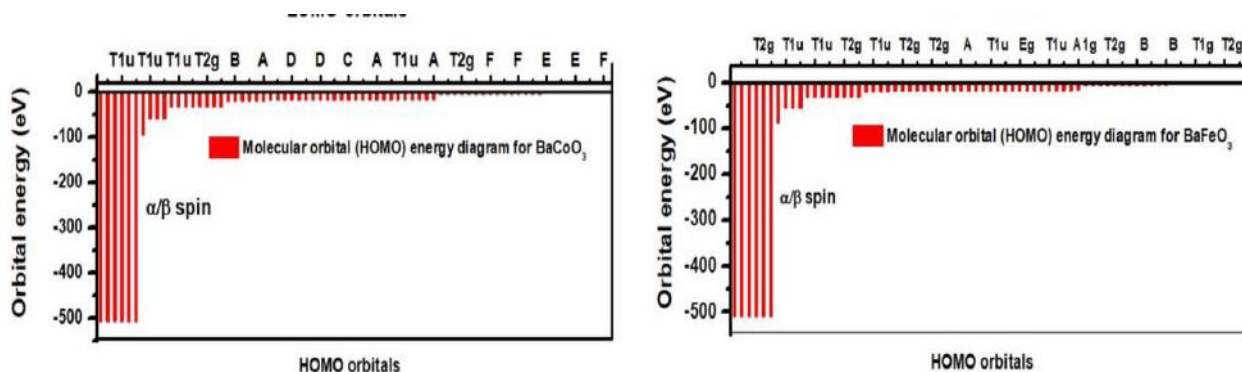
As expected, irrespective of the composition, the population density of participating metal orbitals is high in highest occupied molecular orbitals. Electronic structure is determined for pristine and doped perovskites using Gaussian 09 suite of quantum chemical program. Reaction mechanism involve simultaneous route 1, 2



and 3 wherein charge compensation proceeds through a  $e^-$  transfer and/or oxygen vacancy. For pristine system, irrespective of B-site element, incorporation of La and Sr tend to have more attractive/stable HOMO which results in much higher single point interactive energy of  $-23 \times 10^3$  eV compared to Ba based oxides ( $-21 \times 10^3$  eV). Incorporation of less penetrating  $f$  orbital in LUMO is more prevalent with La family after spitting degeneracy owing to which accelerated electronic conduction/MIEC behavior through ion pair is more pronounced in LSCF. The single point optimized energy for doped system is still higher compared to the pristine compositions which support further stability of the systems through loss in orbital degeneracy. However, during the computation of DOS, the doped systems are iterated and found to be devoid of any symmetry operation owing to which the splitted orbital degeneracy are all denoted to be of even singular symmetry (denoted by A). The lesser stabilization of BSCF system (low single point energy compared to LSCF) and presence to more screened orbitals at the LUMO level restricts the charge migration through aliovalency. However, as seen from the orbital plot of pristine  $\text{BaBO}_3$  and  $\text{SrBO}_3$  [B refers to either Co/Fe], the high energy LUMO is composed of single (odd or even symmetry), double and triple (A, B, C and T) symmetry orbitals (as shown in Figure 1) which are reported to be more compatible to be hybrid orbital thereby allowing relaxation of quantum selection rules. Owing to such fact, generation of oxygen vacancy and charge compensation is more probable. It is further noted that HOMO configuration for a perovskite oxide system is also same for Sr, La and Ba in terms of energy. However, the energy of LUMO is primarily governed by A site. In LSCF and BSCF, surprisingly the energy of LUMO is governed by La and Ba and not Sr. So, the deciding parameter for charge tunneling within the  $\text{ABO}_3$  and oxygen vacancy propagation within  $\text{BO}_6$  octahedra is governed by configuration of LUMO state.

The theoretical studies form the basis of understanding the functionality of LSCF and BSCF in terms of their better applicability as SOFC/SOEC air electrodes. In order to establish the efficacy of the MIEC perovskite as air electrode material in conjunction with the GDC interlayer impedance spectroscopic analysis have been carried out by using the symmetric cells of configuration in the temperature range of SOC operation ( $800^\circ\text{C}$ - $850^\circ\text{C}$ ). The electrode polarization losses involving the diffusion are primarily being represented in the lower frequency region wherein the higher frequency region attributed to the overall bulk impedance associated with electron transfer through grain interior and ion transfer process throughout defects in the grain boundaries. From the temperature dependent impedance analyses, it is further observed that with increase in temperature from 800 to  $850^\circ\text{C}$ , ohmic resistance ( $R_0$ ) and interfacial polarization resistance ( $R_p$ ) of BSCF electrode are found to reduce from  $8.94\Omega\cdot\text{cm}^2$  and  $0.22\Omega\cdot\text{cm}^2$  to  $6.86\Omega\cdot\text{cm}^2$  and  $0.17\Omega\cdot\text{cm}^2$  and the same  $R_0$  and  $R_p$  values of LSCF electrode are reduced from  $1.63\text{ohm}\cdot\text{cm}^2$  and  $0.02\text{ohm}\cdot\text{cm}^2$  to  $1.37\Omega\cdot\text{cm}^2$  and  $0.017\Omega\cdot\text{cm}^2$ . It is also observed that  $R_0$  of LSCF is much smaller than that of BSCF in both the temperature. This should be attributed to the presence of aliovalent substitution of  $\text{Sr}^{2+}$  in the A site of  $\text{La}^{3+}$  creating sufficient metal ion pairs of  $\text{Co}^{3+}/\text{Co}^{4+}$  and thus optimizing the disproportionation reactions of  $\text{Co}^{3+}$  rather than BSCF. The lower values of  $R_p$  for both the electrodes at  $800^\circ\text{C}$ - $850^\circ\text{C}$  dictates their effective application as an air electrode in conjunction with the GDC interlayer for SOCs. Irrespective of the temperature of operations, BSCF is found to have higher hydrogen flux because of the intrinsically higher charge transfer reaction for OER as indicated by the presence of higher oxygen vacancies in the reaction:  $\text{O}_2 + 2\text{V}_\text{o}^{\bullet\bullet} + 4e^- = 2\text{O}_\text{o}^{\times}$ .





**Figure 1.** Highest occupied and lowest unoccupied molecular orbitals for BaCoO<sub>3</sub> and BaFeO<sub>3</sub> as derived from ab initio first principle analyses

As also envisaged from the quantum chemistry calculations, the B site composition is also important, with the Co-rich compositions displaying faster kinetic coefficients than the Fe-rich compositions. For example, Cobalt-doping in BSCF decreases the energy for O-vacancy formation due to the proximity of the density of electronic states to the Fermi level, which facilitates easier reduction of Co<sup>4+</sup> to Co<sup>3+</sup> than Fe<sup>4+</sup> to Fe<sup>3+</sup> [7].

#### 4. Conclusions:

In a nutshell, it can be stated that, the present investigation reports the analyses of electronic structure of isovalent and aliovalent doped multicomponent perovskite oxides viz. La<sub>1-x</sub>Sr<sub>x</sub>Co<sub>y</sub>Fe<sub>1-y</sub>O<sub>3</sub> (LSCF), Ba<sub>1-x</sub>Sr<sub>x</sub>Co<sub>y</sub>Fe<sub>1-y</sub>O<sub>3</sub> (BSCF) system by means of ab initio first principle studies based on quantum calculation wherein the orbital splitting pattern is undertaken using linear combination of atomic orbitals (LCAO). The theoretical studies form the basis of understanding the functionality of LSCF and BSCF in terms of their better applicability as SOFC/SOEC air electrodes. It is observed that, in LSCF and BSCF, surprisingly the energy of LUMO is governed by La and Ba and not Sr. So, the deciding parameter for charge tunneling within the ABO<sub>3</sub> and oxygen vacancy propagation within BO<sub>6</sub> octahedra is governed by configuration of LUMO state. In conjunction with the theoretical studies, the efficacy of the MIEC perovskite as air electrode material in conjunction with the GDC interlayer impedance spectroscopic analysis have been carried out by using the symmetric cells of configuration in the temperature range of SOC operation (800°-850°C). It is also observed from impedance studies that, R<sub>0</sub> of LSCF is much smaller than that of BSCF in both operating temperature regime. This should be attributed to the presence of aliovalent substitution of Sr<sup>2+</sup> in the A site of La<sup>3+</sup> creating sufficient metal ion pairs of Co<sup>3+</sup> / Co<sup>4+</sup> and thus optimizing the disproportionation reactions of Co<sup>3+</sup> rather than BSCF. Therefore, the phenomena of ion conduction, associated polarization of air electrode (s) viz. LACF and BSCF is studied using a coherent theoretical and experimental finding.

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## THE UPPER TOTAL RESTRAINED GEODETIC DOMINATION NUMBER OF A GRAPH

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### **Abstract:**

A set  $S$  of vertices of a connected graph  $G$  is a restrained geodetic dominating set, if either  $S = V$  or  $S$  is a geodetic dominating set with the subgraph  $G[V - S]$  induced by  $V - S$  has no isolated vertices. The minimum cardinality of a restrained geodetic dominating set of  $G$  is called the restrained geodetic domination number and is denoted by  $\gamma_{gr}(G)$ . A total restrained geodetic dominating set  $S$  in a connected graph  $G$  is called a minimal total restrained geodetic dominating set of  $G$ , if no proper subset of  $S$  is a total restrained geodetic dominating set of  $G$ . The upper total restrained geodetic domination number  $\gamma_{grt}^+(G)$  is the maximum cardinality of a minimal total restrained geodetic dominating set of  $G$ . The upper total restrained geodetic domination number of certain classes of graphs are determined. It is shown that for every pair  $a, b$  of integers with  $3 \leq a \leq b$ , there exists a connected graph  $G$  such that  $\gamma_{grt}(G) = a$  and  $\gamma_{grt}^+(G) = b$ . Also, for every pair  $a, b$  of integers with  $3 \leq a \leq b$ , there exists a connected graph  $G$  such that  $\gamma_{grt}^+(G) = a$ . It is also shown that for any five integers  $a, b, c, d$  and  $e$  with  $2 \leq a \leq b \leq c \leq d \leq e$  there exists a connected graph  $G$  such that  $g(G) = a$ ,  $\gamma_g(G) = b$ ,  $\gamma_{gr}(G) = c$ ,  $\gamma_{grt}(G) = d$  and  $\gamma_{grt}^+(G) = e$ .

**Keywords** restrained geodetic dominating set, restrained geodetic domination number, upper total restrained geodetic dominating set, upper total restrained geodetic domination number.

AMS subject classification: 05C12.

### **1. Introduction:**

By a graph  $G = (V, E)$ , we mean a finite undirected connected graph without loops or multiple edges. The order and size of  $G$  are denoted by  $p$  and  $q$  respectively. For basic graph theoretic terminology, we refer [8,9]. The neighborhood of a vertex  $v$  is the set  $N(v)$  consisting of all vertices  $u$  which are adjacent with  $v$ . The closed neighborhood of a vertex  $v$  is the set  $N[v] = N(v) \cup \{v\}$ . A vertex  $v$  is an extreme vertex if the subgraph induced by its neighbors is complete. A vertex  $v$  is a semi-extreme vertex of  $G$  if the subgraph induced by its neighbors has a full degree vertex in  $N(v)$ . In Particular, every extreme vertex is a semi-extreme vertex and a semi-extreme vertex need not be an extreme vertex, we refer [10]. For vertices  $u$  and  $v$  in a connected graph  $G$ , the distance  $d(u, v)$  is the length of a shortest  $u - v$  path in  $G$ . A  $u - v$  path of length  $d(u, v)$  is called a  $u - v$  geodesic. A geodetic set of  $G$  is a set  $S \subseteq V(G)$  such that every vertex of  $G$  is contained in a geodesic joining some pair of vertices of  $S$ . The geodetic number  $g(G)$  of  $G$  is the minimum cardinality of its geodetic sets. The geodetic number of a graph was introduced in [10,12].

A *dominating set* in a graph  $G$  is a subset of vertices of  $G$  such that every vertex outside the subset has neighbor in it. The size of a minimum dominating set in a graph  $G$  is called the *domination number* of  $G$  and is denoted by  $\gamma(G)$ . A *geodetic dominating set* of  $G$  is a subset of  $V(G)$  which is both geodetic and dominating set of  $G$ . The minimum cardinality of a geodetic dominating set is a *geodetic domination number* and is denoted by  $\gamma_g(G)$ . The geodetic domination number of a graph was introduced in [12]. A set  $S$  of vertices of a connected graph  $G$  is a *restrained geodetic dominating set*, if either  $S = V$  or  $S$  is a geodetic dominating set with the subgraph  $G[V - S]$  induced by  $V - S$  has no isolated vertices. The minimum cardinality of a restrained geodetic dominating set of  $G$  is called the *restrained geodetic domination number* and is denoted by  $\gamma_{gr}(G)$ , we refer [1].

The following Theorems will be used in sequel.

**Theorem 1.1.** [1]. Each extreme vertex of a connected graph  $G$  belongs to every restrained geodetic dominating set of  $G$ .

**Theorem 1.2.** [1]. Every restrained geodetic dominating set of a connected graph  $G$  contains its semi-extreme vertex of  $G$ .

**Theorem 1.3** [1]. For a complete graph  $K_p$  ( $p \geq 2$ ),  $\gamma_{gr}^+(K_p) = p$ .

Throughout the following  $G$  denotes a connected graph with at least two vertices.

## 2. The Upper Total Restrained Geodetic Domination Number of a Graph:

**Definition 2.1.** A total restrained geodetic dominating set  $S$  in a connected graph  $G$  is called a *minimal total restrained geodetic dominating set* of  $G$ , if no proper subset of  $S$  is a total restrained geodetic dominating set of  $G$ . The *upper total restrained geodetic domination number*  $\gamma_{grt}^+(G)$  is the maximum cardinality of a minimal total restrained geodetic dominating set of  $G$ .

**Example 2.2.** For the graph  $G$  given in Figure 2.1,  $S_1 = \{v_1, v_2, v_3, v_6, v_7\}$  is a minimum total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}(G) = 5$ . The set  $S_2 = V(G) - \{v_7, v_8\}$  is a minimal total restrained geodetic dominating set of  $G$ , so that  $\gamma_{grt}^+(G) \geq 7$ . It is easily verified that no eight elements set of  $G$  is a total restrained geodetic dominating set of  $G$ . Hence  $\gamma_{grt}^+(G) = 7$ .

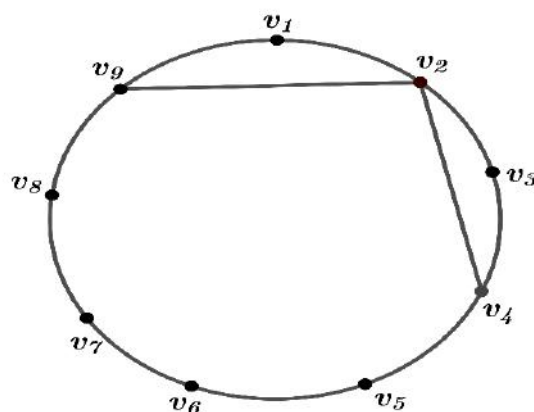


Figure 2.1: A graph  $G$  with  $\gamma_{grt}^+(G) = 7$

**Theorem 2.3.** Each extreme vertex of a connected graph  $G$  belongs to every minimal total restrained geodetic dominating set of  $G$ .

**Proof.** This follows from Theorem 1.1

**Theorem 2.4.** Each semi-extreme vertex of a connected graph  $G$  belongs to every minimal total restrained geodetic dominating set of  $G$ .

**Proof.** This follows from Theorem 1.2.

**Theorem 2.5.** Let  $G$  be a connected graph of order  $p$ . If  $G$  has a semi-extreme vertex of order  $p$  then  $\gamma_{grt}^+(G) = p$ .

**Proof.** If  $G$  has a semi-extreme vertex of order  $p$  and by Theorem 2.4, it belongs to every minimal total restrained geodetic dominating set. The result follows.

**Theorem 2.6.** If  $G$  is a connected graph with extreme vertices and if the set  $S$  of all extreme vertices is a total restrained geodetic dominating set of  $G$  then  $\gamma_{grt}(G) = \gamma_{grt}^+(G)$ .

**Proof.** Suppose that  $G$  is a graph with extreme vertices and the set of all extreme vertices forms a total restrained geodetic dominating set of  $G$ . Since any minimal total restrained geodetic dominating set of  $G$  contains all the extreme vertices, it follows that the minimum total restrained geodetic dominating sets are nothing but the minimal total restrained geodetic dominating sets. Hence  $\gamma_{grt}(G) = \gamma_{grt}^+(G)$ .

**Theorem 2.7.** Let  $G$  be a connected graph with cut-vertices and let  $S$  be a minimal total restrained geodetic dominating set of  $G$ . If  $v$  is a cut-vertex of  $G$ , then every component of  $G - v$  contains an element of  $S$ .

**Proof.** Let  $v$  be a cut-vertex of  $G$  and  $S$  be a minimal total restrained geodetic dominating set of  $G$ . Suppose there is a component  $G_1$  of  $G - v$  such that  $G_1$  contains no vertices of  $S$ . By Theorem “Let  $v$  be a cut-vertex of a connected graph  $G$ , and let  $u$  and  $w$  be vertices in distinct components of  $G - v$ , then  $v$  lies on every  $u - w$  path in  $G$ ”,  $G_1$  contains at least one vertex, say  $u$ . Since  $S$  is a minimal total restrained geodetic dominating set, there exist vertices  $x, y \in S$  such that  $u$  lies on the  $x - y$  geodesic path  $P: x = u_0, u_1, \dots, u_t = y$  in  $G$ . Let  $P_1$  be a  $x - u$  subpath of  $P$  and  $P_2$  be a  $u - y$  subpath of  $P$ . Since  $v$  is a cut-vertex of  $G$ , both  $P_1$  and  $P_2$  contain  $v$  so that  $P$  is not a path, which is a contradiction. Thus, every component of  $G - v$  contains an element of  $S$ .

**Theorem 2.8.** For any connected graph  $G$ ,  $3 \leq \gamma_{grt}(G) \leq \gamma_{grt}^+(G) \leq p$ .

**Proof.** A total restrained geodetic dominating set needs at least three vertices and so  $\gamma_{grt}(G) \geq 3$ . Since every minimal total restrained geodetic dominating set is a total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}(G) \leq \gamma_{grt}^+(G)$ . Also, since  $V(G)$  is a total restrained geodetic dominating set of  $G$ , it is clear that  $\gamma_{grt}^+(G) \leq p$ . Thus  $3 \leq \gamma_{grt}(G) \leq \gamma_{grt}^+(G) \leq p$ .

**Theorem 2.9.** For any connected graph  $G$ ,  $\gamma_{grt}(G) = p$  if and only if  $\gamma_{grt}^+(G) = p$ .

**Proof.** Let  $\gamma_{grt}^+(G) = p$ . Then  $S = V(G)$  is the unique minimal total restrained geodetic dominating set of  $G$ . Since no proper subset of  $S$  is a total restrained geodetic dominating set, it is clear that  $S$  is the minimum total restrained geodetic dominating set of  $G$  and so  $\gamma_{grt}(G) = p$ . The converse follows from Theorem 2.9.

**Theorem 2.10.** For a complete graph  $K_p (p \geq 2)$ ,  $\gamma_{grt}^+(K_p) = p$ .

**Proof.** This follows Theorem 1.3 and Theorem 2.9.

**Theorem 2.11.** Let  $G$  be a connected graph of order  $p$  and  $u \in V(G)$ . If  $\deg(u) = 1$  then  $\gamma_{grt}^+(G - u) \leq \gamma_{grt}^+(G)$ .

**Proof.** Let  $u \in V(G)$  and  $\deg(u) = 1$ . Let  $S$  be a minimal total restrained geodetic dominating set of  $G - u$  with maximum cardinality, so that  $\gamma_{grt}^+(G) = |S|$ . Since  $\deg(u) = 1$ ,  $u$  is an end vertex and  $u$  adjacent to exactly one vertex, say  $v$ . By Theorem 2.3, every minimal total restrained geodetic dominating set of  $G$  contains  $u$ . We consider two cases.



**Case (i).** Let  $v \in S$ . Since  $S$  is a total restrained geodetic dominating set of  $G - u$ , there exists a vertex  $w \in V(G - u)$  such that  $w \in I[v, x] \subseteq I[S]$ ,  $w \in N(S)$  and  $d(v, x) \leq 3$ . If  $d(v, x) = 3$ , then consider the set  $S_1 = S - \{v\} \cup \{u, w\}$ . If  $d(v, x) \leq 2$  then consider the set  $S_2 = S - \{v\} \cup \{u\}$ . It is straightforward to verify that  $S_1$  is a minimal total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}^+(G - u) = |S| \leq |S_1| \leq \gamma_{grt}^+(G)$ .

**Case (ii).** Let  $v \notin S$ . Then consider the set  $S_1 = S \cup \{u\}$ . It is straight forward to verify that  $S_1$  is a minimal total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}^+(G - u) = |S| \leq |S_1| \leq \gamma_{grt}^+(G)$ . Hence in both cases,  $\gamma_{grt}^+(G - u) \leq \gamma_{grt}^+(G)$ .

**Theorem 2.12.** Let  $G$  be a connected graph of order  $p$  with  $\gamma_{grt}(G) \leq p - 2$ . Then  $\gamma_{grt}^+(G) = p - 2$ .

**Proof.** Given  $\gamma_{grt}(G) = p - 2$ . By Theorem 2.8,  $\gamma_{grt}^+(G) \geq p - 2$ , therefore  $\gamma_{grt}^+(G)$  is either  $p$  or  $p - 2$ . If  $\gamma_{grt}^+(G) = p$  then by Theorem 2.9,  $\gamma_{grt}(G) = p$  which is a contradiction. Therefore  $\gamma_{grt}^+(G) = p - 2$ .

**Theorem 2.13.** For the connected graph  $G$  of order  $p$ , the following are equivalent

- (i)  $\gamma_{grt}^+(G) = p$
- (ii)  $\gamma_{grt}(G) = p$
- (iii)  $G = K_p$

**Proof.** (i)  $\Rightarrow$  (ii). Let  $\gamma_{grt}^+(G) = p$ . Then  $S = V(G)$  is the unique minimal total restrained geodetic dominating set of  $G$ . Since no proper subset of  $S$  is a total restrained geodetic dominating set of  $G$ , it is clear that  $S$  is the unique minimum total restrained geodetic dominating set of  $G$  and so  $\gamma_{grt}(G) = p$ .

(ii)  $\Rightarrow$  (iii). Let  $\gamma_{grt}(G) = p$ . If  $G \neq K_p$ , then by Theorem 2.10,  $\gamma_{grt}(G) \leq p - 2$ , which is a contradiction. Therefore  $G = K_p$ .

(iii)  $\Rightarrow$  (i). Let  $G = K_p$ . Then by Theorem 2.9,  $\gamma_{grt}^+(G) = p$ .

**Theorem 2.14.** For a connected graph  $G$ ,  $2 \leq g(G) \leq \gamma_g(G) \leq \gamma_{gr}(G) \leq \gamma_{grt}(G) \leq \gamma_{grt}^+(G) \leq p$ .

**Proof.** A geodetic set needs at least two vertices and therefore  $g(G) \geq 2$ . Also, every geodetic dominating set is a geodetic set of  $G$  and so  $g(G) \leq \gamma_g(G)$ . If  $\gamma_g(G) = p$  or  $p - 1$  then  $\gamma_{gr}(G) = p$ . The complement of each restrained geodetic dominating set has cardinality different from 1 we have  $\gamma_{gr}(G) \neq p - 1$ . Hence  $\gamma_{gr}(G) = p$ . Also, since every restrained geodetic dominating set of  $G$  is a geodetic dominating set of  $G$  and then  $\gamma_g(G) \leq \gamma_{gr}(G)$ . Also, since every total restrained geodetic dominating set of  $G$  is a restrained geodetic dominating set of  $G$  so that  $\gamma_{gr}(G) \leq \gamma_{grt}(G)$ . Also, every minimal total restrained geodetic dominating set is a total restrained geodetic dominating set of  $G$ , but the converse is not true and therefore  $\gamma_{grt}(G) < \gamma_{grt}^+(G)$ . Also, since  $V(G)$  is a total restrained geodetic dominating set of  $G$ , it is clear that  $\gamma_{grt}^+(G) \leq p$ . It follows that  $2 \leq g(G) \leq \gamma_g(G) \leq \gamma_{gr}(G) \leq \gamma_{grt}(G) \leq \gamma_{grt}^+(G) \leq p$ .

### 3. Realization results:

**Theorem 2.15.** For every pair  $a, b$  of integers with  $3 \leq a \leq b$ , there exists a connected graph  $G$  such that  $\gamma_{grt}(G) = a$  and  $\gamma_{grt}^+(G) = b$ .

**Proof.** Let  $K_{2, b-a+2}$  be the complete bipartite graph with partite sets,  $X = \{x_1, x_2\}$  and  $Y = \{y_1, y_2, \dots, y_{b-a+2}\}$ . Let  $P: u, v, w$  be a path of order 3. Let  $H_1$  be the graph obtained from  $K_{2, b-a+2}$  and  $P$  by joining  $u$  with the vertex  $x_2$ . Let  $G$  be the graph obtained from  $H_1$  by adding a set of  $a - 5$  new

vertices  $v_i$  ( $1 \leq i \leq a-5$ ) and join each  $v_i$  ( $1 \leq i \leq a-5$ ) with the vertex  $w$ . The resulting graph  $G$  is given in Figure 2.2.

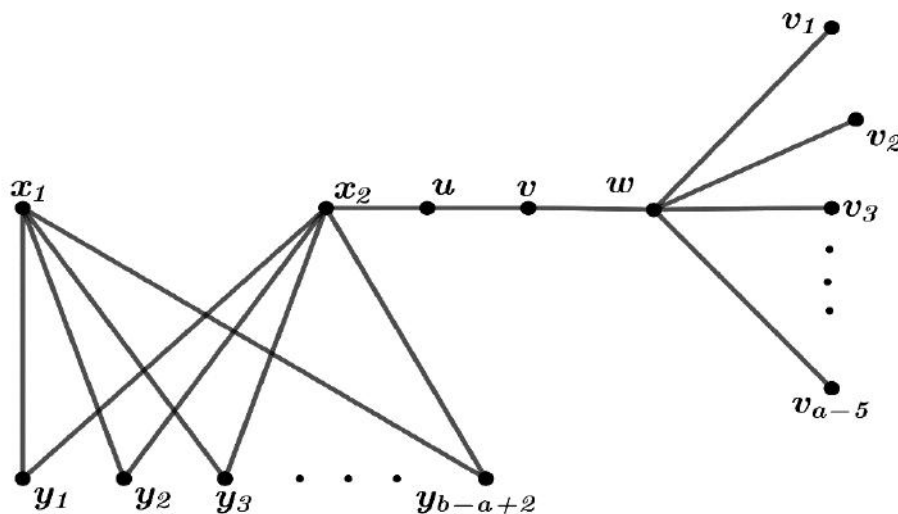


Figure 2.2: A graph  $G$  with  $\gamma_{grt}(G) = a$  and  $\gamma_{grt}^+(G) = b$

Let  $S = \{v_1, v_2, v_3, \dots, v_{a-5}\}$  be the set of all extreme vertices of  $G$ . By Theorem 2.3,  $S$  is the subset of every geodetic set, geodetic dominating set, restrained geodetic dominating set, total restrained geodetic dominating set and minimal total restrained geodetic dominating set of  $G$  and it is not a geodetic set of  $G$ . It is shown that  $S_1 = S \cup \{x_1, y_1, u, v, w\}$  is a minimum total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}(G) = a-5+5 = a$ . Now, we seen that  $S_2 = S \cup \{x_1, x_2, y_1, y_2, y_3, \dots, y_{b-a+2}, w\}$  is a minimal total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}^+(G) = a-5+3+b-a+2 = b$ .

**Theorem 2.16.** For every pair  $a, b$  of integers with  $3 \leq a \leq b$ , there exists a connected graph  $G$  such that  $\gamma_{grt}^+(G) = a$ .

**Proof.** Let  $K_{2,2}$  be a complete bipartite graph with partite sets,  $X = \{x_1, x_2\}$  and  $Y = \{y_1, y_2\}$ . Let  $P: v_1, v_2, v_3, \dots, v_a$  be a path of order  $a$ . Let  $H_1$  be the graph obtained from  $K_{2,2}$  and  $P$  and join  $v_1$  with the vertex  $x_2$ . Let  $G$  be the graph obtained from  $H_2$  by adding two sets of new vertices  $u_i$  ( $1 \leq i \leq b$ ) and  $w_i$  ( $1 \leq i \leq c-b$ ) and join each  $u_i$  ( $1 \leq i \leq b$ ) with the vertex  $v_a$  and join each  $w_i$  ( $1 \leq i \leq c-b$ ) with the vertices  $v_2$  and  $v_4$ . The resulting graph  $G$  is given in Figure 2.3.

Let  $S = \{u_1, u_2, u_3, \dots, u_b\}$  be the set of all extreme vertices of  $G$ . By Theorem 2.3,  $S$  is the subset of every geodetic set, geodetic dominating set, restrained geodetic dominating set, total restrained geodetic dominating set and minimal total restrained geodetic dominating set of  $G$  and it is not a geodetic set of  $G$ . It is shown that  $S_1 = S \cup \{x_1, x_2, y_1, y_2, v_1, v_2, v_3, v_4, v_7, \dots, v_{a-2}, u_1, u_2, u_3, \dots, u_b, w_1, w_2, w_3, \dots, w_{c-b}\}$  is a minimal total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}^+(G) = b+a-c+c-b = a$ .

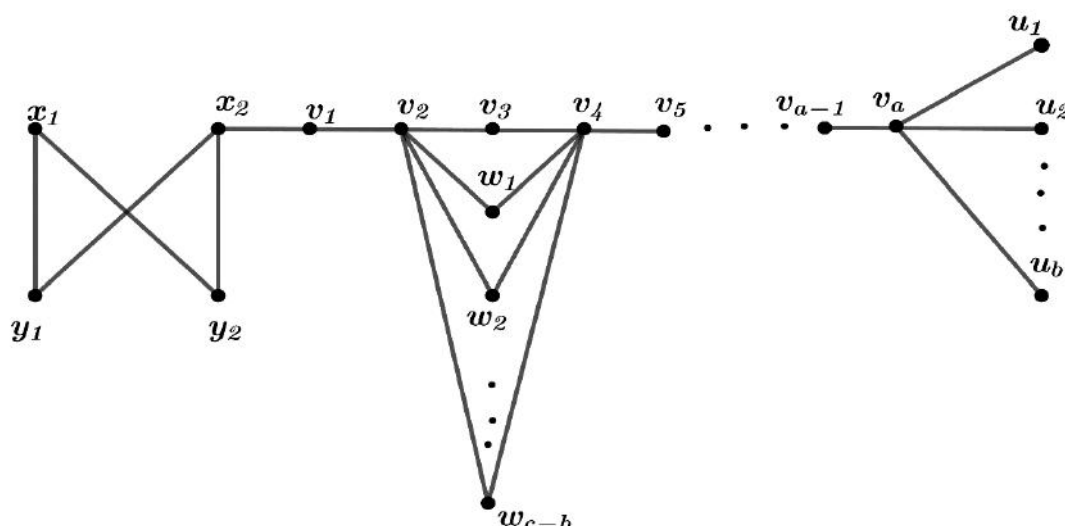


Figure 2.3: A graph  $G$  with  $\gamma_{grt}^+(G) = a$

**Theorem 2.17.** For any five integers  $a, b, c, d$  and  $e$  with  $2 \leq a \leq b \leq c \leq d \leq e$ , there exists a connected graph  $G$  such that  $g(G) = a$ ,  $\gamma_g(G) = b$ ,  $\gamma_{gr}(G) = c$ ,  $\gamma_{grt}(G) = d$  and  $\gamma_{grt}^+(G) = e$ .

**Proof.** Case (i).  $2 < a < b < c < d < e$ . Let  $|V(G) - k| = e$ .

Let  $K_{2,c-b}$  be a complete bipartite graph with partite sets,  $X = \{x_1, x_2\}$  and  $Y = \{y_1, y_2, \dots, y_{c-b}\}$ . Let  $P: u_1, u_2, u_3, \dots, u_b$  be a path of order  $b$ . Let  $H_1$  be the graph obtained from  $K_{2,c-b}$  and  $P$  by joining the vertices  $u_1$  and  $x_2$ . Let  $G$  be the graph obtained from  $H_1$  by adding a set of  $a-1$  new vertices  $z_i$  ( $1 \leq i \leq a-1$ ) and join each  $z_i$  ( $1 \leq i \leq a-1$ ) with the vertex  $u_b$ . The resulting graph  $G$  is given in Figure 2.4.

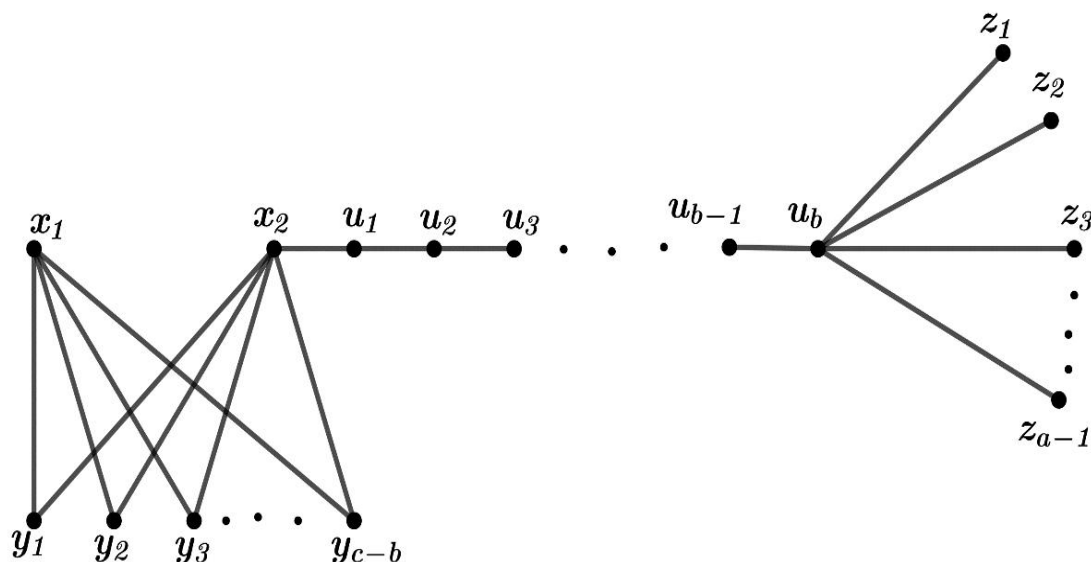


Figure 2.4: A graph  $G$  with case (i) of Theorem 2.17

Let  $S = \{z_1, z_2, z_3, \dots, z_{a-1}\}$  be the set of all extreme vertices of  $G$ . By Theorem 2.3,  $S$  is the subset of every geodetic set, geodetic dominating set, restrained geodetic dominating set total restrained geodetic dominating set and minimal total restrained geodetic dominating set of  $G$  and it is not a geodetic set of  $G$ . Clearly  $S_1 = S \cup \{x_1\}$  is a minimum geodetic set of  $G$  so that  $g(G) = a-1 + 1 = a$ . Also, it is clear that  $S_2 = S_1 \cup \{u_1, u_4, \dots, y_{b-2}\}$  is a minimum geodetic dominating set of  $G$  so that  $\gamma_g(G) = a + b - a =$

$b$  and  $S_2$  is also a minimum restrained geodetic dominating set of  $G$  so that  $\gamma_{gr}(G) = b = c$ . Now, we observe that  $S_3 = S_2 \cup \{y_1, u_2, u_5, \dots, u_{b-3}\}$  is a minimum total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}(G) = c + d - c = d$ . Also, it is easily verified that  $S_4 = V(G) - \{u_1, u_2, u_7, u_8, u_{13}, \dots, u_{b-1}, u_b\}$  is a minimal total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}^+(G) = |V(G) - k| = e$ .

**Case (ii).**  $2 < a + 1 = b < c = d < e$ , let  $|V(G) - 2| = e$

Consider the cycle  $C_4 : v_1, v_2, v_3, v_4, v_1$ . Let  $H_1$  be the graph obtained from  $C_4$  by adding a path  $P : u_1, u_2, u_3, u_4$  and join the vertices  $u_1$  and  $v_2$ . Let  $G$  be the graph obtained from  $H_1$  by adding two sets of new vertices  $w_i$  ( $1 \leq i \leq a - 2$ ) and  $z_i$  ( $1 \leq i \leq c - b - 1$ ) and join each  $w_i$  ( $1 \leq i \leq a - 2$ ) with the vertex  $u_4$  and join each  $z_i$  ( $1 \leq i \leq c - b - 1$ ) with the vertices  $v_1$  and  $v_4$ . The resulting graph  $G$  is given in Figure 2.5.

Let  $S = \{w_1, w_2, w_3, \dots, w_{a-2}\}$  be the set of all extreme vertices of  $G$ . By Theorem 2.3,  $S$  is the subset of every geodetic set, geodetic dominating set, restrained geodetic dominating set, total restrained geodetic dominating set and minimal total restrained geodetic dominating set of  $G$  and it is not a geodetic set of  $G$ . Clearly  $S_1 = S \cup \{v_1, v_3\}$  is a minimum geodetic set of  $G$  so that  $g(G) = a - 2 + 2 = a$ . Also, it is clear that  $S_2 = S_1 \cup \{u_2\}$  is a minimum geodetic dominating set of  $G$  so that  $\gamma_g(G) = a + 1 = b$ . Now, we observe that  $S_3 = S_2 \cup \{v_4, z_1, z_2, z_3, \dots, z_{c-b-1}\}$  is a minimum restrained geodetic dominating set of  $G$  so that  $\gamma_{gr}(G) = b + c - b - 1 + 1 = c$  and  $S_3$  is also a minimum total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}(G) = c = d$ . Now, it is easily verified that  $S_4 = V(G) - \{u_2, u_3\}$  is a minimal total restrained geodetic dominating set of  $G$  so that  $\gamma_{grt}^+(G) = |V(G) - 2| = e$ .

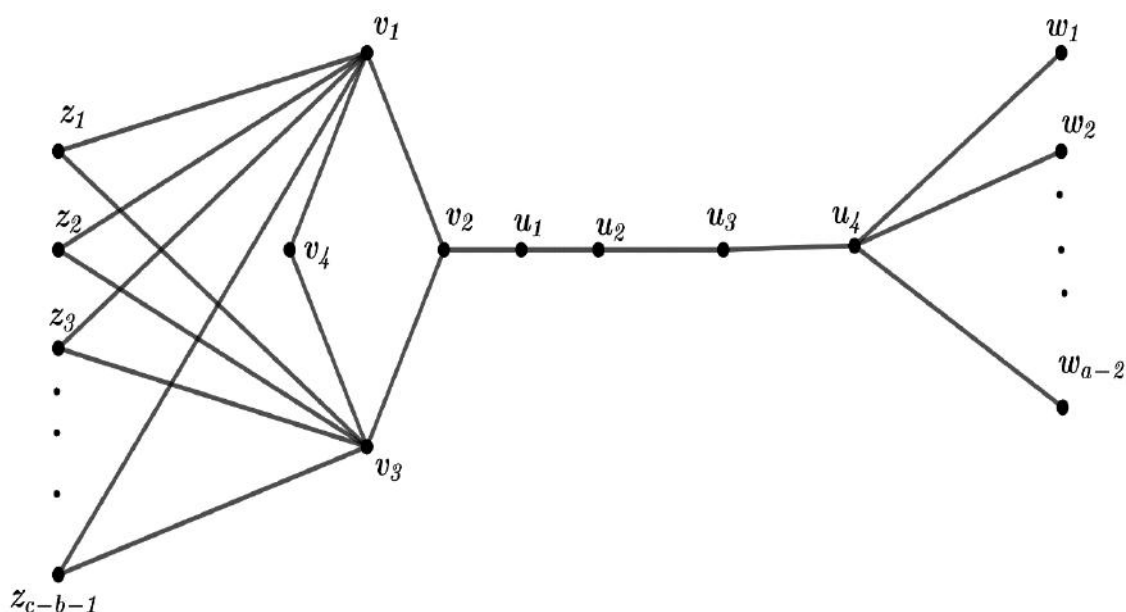


Figure 2.5: A graph  $G$  with case (ii) of Theorem 2.17

## 4. Conclusion:

Every communication network can be demonstrated by the help of connected graphs. This work can be used to upgrade the different communication networks. We can extend this concept to define forcing total restrained geodetic domination number, forcing connected total restrained geodetic domination number and so on.

## Declaration.

I hereby declare that the above information is correct and true to the best of my knowledge and belief.

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## International E-Conference on Science, Engineering & Technological Innovation

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Automation, Computer Science and Technology Department,  
Kryvyi Rih National University, Ukraine and 'Research Culture Society'.

# Total Outer Independent Geodetic Domination Number of a Graph

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**Abstract:** In this paper we learn the new idea of total outer independent geodetic domination number of a graph. A geodetic set  $R \subseteq V$  is said to be total outer independent geodetic dominating set [TOIGDS] if it is a total geodetic dominating set and  $\langle V - R \rangle$  is an independent set. The minimum cardinality of a total outer independent geodetic dominating set, denoted by  $\gamma_{gt}^{oi}(G)$  is called the total outer independent geodetic domination number of  $G$ . We look over the total outer independent geodetic domination number of some standard graphs. It is shown that for every couple of integers  $m, n$  with  $2 \leq m \leq n$  and  $n \geq 2$ , there exists a connected graph  $G$  such that  $\gamma_g(G) = m$  and  $\gamma_{gt}^{oi}(G) = n$ .

**AMS subject classification:** 05C12.

**Keywords:** geodetic number, independent geodetic number, total outer independent geodetic number, total outer independent geodetic domination number.

## 1. Introduction :

By a graph  $G = (V, E)$ , we denote a finite undirected graph in the absence of loops or multiple lines. The order and size of  $G$  are denoted by  $p$  and  $q$  consecutively. For basic graph theoretic expressions we refer to Harary [3, 9]. The distance  $d(a, b)$  between two points  $a$  and  $b$  in a connected graph  $G$  is the length of a shortest  $a - b$  path in  $G$ . An  $a - b$  path of length  $d(a, b)$  is known as  $a - b$  geodesic. A point  $u$  is said to lie on a  $a - b$  geodesic  $Q$  if  $u$  is a point of  $Q$  including the points  $a$  and  $b$ . The eccentricity  $e(x)$  of a point  $x$  in  $G$  is the maximum distance from  $x$  and a point of  $G$ . The minimum eccentricity among the points of  $G$  is the radius,  $rad G$  or  $r(G)$  and the maximum eccentricity is the diameter,  $diam G$  of  $G$ . A geodetic set of  $G$  is a set  $R \subseteq V(G)$  such that every point of  $G$  is contained in a geodesic joining some couple of points in  $R$ . The geodetic number  $g(G)$  of  $G$  is the minimum order of its geodetic sets and any geodetic set of order  $g(G)$  is a geodetic basis. The geodetic number of a graph was introduced in [10] and further studied in [5, 12].  $N(x) = \{y \in V(G) : xy \in E(G)\}$  is called the neighborhood of the point  $x$  in  $G$ . For any set  $N$  of points of  $G$ , the induced subgraph  $\langle N \rangle$  is the maximal subgraph of  $G$  with point set  $N$ . A vertex  $x$  is a extreme vertex of a graph  $G$  if  $\langle N(x) \rangle$  is complete. A point in a graph  $G$  dominates itself and its neighbours. A set of points  $B$  in a graph  $G$  is a dominating set if each point of  $G$  is dominated by some point of  $B$ . The domination number  $\gamma(G)$  of  $G$  is the minimum cardinality of a dominating set of  $G$ . For references on domination parameters in graphs see [4, 6]. A set of points  $R$  in  $G$  is known as a geodetic dominating set if  $R$  is both a geodetic set and a dominating set. The minimum cardinality of a geodetic dominating set of  $G$  is its geodetic domination number and is indicated by  $\gamma_g(G)$ . A geodetic dominating set of size  $\gamma_g(G)$  is said to be a  $\gamma_g$ -set. The geodetic domination number of a graph was introduced in [8]. A set of points of  $G$  is an independent geodetic set if  $R$  is an

independent set and  $I[R] = V$ . The minimum cardinality of an independent geodetic set is the independent geodetic number  $g_i(G)$ , it was introduced by P. Kazemi and doost Ali mojde [11]. A geodetic set  $R \subseteq V(G)$  is a total geodetic set if the subgraph  $G[R]$  induced by  $R$  has no isolated points. The minimum cardinality of a total geodetic set is the total geodetic number  $g_t(G)$  and it was introduced by Abdollahzadeh Ahangar and Vladimir Samodivkin[1]. A geodetic set  $R \subseteq V(G)$  is a total geodetic dominating set if the subgraph  $G[R]$  induced by  $R$  has no isolated points and a dominating set. The minimum cardinality of a total geodetic dominating set is the total geodetic domination number  $\gamma_{gt}(G)$ [2]. A geodetic set  $R \subseteq V$  is said to be total outer independent geodetic set if  $\langle R \rangle$  has no isolated points and  $\langle V - R \rangle$  is an independent set. The minimum cardinality of a total outer independent geodetic set and it is denoted by  $g_{toi}(G)$  is called the total outer independent geodetic number of  $G$ [7]. In this paper we define total outer independent geodetic dominating set.

The following theorem is used in the consequences.

**Theorem 1.1.** [5] Each geodetic set of a graph contains its extreme vertices.

**Theorem 1.2.** [5] For any cycle  $C_n$  of order  $n \geq 3$ ,  $g(C_n) = \begin{cases} 2 & \text{if } n \text{ is even} \\ 3 & \text{if } n \text{ is odd.} \end{cases}$

## 2. Total Outer Independent Geodetic Domination Number of a Graph :

**Definition 2.1.** A geodetic set  $R \subseteq V$  is said to be total outer independent geodetic dominating set [TOIGDS] if it is a total geodetic dominating set and  $\langle V - R \rangle$  is an independent set. The minimum cardinality of a total outer independent geodetic dominating set, indicated by  $\gamma_{gt}^{oi}(G)$  is known as the total outer independent geodetic domination number of  $G$ .

**Example 2.2.** For the graph  $G$  given in Figure 2.1, it is observed that  $R_1 = \{a_1, a_5\}$  is the geodetic set of  $G$  so that  $g(G) = 2$ . It is verified that the set  $R_2 = \{a_1, a_2, a_5\}$  is the minimum geodetic dominating set so that  $\gamma_g(G) = 3$ . Also, the set  $R_3 = \{a_1, a_2, a_5, a_6\}$  is the total geodetic dominating set and so  $\gamma_{gt}(G) = 4$  and the set  $R_4 = \{a_1, a_2, a_4, a_5, a_6, a_8\}$  is the total outer independent geodetic dominating set of  $G$  so that  $\gamma_{gt}^{oi}(G) = 6$ .

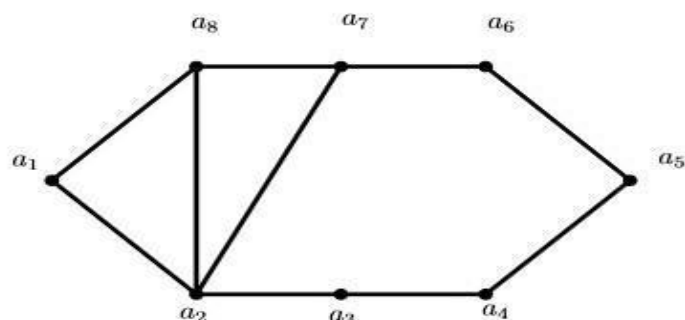


Figure 2.1: A Graph  $G$  with  $\gamma_{gt}^{oi}(G) = 6$ .

**Observation 2.3.** For any connected graph  $G$ ,  $2 \leq g(G) \leq \gamma_g(G) \leq \gamma_{gt}(G) \leq \gamma_{gt}^{oi}(G)$ .

**Observation 2.4.** Each extreme vertex of a connected graph  $G$  belongs to every total outer independent geodetic dominating set of  $G$ .

**Observation 2.5.** For any complete graph  $K_p$  ( $p \geq 2$ ),  $\gamma_{gt}^{oi}(G) = p$ .

**Theorem 2.6.** If  $G = W_n$  ( $n \geq 5$ ) is a wheel graph,

$$\text{then } \gamma_{gt}^{oi}(G) = \begin{cases} \frac{n+2}{2} & \text{if } n \text{ is even,} \\ \frac{n+1}{2} & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** Let  $G = W_n$  ( $n \geq 5$ ), be the wheel graph.  $V(G) = \{a, b_1, b_2, \dots, b_{n-1}\}$ , where  $\deg(a) = n - 1$  and  $\deg(b_k) = 3$  for each  $k = 1, 2, \dots, n - 1$ . We have two cases.

Case (1). If  $n$  is even.

Consider  $R = \{b_1, b_3, \dots, b_{n-1}\}$ , Clearly  $R$  is the geodetic dominating set of  $G$ . But  $\langle R \rangle$  has isolated points and  $\langle V - R \rangle$  is connected. Take  $R_1 = R \cup \{a\}$ . It is observed that  $\langle R_1 \rangle$  is connected so that  $R_1$  become a total geodetic dominating set and  $\langle V - R_1 \rangle$  is an independent set. Then  $R_1$  is the total outer independent geodetic dominating set of  $G$ . Hence  $\gamma_{gt}^{oi}(G) = |R_1| = |R| + \{a\} = \frac{n}{2} + 1 = \frac{n+2}{2}$ .

Case (2). If  $n$  is odd.

Let  $R = \{b_1, b_3, \dots, b_{n-2}\}$  be the geodetic dominating set of  $G$ . But  $\langle R \rangle$  has isolated points and  $\langle V - R \rangle$  is connected. Consider  $R_1 = \{a, b_1, b_3, \dots, b_{n-2}\}$ . Clearly  $\langle R_1 \rangle$  is connected so that  $R_1$  become a total geodetic dominating set and also  $\langle V - R_1 \rangle$  is an independent set. Therefore,  $R_1$  become a total outer independent geodetic dominating set of  $G$ . Hence  $\gamma_{gt}^{oi}(G) = |R_1| = |R| + \{a\} = \frac{n-1}{2} + 1 = \frac{n+1}{2}$ . ■

**Theorem 2.7.** In any graph  $G$ ,  $\gamma_{gt}^{oi}(G) \geq \delta(G)$ .

**Proof.** Let  $R$  be any  $\gamma_{gt}^{oi}(G)$  - set. If  $R = V(G)$ , then obviously the result is true. Suppose  $R \neq V(G)$ . Let  $x$  be any point which does not belong to  $R$ . Since  $\langle V - R \rangle$  is independent, all neighbors of  $x$  belong to the set  $R$ . Then  $|R| > \deg(x)$ . By definition we have  $\delta(G) \leq \deg(x)$ . Hence  $\gamma_{gt}^{oi}(G) \geq \deg(x) \geq \delta(G)$ , that is  $\delta(G) \leq \gamma_{gt}^{oi}(G)$ . ■

**Definition 2.8.** An alternate triangular snake  $AT_m$  is derived from a path  $P_m$  by joining  $a_k$  and  $a_{k+1}$  alternatively to a new point  $b_k$  where  $1 \leq k \leq m$  for  $m$  even and  $1 \leq k \leq m - 1$  for  $m$  odd.

**Definition 2.9.** The double alternate triangular snake  $DAT_m$  consists of two alternate triangular snake which have a common path.

**Theorem 2.10.** For the double alternate triangular snake  $G = DAT_m$  ( $m \geq 3$ ),

$$\gamma_{gt}^{oi}(G) = \begin{cases} \frac{3m}{2} & \text{if } m \text{ is even,} \\ \frac{3m-1}{2} & \text{if } m \text{ is odd.} \end{cases}$$

**Proof.** Let  $G = DAT_m$  and  $V(G) = \{a_1, a_2, \dots, a_m, b_1, b_2, \dots, b_{\frac{m}{2}}, c_1, c_2, \dots, c_{\frac{m}{2}}\}$  be the point set of  $G$ . We discuss two cases:

Case (1). If  $m$  is even.

Consider  $R_1 = \{b_1, b_2, \dots, b_{\frac{m}{2}}, c_1, c_2, \dots, c_{\frac{m}{2}}\}$ . Clearly  $R_1$  is the geodetic dominating set of  $G$ . But it is not a total geodetic dominating set of  $G$ . So we add a point set  $\{a_2, a_4, \dots, a_{m-2}, a_m\}$  to  $R_1$ , that is  $R_2 = R_1 \cup \{a_2, a_4, \dots, a_{m-2}, a_m\}$ . Hence  $\langle R_2 \rangle$  is connected so that  $R_2$  become a total geodetic dominating set and  $\langle V - R_2 \rangle$  is an independent set. Thus  $R_2$  is a total outer independent geodetic dominating set of  $G$ . Therefore,

$$\gamma_{gt}^{oi}(G) = |R_2| = |R_1| + \frac{m}{2} = m + \frac{m}{2} = \frac{3m}{2}.$$

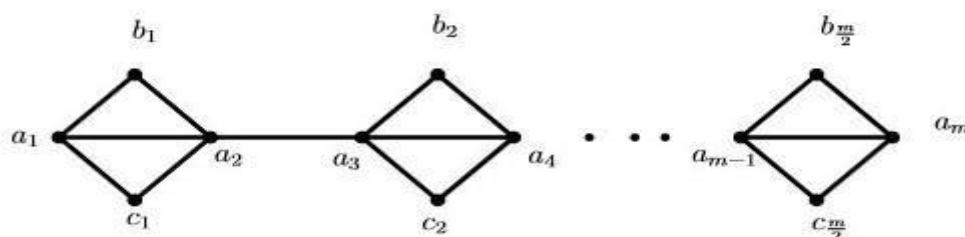


Figure 2.2: Double alternate triangular snake when  $m$  is even

Case (2). If  $m$  is odd. Consider  $R_1 = \{b_1, b_2, \dots, b_{\frac{m-1}{2}}, c_1, c_2, \dots, c_m, a_m\}$ . Obviously  $R_1$  is the geodetic

dominating set of  $G$ . But  $\langle R_1 \rangle$  has isolated points and  $\langle V - R_1 \rangle$  is connected. Take  $R_2 = R_1 \cup \{a_2, a_4, \dots, a_{m-1}\}$ . It is observed that  $\langle R_2 \rangle$  is connected so that  $R_2$  is a total geodetic dominating set and  $\langle V - R_2 \rangle$  is an independent set. Hence  $R_2$  is the total outer independent geodetic dominating set of  $G$ .

$$\text{Hence } \gamma_{gt}^{oi}(G) = |R_2| = |R_1| + \frac{m-1}{2} = \frac{m-1}{2} + \frac{m-1}{2} + 1 + \frac{m-1}{2} = \frac{m-3}{2} + 1 = \frac{3m-1}{2}. \quad \blacksquare$$

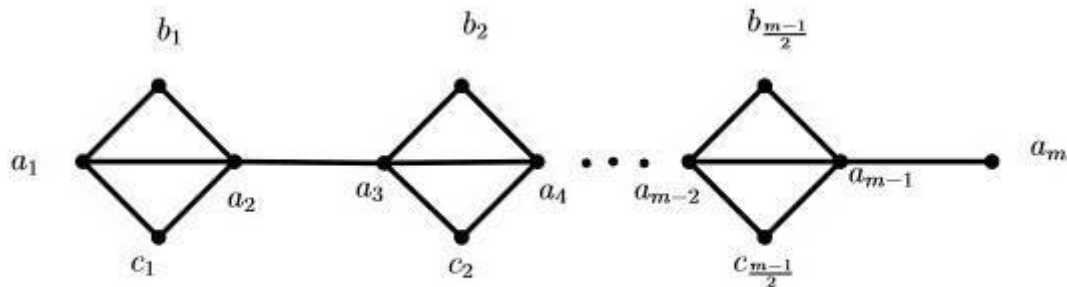


Figure 2.3: Double alternate triangular snake when  $m$  is odd

**Theorem 2.11.** For any path  $P_n$  of order  $n \geq 8$ ,

$$\gamma_{gt}^{oi}(P_n) = \begin{cases} \frac{2n}{3} + 1 & \text{if } n \text{ is a multiple of } 3 \\ \lceil \frac{2n-1}{3} \rceil + 1 & \text{if } n \text{ is not a multiple of } 3 \end{cases}$$

**Proof.** Let  $P_n: a_1, a_2, \dots, a_n$  be the points of path for  $n \geq 8$ . We have two cases.

Case (1). If  $n$  is a multiple of 3.

Consider  $R = \{a_1, a_2, a_{n-1}, a_n\}$ . Clearly  $R$  is the total geodetic set, such that  $R$  is not a dominating set as well as  $\langle V - R \rangle$  is not an independent set. Take  $R_1 = R \cup B$ , where  $B \subseteq V(P_n) - R$ ,  $B = \cup a_k$ ,  $k = 3h$ , for all  $h \in N$ . Now,  $R_1$  is the total geodetic dominating set and  $\langle V - R_1 \rangle$  is an independent set. Hence  $R_1$  is a total outer independent geodetic dominating set. Therefore,  $\gamma_{gt}^{oi}(P_n) = |R_1| = |R \cup B| = |R| + |B| = 4 + \frac{2n}{3} - 3 = \frac{2n}{3} + 1$ .

Case (2). If  $n$  is not a multiple of 3.

Let  $R = \{a_1, a_2, a_{n-1}, a_n\}$  be the total geodetic set, such that  $R$  is not a dominating set and  $\langle V - R \rangle$  is not an independent set. Consider  $R_1 = R \cup B$ , where  $B = \{a_4, a_5, \dots, a_k \mid 4 \leq k \neq 3h < n-1\}$  for all  $h \in N$  with  $|R_1| = \lceil \frac{2n-1}{3} \rceil + 1$ . It is observed that the set  $R_1$  is a total outer independent geodetic dominating set of  $P_n$ . Because  $\langle R_1 \rangle$  has no isolated points and  $\langle V - R_1 \rangle$  is an independent set. Therefore,

$$\gamma_{gt}^{oi}(P_n) = \lceil \frac{2n-1}{3} \rceil + 1. \quad \blacksquare$$

**Theorem 2.12.** For any cycle  $C_n$  of order  $n \geq 6$ ,

$$\gamma_{gt}^{oi}(C_n) = \begin{cases} \frac{2n}{3} & \text{if } n \equiv 0 \pmod{6} \\ \frac{2n+1}{3} & \text{if } n \equiv 1 \text{ or } 4 \pmod{6} \\ \frac{2n+2}{3} & \text{if } n \equiv 2 \text{ or } 5 \pmod{6} \\ \frac{2n+3}{3} & \text{if } n \equiv 3 \pmod{6} \end{cases}$$

**Proof.** Let  $G = C_n$  be the cycle of order  $n \geq 6$ , and let  $V(G) = \{a_1, a_2, \dots, a_n\}$  be the point set of  $G$ . We have to consider four cases.

Case (1). If  $n \equiv 0 \pmod{6}$ .

Consider  $R = \{a_1, a_2, a_{\frac{n}{2}+1}, a_{\frac{n}{2}+2}\}$ . Clearly  $R$  is the total geodetic set of  $G$ . But  $R$  is not a dominating set also  $\langle V - R \rangle$  is not an independent set. Let  $K = \cup a_j, j \neq 3h$  for all  $h \in N$  and  $R_1 = R \cup K$  be the total outer independent geodetic dominating set of  $G$ . Because  $R_1$  is a dominating set,  $\langle R_1 \rangle$  is connected and  $\langle V - R_1 \rangle$  is an independent set.

Therefore,  $\gamma_{gt}^{oi}(G) = |R_1| = |R \cup K| = |R| + |K| = 4 + 2(\frac{n-6}{3}) = \frac{2n}{3}$ .

Case (2). If  $n \equiv 1$  or  $4 \pmod{6}$ . Let  $R = \{a_1, a_2, a_{\frac{n+1}{2}}, a_{\frac{n+1}{2}+1}\}$  and  $\{a_1, a_2, a_{\frac{n}{2}+1}, a_{\frac{n}{2}+2}\}$  are the total geodetic set for  $n \equiv 1 \pmod{6}$ , and  $n \equiv 4 \pmod{6}$  respectively. But  $R$  is not a dominating set and  $\langle V - R \rangle$  is not an independent set.

Take  $K = \begin{cases} \{a_4, a_5, \dots, a_k\} & \text{for } n \equiv 1 \pmod{6} \\ \{a_4, a_5, \dots, a_k\} \cup \{a_{\frac{n}{2}+3}, a_{\frac{n}{2}+4}, \dots, a_l\} & \text{for } n \equiv 4 \pmod{6} \end{cases}$  with  $|K| = \frac{2n-11}{3}$ , where  $k \neq 3h$  for

all  $h \in N$  for  $n \equiv 1 \pmod{6}$  and  $k \neq 3h < \frac{n}{2}, l \neq 3h + 1, \frac{n}{2} + 2 \leq l < n$  for all  $h \in N$  for  $n \equiv 4 \pmod{6}$ . Consider  $R_1 = R \cup K$ . Now,  $R_1$  is the total outer independent geodetic dominating set of  $G$ . Since  $R_1$  is a dominating set,  $\langle R_1 \rangle$  has no isolated points and  $\langle V - R_1 \rangle$  is an independent set. Hence,  $\gamma_{gt}^{oi}(G) = |R_1| = |R \cup K|$

$$= |R| + |K| = 4 + \frac{2n-11}{3} = \frac{2n+1}{3}.$$

Case (3). If  $n \equiv 2$  or  $5 \pmod{6}$ .

Let  $R = \{a_1, a_2, a_{\frac{n}{2}+1}, a_{\frac{n}{2}+2}\}$  and  $\{a_1, a_2, a_{\frac{n+1}{2}}, a_{\frac{n+1}{2}+1}\}$  are the total geodetic set for  $n \equiv 2 \pmod{6}$  and  $n \equiv 5 \pmod{6}$  respectively. But  $R$  is not a dominating set and  $\langle V - R \rangle$  is not an independent set.

Take  $K = \begin{cases} \{a_4, a_5, \dots, a_k\} & \text{for } n \equiv 2 \pmod{6} \\ \{a_4, a_5, \dots, a_k\} \cup \{a_{\frac{n+1}{2}+3}, a_{\frac{n+1}{2}+4}, \dots, a_l\} & \text{for } n \equiv 5 \pmod{6} \end{cases}$  with  $|K| = \frac{2n-10}{3}$ , where  $k \neq$

$3h$  for all  $h \in N$  for  $n \equiv 2 \pmod{6}$  and  $k \neq 3h < \frac{n}{2}, \frac{n+1}{2} < l \neq 3h + 2 < n$  for all  $h \in N$  for  $n \equiv 5 \pmod{6}$ . Consider  $R_1 = R \cup K$ . Now  $R_1$  become total outer independent geodetic dominating set of  $G$ . Because  $R_1$  is a dominating set,  $\langle R_1 \rangle$  has no isolated points and  $\langle V - R_1 \rangle$  is an independent set. Therefore,  $\gamma_{gt}^{oi}(G) = |R_1| = |R \cup K| = |R| + |K| = 4 + \frac{2n-10}{3} = \frac{2n+2}{3}$ .

Case (4). If  $n \equiv 3 \pmod{6}$ .

Let  $R = \{a_1, a_2, a_{\frac{n+1}{2}}, a_{\frac{n+1}{2}+1}\}$  be the total geodetic set. But  $R$  is not a dominating set and  $\langle V - R \rangle$  is not an independent set.

Take  $K = \{a_4, a_5, \dots, a_k\} \cup \{a_{\frac{n+1}{2}+3}, a_{\frac{n+1}{2}+4}, \dots, a_l\}$  with  $|K| = \frac{2n-9}{3}$  where  $k \neq 3h < \frac{n+1}{2}$  and  $\frac{n+1}{2} + 1 < l \neq 3h + 1 < n$ . Consider  $R_1 = R \cup K$ . It is observed that  $R_1$  is the total outer independent geodetic dominating set of  $G$ . Because  $R_1$  is a dominating set,  $\langle R_1 \rangle$  has no isolated points and  $\langle V - R_1 \rangle$  is an independent set. Therefore,  $\gamma_{gt}^{oi}(G) = |R_1| = |R \cup K| = |R| + |K| = 4 + \frac{2n-9}{3} = \frac{2n+3}{3}$ . ■

### 3. Realization Result:

**Theorem 3.1.** For any pair  $m, n$  of integers with  $2 \leq m \leq n$  and  $n \geq 2$ , there exists a connected graph  $G$  such that  $\gamma_g(G) = m$  and  $\gamma_{gt}^{oi}(G) = n$ .

**Proof.** Case (1). If  $m = n$ . Let  $G = K_2$ , then  $\gamma_g(G) = 2$  and  $\gamma_{gt}^{oi}(G) = 2$ .

Case (2). If  $m = 2, n = 3$ . Let  $C_4: a_1, a_2, a_3, a_4$  be a cycle of length 4. Consider the graph  $C_4$  as  $G$ . The resulting graph  $G$  is given in Figure 3.1. Take  $R_1 = \{a_1, a_3\}$ . Clearly  $R_1$  is the minimum geodetic dominating



set of  $G$ , so that  $\gamma_g(G) = 2$ . Let  $R_2 = R_1 \cup \{a_2\}$ . Then  $R_2$  become a total outer independent geodetic dominating set of  $G$ . Therefore,  $\gamma_{gt}^{oi}(G) = 3$ .

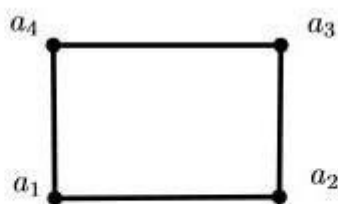


Figure 3.1: A graph  $G$  with case 2 of theorem 3.1

Case (3). If  $m \geq 3, n \geq 4, n \neq m + 3$ . Let  $P_3 : a_1, a_2, a_3$  be a path of length 3. Let  $G$  be the graph obtained from  $P_3$  by adding the new points  $c_1, c_2, \dots, c_{m-1}$  and  $b_1, b_2, \dots, b_l$  and joining each  $c_k$  ( $1 \leq k \leq m-2$ ) with  $a_1$  and  $a_2$  and also joining each  $b_k$  ( $1 \leq k \leq l$ ) with  $a_1$  and  $a_3$ . The resulting graph  $G$  is given in Figure 3.2. Take  $R_1 = \{c_1, c_2, \dots, c_{m-2}, a_3, a_1\}$ . It is observed that  $R_1$  is the minimum geodetic dominating set of  $G$ , so that  $\gamma_g(G) = m - 2 + 1 - 1 = m$ . Consider  $R_2 = R_1 \cup \{a_2\}$ . Clearly  $\langle R_2 \rangle$  has no isolated points and  $\langle V - R_2 \rangle$  is an independent set. Hence  $R_2$  is the total outer independent geodetic dominating set of  $G$ . Therefore,  $\gamma_{gt}^{oi}(G) = |R_2| = |R_1| + 1 = m + 1 \neq m + 3 = n$ .

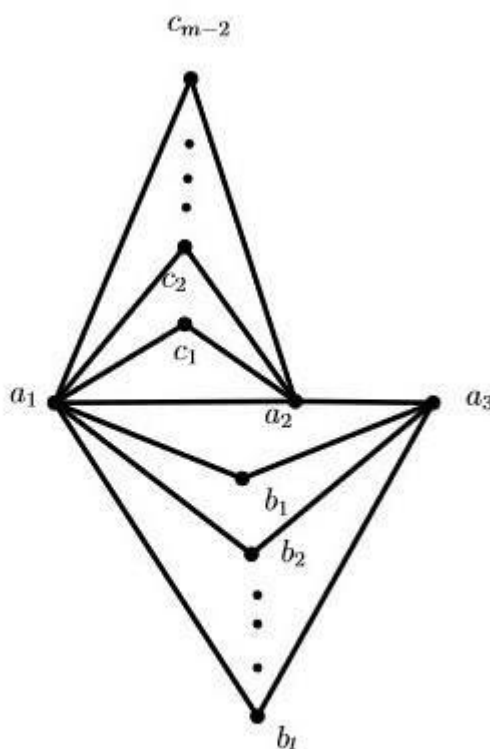


Figure 3.2: A graph  $G$  with case 3 of theorem 3.1

Case (4). If  $m \geq 3, n \geq 4, n = m + 3$ . Let  $P_5 : a_1, a_2, a_3, a_4, a_5$  be a path of length 5. Let  $G$  be the graph obtained from  $P_5$  by adding the new points  $c_1, c_2, \dots, c_{m-2}$  and  $b_1, b_2, \dots, b_l$  and joining each  $c_k$  ( $1 \leq k \leq m-2$ ) with  $a_3$  and joining each  $b_k$  ( $1 \leq k \leq l$ ) with  $a_2$  and  $a_4$ . The resulting graph  $G$  is given in Figure 3.3. Consider  $R_1 = \{a_1, a_5, c_1, c_2, \dots, c_{m-2}\}$ . Clearly  $R_1$  is the geodetic dominating set of  $G$ , so that  $\gamma_{gt}^{oi}(G) = |R_1| = 2 + m - 2 = m$ . Let  $R_2 = \{a_1, a_2, a_3, a_4, a_5, c_1, c_2, \dots, c_{m-2}\}$ . It is observed that  $\langle R_2 \rangle$  has no isolated points and  $\langle V - R_2 \rangle$  is an independent set. Hence  $R_2$  is the total outer independent geodetic dominating set of  $G$ . Therefore,  $\gamma_{gt}^{oi}(G) = |R_2| = |R_1| + 3 = m + 3 = n$ . ■

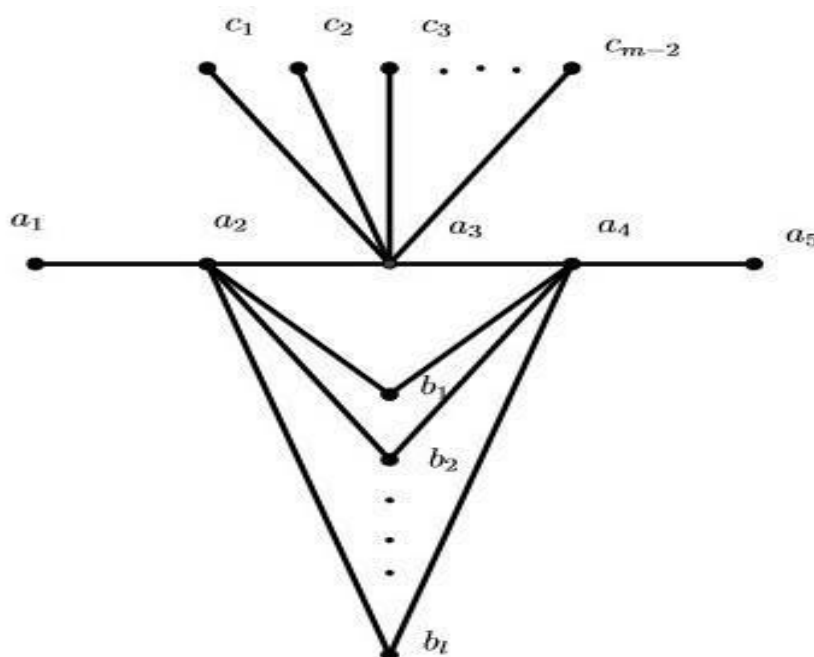


Figure 3.3: A Graph  $G$  with Case 4 of theorem 3.1

#### 4. Conclusion:

In this paper we define and study the concept Total outer independent geodetic domination number of a graph. This work can be extended to find upper total outer independent geodetic domination number of a graph, connected total outer independent geodetic domination number of a graph. The findings united in this paper would support the readers to develop various useful applications to the world of science and technology.

#### 5. Acknowledgment

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Kryvyi Rih National University, Ukraine and 'Research Culture Society'.**

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**ACHIEVING SOCIAL AND ECONOMIC REVIVALS BY  
EMPLOYING SUSTAINABLE AGRICULTURE DEVELOPMENT**

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**Abstract:** *The Economics development and growth of a country like India are supported largely by the agricultural practices performed by the potential farmers. The role of the agricultural sector in the Indian economy can be seen through its contribution to GDP. The performance of agriculture and the economy is quite related. So it is quite obvious that the investment in agriculture must be linked with the objective of increasing productivity. This paper will attempt to discuss the various issues and challenges of Sustainable Agriculture Development in India. Sustainability means the practices of farming for ensuring policy frameworks that will be designed and equipped in such a manner that gives quality wise good products and as well as gives profitability through agriculture practices. Due to the increasing population, there has been a challenge to meet the demand for food; hence to secure food security there is a need to increase the productivity of agricultural land. The monsoon in India is quite unpredictable and hence this paper will discuss the various priority areas for solving the issue which in turn increase productivity to support the livelihood of the rural population. The aim of sustainable development in agriculture should also provide employment opportunities. The farmers performing agriculture have to take care of maintaining the soil quality and should try to protect and preserve the quality of resources. The land being cultivated time and again loses its fertility. The multiple cropping has its own importance in maintaining in the field of agriculture. The paper will conclude on how economic prosperity and livelihood sustainability is related to agricultural production.*

**Keywords:** *Economics development, growth, agricultural practices, GDP, Sustainable development*

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## **1. INTRODUCTION:**

In India, food security is the major issue and many in part of the country the people are still not getting sufficient food for their survival. The food challenges are a great threat and a challenge for the country because people deprive of even the basics of life. In the digital era, the country has witnessed the paradigm shift from conventional practices to modern practices in every field. Agriculture should also develop in the lines of adopting the latest technology. The major issues with our system are delays in adopting technology and changing policies. We still find the existence of insufficient rural transport system, lack of awareness of the new policies among the farmers. The people have limited knowledge of the treatment of crops, limited access to modern farming technology. In our country, due to the increasing population, there is a shrinking of agricultural land due to urbanization.

## **2. NEED FOR THE STUDY:**

There is increasing pressure on agriculture due to the increasing pressure of the population. There is a lack of food security. Even if there has been a lot of investment in this sector, still the

benefit is not reaching everyone. Hence, there is a need to understand the importance and scope of introducing sustainable agriculture. The sustainable agriculture will bring the targeted profit and ensure food security. Thus investments in agriculture should be targeted to areas that are likely to attain high productivity.

### **3. OBJECTIVES:**

- To role of intervention by means of achieving sustainable agricultural growth.
- To find the emerging challenges and opportunities for betterment of agricultural produce.

### **4. METHODOLOGY:**

This research was primarily descriptive research emphasizes on explaining the importance of sustainable agriculture and its related challenges and opportunities. Information regarding this concept has been collected from the website, online articles, and ideas from the abstract, journal. Based on the conceptual study the paper discusses the various interpretations. Based on the analysis discussion the conclusions were drawn.

### **ROLE OF INDIAN AGRICULTURE SECTOR**

The agriculture sector is the backbone of any economy. There is an interdependence of industries on agriculture. The produce of agriculture gives large support to the Indian industries. Hence, our export can be increased and our GDP and balance of trade situation will also be improved. Agriculture is considered the most important industries in the Indian economy. Agriculture provides employment to a large section of society. Approximately 60 percent of the Indian population is engaged in the industry, contributing about 18 percent to India's GDP. This share decreases gradually with each year, with development in other areas of the country's economy.

### **ATTAINING VIABLE FUTURE THROUGH SUSTAINABLE AGRICULTURE DEVELOPMENT**

The sustainable agriculture provides is a major step forward initiative to ensure food and livelihood security and would require a multi-functional/multi-tier institutional mechanism for ensuring convergence and establishing linkage at all levels. The thrust areas to be addressed in the plan of sustainable development can be supporting dryland agriculture, access to information, biotechnology and risk management. The strategies must be developed to make Indian agriculture more self-sufficient.

The policies must focus on resilience to address the issues of climate change. The objective is to increase and improve the productivity of rainfed agriculture. There has been continuous research in these areas for improvement. The purpose of Sustainable agricultural practices is to provide balance environmental health and economic profitability in order to promote social and economic equity. Sustainable Agriculture involves the processes that would help the policy-makers to plans for longer terms. It can meet the needs of the present as well as future people. It helps to build the entire ecosystem.

### **EMERGING CHALLENGES AND OPPORTUNITIES**

The soil and water management are the greater thrust areas. There is a need of better seed management to boost productivity and to improve the health of the crop. The fertility of the soil and the quality of the seeds are of great importance to bring significant crop health and boost productivity. Not only these there is a big challenge of the crops getting wasted every year the unwanted fungi and parasites also damage the crop and reduce the productivity to a greater extent that can damage crops or hinder growth, and increase productivity. Food security can also be ensured in a better manner if there is proper soil, water and seed management. In order to work towards achieving a

thriving ecosystem, productive economy and socio-economic parity, sustainable agriculture has a major role to play.

The support of the government is still not reaching for the proper running of the warehousing. The uncertain climate change poses another challenge and threat to agricultural growth. Another, challenge for the agriculture sector to match the changing need of the industrial demand of raw materials because there is a greater threat due to the changing long-term intensive industrial growth and high-changing consumer lifestyles and preferences. India is also trying to frame different strategies to deal with these changing consumption patterns and frequently changing international markets. In order to ensure the socio-economic and developmental priorities

## **FUTURE PROSPECTS AND PRIORITY AREAS FOR SUPPORT**

In the present scenario, it is important that agricultural produce must be enhanced to meet the, competitiveness, and the need for rural growth. Training must be provided regarding the new technology. The new technologies must be promoted and supported by the government. The reforms can be possible with the extension of agricultural research and developments. The most important needs for agricultural growth are to bring the major reform and strengthening of India's agricultural research. The policy frame for developing sustainable agriculture must be economically feasible. The earlier practice of agriculture was more exposed to failure and risk. But now the orientation of agriculture produces can be more export-oriented. The domestic supply of agriculture produce is now channelized for foreign markets. The sustainable agriculture will not only meet the existing demand or say the local demand for food grains but will also be in form of positive and visible trade balance.

Any development policies must be accepted by the farming community and focused to reduce rural poverty. Any policies must reduce the gap between the 'haves and 'have-nots', then only we can label it as a robust system. Sustainable agriculture practices are useful as they are based on the adoption of the latest technique and innovation. The success of any policy depends upon the knowledge of the people engaged in that activity and regarding the environment crops and livestock. Further, we can compare them across three dimensions, ecological, economic, and social sustainability. The government is also playing a vital role in revitalization the entire institution. The numbers of education programmers are launched by the government to support literacy regarding the agricultural reform taking place in the agriculture sector for achieving sustainable development. It can also be achieved by the full utilization of human resources. A large part of the poor population of the country is engaged in agriculture, unless we increase their living standard, the overall growth of this country is not possible. Due to the increasing Debt in farmers are committing suicides. The People with dreams of prosperity and better life are migrating towards the city. They wanted a better livelihood but due to poor situation of agriculture, the development is at very slow pace.

## **5. CONCLUSION :**

The paper brought the major challenges being faced by the farmers in adopting the technology. Though they are adopting the technology the pace of adoption is very slow compared to the increasing demand. But gradually the farmers are realizing that times have come to replace the unscientific agriculture practices. It is the time when basics issues of development of the Indian agriculture sector must be planned again with the new framework, need and situation in demand.

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**Corrosion Inhibition Studies of Triazinedithiol Inhibitors for Mild  
steel in a Acid Chloride Solution**

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**Abstract:** Two environmental pleasant triazinedithiol inhibitors 6-diallylamino-1, 3, 5-triazine-2, 4-dithiol monosodium (DAN) and 6-dibutylamino-1,3,5-triazine-2,4 dithiol monosodium (DBN) were synthesized and their corrosion inhibition for slight metallic in a 1 M HCl solution turned into studied the usage of weight reduction methods, electrochemical measurements, and scanning electron microscopy (SEM) techniques.[1-5] The inhibition efficiency of both DAN and DBN improved with increases in inhibitor concentration but decreased with increases in temperature. Results from potentiodynamic polarization and EIS confirmed that the corrosion inhibition performance of DAN and DBN became excellent.

**Keywords:** mild steel; potentiodynamic polarization; corrosion inhibition.

**1. Introduction:**

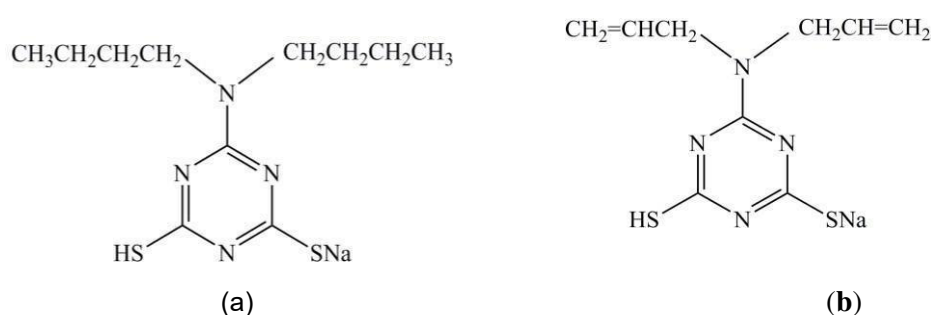
Corrosion of mild steel and its alloys has attracted much attention from many researchers due to their high mechanical intensity, low cost, low density, and good machinability, and they have been widely used in industrial applications, especially in constructions, electronics, packing, storage, and transportation equipment and machinery. Corrosion is an electrochemical process and is often activated by industrial processes such as acid descaling, acid pickling, acid cleaning, and oil well acidizing. Efforts have been made to protect the integrity of the aluminum surface in an aggressive acid medium or other corrosive environment. In recent decades, the addition of inhibitors has been considered to be the most common approach to hinder the corrosion of mild steel. [6-10]

Many organic compounds have been widely reported as corrosion inhibitors of mild steel in acid solution, such as aliphatic, aromatic amines, and nitrogen heterocyclic molecules. However, some of these compounds are costly and not easily biodegradable. As excessive reactive, low cost, excessive solubility, and environmentally pleasant compounds, triazinedithiol, and its monosodium salt had been mentioned to put together the powerful corrosion inhibitive movie on metal surfaces through electrochemical deposition. The unique tautomer of thiol–thione with quite electronegative atoms like S and O, and the N-containing heterocyclic conjugate system, gain the triazinedithiol molecules to adsorb on metal surface. [11-13] However, the research on triazinedithiol inhibitors for mild steel is seldom reported. The purpose of present work is to investigate and compare the corrosion inhibition action of 6-diallylamino-1,3,5-triazine-2,4-dithiol monosodium (DAN) and 6-dibutylamino-1,3,5-triazine-2,4-dithiolmonosodium (DBN), and their protective performance for mild steel in 1 M HCl was studied utilizing a variety of electrochemical tests, weight loss methods, scanning electron microscopy (SEM) techniques, and quantum chemistry analysis.

## 2. Materials and Methods:

### 2.1. Materials and Sample Preparation

The mild steel sheet AA5052 (Cu: 0.1%, Si: 0.2%, Fe: 88%, Mn: 0.1%, Mg: 2.8%, Zn: 0.1%, Cr: %, others: 0.15%) was mechanically press-cut into specimens of dimension 30 mm × 50 mm × 0.3 mm. All test plates of AA5052 were ultrasonically degreased in the acetone for 15 min, and treated by the immersion in alkaline solution (15 g Na<sub>2</sub>CO<sub>3</sub> + 15 g Na<sub>2</sub>PO<sub>4</sub> per liter) at 60 °C for the debinding process [14-17]. After that, the mild steel specimens were washed thoroughly with distilled water and dried with nitrogen. The specimens with an exposed area of 1 cm<sup>2</sup> were used for potentiodynamic polarization and electrochemical impedance spectroscopy. AR (analytical reagent) grade hydrochloric acid and double distilled water were used to prepare the corrosive media. Molecular structures of DAN and DBN are displayed in Figure 1. In this paper, DAN was synthesized by the reaction between 6-*N,N*-diallylamino-1,3,5-triazine-2,4-dichloride and NaSH, while DBN was synthesized by the reaction between 6-*N,N*-dibutylamino-1,3,5-triazine-2,4-dichloride and NaSH according to the method in previous studies.



**Figure 1.** Molecule structures of two triazinedithiols of (a) 6-diallylamino-1,3,5-triazine-2,4-dithiol monosodium (DAN) and (b) 6-dibutylamino-1,3,5-triazine-2,4-dithiol monosodium (DBN). [18-20]

### 2.2. Weight Loss Test

The mild steel specimens in triplicate were immersed in a 1 M HCl solution with different concentration (0.01–1.00 mM) of inhibitors for 2 h. The temperature was controlled by a thermostat aqueous bath at 30 °C. Furthermore, the mild steel specimens were immersed into a 1 M HCl solution with the presence of 1 mM inhibitors, and the experiments were conducted over the temperature range from 30 °C to 50 °C. For all weight loss tests, the volume of prepared solution is 200 mL, and buffer solutions of citric acid/sodium citrate were used to adjust the pH value of tested solution rectangular piece of graphite on between 6 and 6.5. After the immersion, all specimens were brought out from the solution, scrubbed with bristle brush under running water, then washed thoroughly with distilled water, dried in acetone, and weighed accurately. At least three samples were tested and the average value was obtained. [21-23]

### 2.3. Electrochemical Measurements

The potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) measurements were carried out using CHI 608E electrochemical work station (CHI Instruments; USA) in a three-electrode cell system with a saturated calomel electrode (SCE) as reference electrode and a square piece of graphite as counter electrode. The working electrode was mild steel. Prior to any electrochemical measurements, the immersion in the solution for 1 h was necessary for the open circuit potential to reach a steady state. EIS was carried out at steady open circuit potential disturbed with amplitude of 10 mV alternative current sine wave in the frequency range of 100 mHz to 10 kHz. The polarization curves were obtained by changing potential from –250 mV to +250 mV versus OCP with a scan rate of 0.5 mV/s.

## 2.4. Scanning Electron Microscopy (SEM)

The surfaces morphologies of the mild steel immersed in a 1 M HCl solution for 2 h with and without the triazinethiol inhibitors were observed via SEM (JSM-6360LV, JEOL, Tokyo, Japan) at an accelerating voltage of 20 kV, respectively. [25-27]

## 3. Results:

### 3.1. Weight Loss Study

#### 3.1.1. Effect of Concentration

The inhibition efficiency ( $\eta_w$ ) and corrosion rate ( $C_R$ ) of mild steel acquired from the weight loss method in a 1 M HCl solution contained different concentrations of inhibitors (0.01–1.00 mM) at 30 °C are presented in Table1. The results clearly show that the inhibition efficiency increases and the corrosion rate decrease by increasing the concentration of studied inhibitors. When concentration of inhibitors varies from 0.01 mM to 1 mM, there is an increase in efficiency from 78.41% to 98.56% for DAN, and an increase in efficiency from 43.79% to 99.21% for DBN (Table1). This indicates that the presence of DAN or DBN acts as inhibitor retarding the corrosion of aluminum in a hydrochloric acid solution. When the concentration of inhibitor is low, more molecules are needed to adequately cover the aluminum surface. We also found that further enhancement in concentration did not bring any significant changes in the performance of inhibitors, indicating that the achievement of a limiting value. The effect is attributed to the amassing of inhibitor molecules onto the positively charged metal surface leading a decrease in direct contact with metal and corrosive environment. Similar results were found in other studies about different inhibitors for mild steel in hydrochloric acid. [27-30]

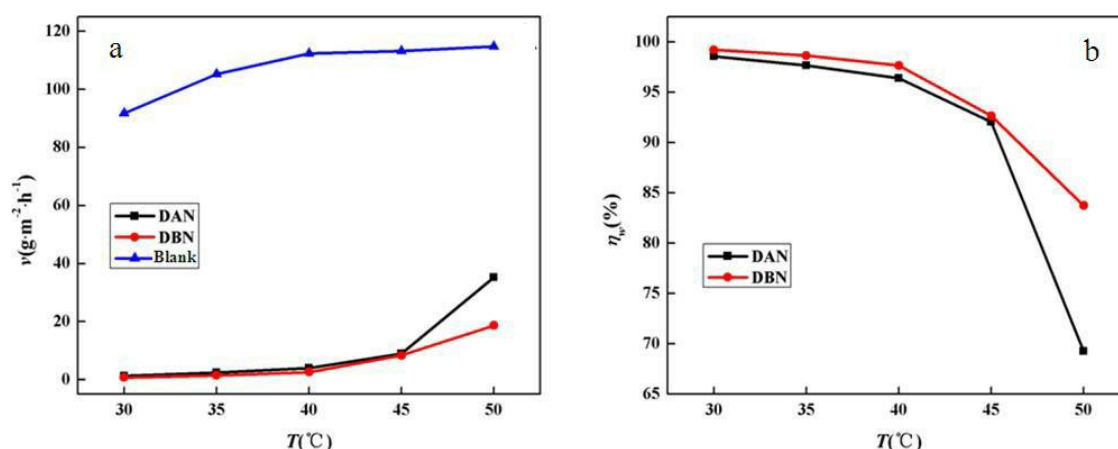
**Table 1.** Corrosion parameters for mild steel in a 1 M HCl solution with inhibitors concentrations range from 0.01 mM to 1.00 mM at 30 °C.

Conc.	DAN		DBN	
(mM)	CR (g·m <sup>-2</sup> ·h <sup>-1</sup> )	$\eta_w$ (%)	CR (g·m <sup>-2</sup> ·h <sup>-1</sup> )	$\eta_w$ (%)
Blank	80.90		92.15	
0.01	40.00	88.41	66.18	63.79
0.03	20.57	71.60	41.94	74.25
0.05	10.98	64.56	30.40	85.86
0.10	4.04	55.56	10.09	87.46
0.50	1.60	48.24	4.10	88.66
1.00	1.31	38.56	0.95	101.21

#### 3.1.2. Effect of Temperature

Temperature has great influence on the corrosion rate of metals. The effect of solution temperature (30–50 °C) on corrosion rate and inhibition efficiency is shown in Figure 2. Compared with blank solution, the corrosion rate was significantly decreased in presence of inhibitors. It means that the addition of DAN and DBN compounds greatly inhibits the corrosion of mild steel in 1 M HCl. The decrease in inhibition efficiency and increase in corrosion rate was observed with increase in temperature from 30 to 50 °C in the presence of 1 mM inhibitor, which may be attributed to the fact that the adsorption processes were spontaneous and irreversible with heat evolution, and the increase in temperature was not beneficial to the adsorption. The influence may also come from the weakening of electrostatic adsorption on the metal surface and the aggravation of desorption of the inhibitor molecule from the metal surface when the

temperature increases. In addition, the metallic corrosion in acidic environments is usually accompanied by the release of  $H_2$ , and the adsorption process of the inhibitor could be affected by the agitation caused by the acceleration of  $H_2$  evolution rates at higher temperature and lead to the decrease of corresponding inhibition efficiency.

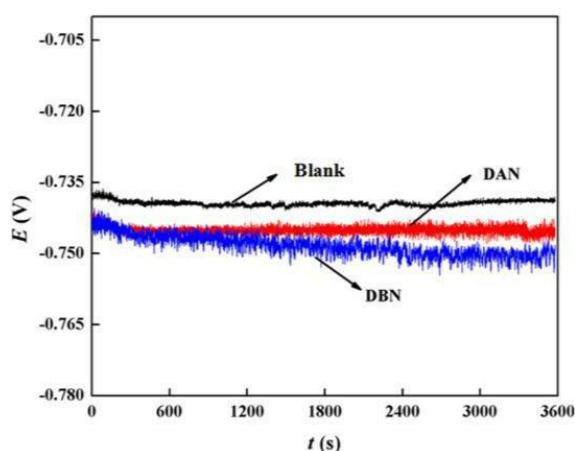


**Figure 2.** Variation of (a) corrosion rate and (b) inhibition efficiency of mild steel in 1 M HCl with 1 mM inhibitor under different temperature (30–50  $^{\circ}C$ ).[29]

### 3.2. Electrochemical Measurements

#### 3.2.1. OCP Measurement

Prior to each polarization or EIS experiment, the working electrodes were immersed in a 1 M HCl solution for 1 h to access the free corrosion potential or the quasi-stationary  $E_{oc}$  value. The plots of  $E_{oc}$  vs. time of AA5052 in the absence and presence of inhibitors for 1 h are given in Figure 3. For all test conditions, open circuit potential change (OCP) initially shifts fast towards a negative direction up to 200 s. However, it shows a very slow decline for the rest of the experiment time and finally attains a steady value in approximately 1 h. The slight oscillations in OCP curves revealed that destruction and formation of corrosion product layer occurred at the metal surface. The gradient shows that the surfaces of metals cannot achieve true steady states. In spite of this, the phenomenon indicates that there is a negligible change of OCP during the measurement period.[30]

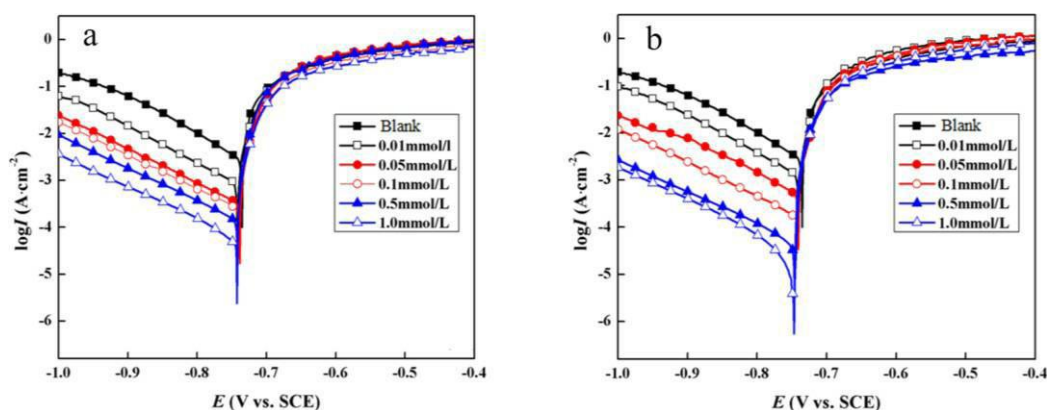


**Figure 3.** Open circuit potential change of AA5052 mild steel in 1 M HCl without inhibitor (Blank) and with different inhibitors added (DAN or DBN), respectively.[32]



### 3.2.2. Potentiodynamic Polarization

Potentiodynamic polarization profiles for AA5052 with different concentrations of DAN and DBN are presented in Figure4. The corrosion kinetics parameters such as corrosion potential ( $E_{\text{corr}}$ ), corrosion current density ( $I_{\text{corr}}$ ), and cathodic and anodic Tafel slopes ( $\beta_a$ ,  $\beta_c$ ) were given in Table 2, where the inhibition efficiency  $\eta_p$  (%) was calculated by the equation: of inhibitor (DAN or DBN), respectively.



**Figure 4.** Tafel plots for mild steel in 1 M HCl containing different concentrations of (a) DAN and (b) DBN.

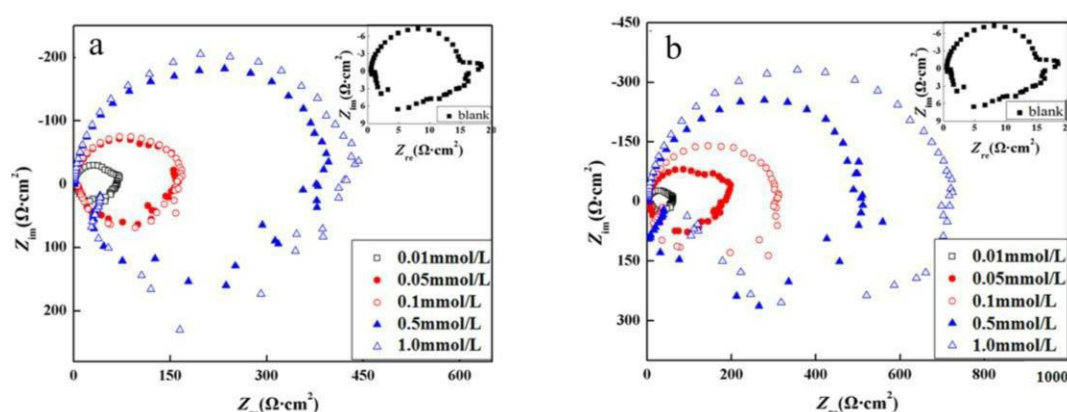
Compared with the blank solution, the cathodic currents were significantly decreased with the presence of inhibitors and the addition of these compounds made  $E_{\text{corr}}$  shifted towards negative potentials (Figure4), which suggested that DAN and DBN greatly reduced the hydrogen evolution reaction, but their inhibition effects on the anodic dissolution were unobvious. Besides, the addition of DAN and DBN shift the cathodic and anodic curves to lower values, while the concentration of inhibitors was increased.

**Table 2.** Tafel polarization parameters of the corrosion for mild steel in 1 M HCl containing different concentrations of DAN and DBN.

Inhibitor	C (mM)	$E_{\text{corr}}$	$I_{\text{corr}}$	$\beta_a$ (mV·dec <sup>-1</sup> )	$\beta_c$ (mV·dec <sup>-1</sup> )	$\eta_p$ (%)
DAN	Blank	-532.23	2562.22	145.25	95.25	
	0.01	-534.12	2003.21	135.21	90.25	70.12
	0.05	-526.25	1586.23	122.12	81.44	78.44
	0.10	-548.24	1322.21	111.01	78.11	85.25
	0.50	-523.25	800.25	95.25	65.21	92.11
	1.00	-539.12	400.28	88.24	58.22	97.54
DBN	0.01	-601.25	1158.22	118.25	85.22	57.21
	0.05	-607.11	958.25	109.25	78.25	62.55
	0.10	-612.14	801.11	95.25	68.24	71.25
	0.50	-625.44	502.88	88.25	55.24	78.25
	1.00	-666.36	310.21	65.44	41.12	81.25

That DAN and DBN belonged to mixed-type inhibitors, mainly inhibiting the cathodic processes. From Table 2, it is clearly seen that, when more inhibitors were added into the corrosive solution, the corrosion current density decreased and the inhibition efficiency increased. When the concentration of DAN or DBN reached 1 mM, the lowest  $I_{\text{corr}}$  values of  $63.6 \mu\text{A}\cdot\text{cm}^{-2}$  and  $33.5 \mu\text{A}\cdot\text{cm}^{-2}$  were obtained, and the inhibition efficiency achieved 97.77% and 98.83%, respectively. Generally, a compound is considered to anodic or cathodic type when the displacement in  $E_{\text{corr}}$  is greater than 85 mV; otherwise, inhibitor is considered as a mixed type. For DAN and DBN, the  $E_{\text{corr}}$  values shift towards more a negative direction compared with the blank solution, but the change is not significant whilst the most displacement of  $E_{\text{corr}}$  values is 10.9 mV, which indicated Electrochemical Impedance Spectroscopy (EIS)

Nyquist plots for mild steel in the absence and presence of various concentrations of DAN and DBN are given in Figure 5. The impedance spectra are consisted of capacitive loops at higher frequency and inductive loops at lower frequency. The presence of depressed semicircle in Nyquist plot across the studied frequency range indicates that a charge transfer process mainly controls the corrosion of aluminum. In different literature, comparable plots had been suggested for the corrosion of aluminum alloys in HCl solutions. The inductive loop is typically attributed to the rest manner with inside the oxide movie protected on steel surface. The reasons behind the deviations from perfect semicircles are usually involved with the frequency dispersion of interfacial impedance, which can be attributed to various kinds of physical phenomena such as active sites, surface roughness, and non-homogeneity of the solids. The diameter of the capacitive loop is enlarging gradually with increasing concentrations of inhibitor, indicating that the charge transfer resistance is increased and the adsorbed inhibitor forms a more compact monolayer on metal surface with an increasing amount of inhibitor.

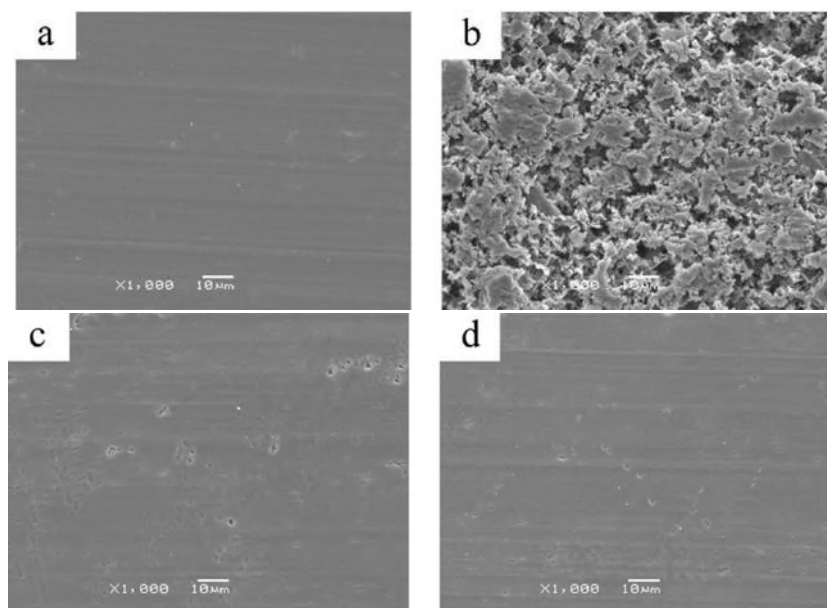


**Figure 5.** Nyquist diagrams for mild steel in 1 M HCl containing different concentrations of (a) DAN and (b) DBN.

### 3.3. Surface Morphology

SEM technique was employed to further prove the corrosion resistance ability of DAN and DBN, and the surface observation images of mild steel after a 2 h exposure in a HCl solution without and with inhibitors are shown in Figure 6. Before immersion, the naked aluminum plate appears very smooth (Figure 6a). In contrast, in the absence of inhibitor, the AA5052 presented a very rough surface covered with a huge amount of deep cracks and large holes, which suggests strong damage and a severe dissolution of mild steel in contact with aggressive solution (Figure 6b). Nevertheless, in Figure 6 c,d, the dissolution rate of mild steel was substantially inhibited by DAN and DBN, exhibiting a comparative smooth surface with a few small pits. Therefore, it is concluded that the regular distribution of the DAN or DBN molecules adsorbed on AA5052 surface generates consistent protective layers, which effectively prevent HCl molecules from penetrating into the aluminum surface.

**Figure 6.** SEM images of AA5052 surface before and after immersing in 1 M HCl for 2 h without and with triazinedithiol inhibitors. (a) Blank before immersion; (b) blank after immersion; (c) with DAN; (d) with DBN.[33]



#### 4. Conclusions

Two triazinedithiol compounds (DAN and DBN) as corrosion inhibitors for mild steel in a 1 M HCl solution were investigated. For DAN and DBN, their inhibition efficiency increased with increases in inhibitor concentration and they belonged to mixed-type inhibitors predominantly retarding the cathodic reaction. The inhibiting efficiencies determined by weight loss methods, potentiodynamic polarization testing, and EIS measurements are all in good agreement.

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## **A STUDY OF ENVIRONMENTAL AWARENESS AMONG THE HIGHER SECONDARY SCHOOL STUDENTS IN BONGAIGAON DISTRICT, ASSAM.**

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**ABSTRACT:** *The study attempts to highlight the environmental awareness among the higher secondary school students of Bongaigaon District in the state of Assam. The researcher, considering the nature of the problem, thought that the Present study comes under the domain of descriptive survey method. Population in the present study comprises of the higher secondary schools students of the Bongaigaon District, Assam. The investigator has collected the sample for his research work from a rural and urban area. For this study a sample of 180 higher secondary school students were selected from higher secondary schools of Bongaigaon District. For selecting the sample the researcher employed simple random sampling because here each and every sample has an equal chance of getting selected. In the present study Questionnaire was used for checking the awareness towards environment. The findings indicated that male students showed greater awareness than female students and urban students showed greater awareness than rural students in environmental awareness. Most of the male students are having better attitude than female students regarding environmental education and majority of the urban students expressed positive attitude than rural students towards environmental education.*

**KEYWORDS:** *Environmental awareness, Environmental education Students, Higher secondary schools, Gender, Locality.*

### **1. INTRODUCTION-**

There has always been a strong interconnection between people and their environment. People are a part of nature and his survival is linked with the quality of the environment. Man has created an imbalanced and immense exploitation of natural resources to fulfil his needs. If environmental pollution keeps on increasing at the present rate, the very existence of life on earth is endangered. There is a vital need to create awareness amongst the people about environment and its allied problems. The educational curricula in schools have been undergoing changes and attempts have been made to make the teaching-learning more environment based. There is a need to promote awareness among the students that the protection of our environment is of utmost importance for maintaining proper ecological balance, commitment to solve environmental problems and for our own survival. There is a great need to bring the students to a heightened awareness of the environmental problems that threaten us and to motivate them to discover favourable solutions to those problems. Students should be helped to develop critical thinking and creative problem-solving ability in order to find the causes of environmental problems and arrive at strategies for environmental protection and preservation.

### **2. LITERATURE REVIEW:**

**Gopinath, G. (2014)** conducted study on the environmental awareness among secondary school students in a District of Kerala State. The investigator was used Random sampling to select 158 secondary school students for the study. Normative survey method was employed for the present investigation. Environmental Awareness Scale constructed by the investigator was used to collect the information. The findings reveal that



female students have a higher level of awareness regarding the environment, urban student's awareness more than rural students and Malayalam Medium students have a higher level of awareness than English medium students regarding the environment.

**H., D., C. and R., P. (2017)** conducted study on environmental awareness among secondary school students. For this study a sample of 300 secondary students were selected by the investigator using simple random sampling technique. The findings reveal that 48% of the students have moderate level of environmental awareness, 26% of the students belong to high level of environmental awareness and the rest 26% of the students belong to low level of environmental awareness. Private school students have more environmental awareness than governmental school students.

**Medhi, R. (2018)** conducted study on environmental awareness among high school students of Kamrup District. Descriptive survey was employed for the present study. The sample consisted of 100 high school students were selected through simple random sampling. This study has found that there exists no significant difference in environmental awareness of boys and girls students and private schools students showed greater environmental awareness than government aided school students.

### 3. SIGNIFICANCE OF THE STUDY:

One of the most crucial situations in the present world is pollution and loss of natural resources. The district of Bongaigaon is no exception to it. The rate of population of this district has increased to a great dimension. As a result natural forest is getting spoilt. So it has a significant effect on environment. The way of coming out of this problem is to create environmental awareness in every step of life. Motivation for awareness about environment should begin at a very early level in schools. It is therefore necessary that such studies that evaluate the awareness about the environment especially among students. So the students of higher secondary level from some schools of Bongaigaon District are included in the present research work to study their environmental awareness.

### 4. OBJECTIVES OF THE STUDY:

- To Study the awareness of environment among the higher secondary school students on the basis of gender.
- To Study the awareness of environment among the higher secondary school students on the basis of locality.
- To study the attitude of the environmental education among the higher secondary school students on the basis of gender.
- To study the attitude of the environmental education among the higher secondary school students on the basis of locality.

### 5. DELIMITATION OF THE STUDY :

- The study is delimited to 180 higher secondary students.
- The present study is delimited to higher secondary school students of District Bongaigaon, Assam.
- The present study has involved rural as well as urban area of District Bongaigaon, Assam.

### 6. METHODOLOGY:

**Research method:** The researcher, considering the nature of the problem, thought that the Present study comes under the domain of descriptive survey method.

**Population:** Population in the present study comprises of the higher secondary schools students of the Bongaigaon District, Assam.

**Sample:** The investigator has collected the sample for his research work from a rural and urban area. For this study a sample of 180 higher secondary school students were selected from higher secondary schools of Bongaigaon District. For selecting the sample the researcher employed simple random sampling because here each and every sample has an equal chance of getting selected.

**Tool:** In the present study Questionnaire was used for checking the awareness towards environment.

## 7. ANALYSIS AND DISCUSSION:

- Table No.1 shows the number and percentages of all respondent's awareness towards environment on the basis of gender.

**Table No. 1 Awareness of students towards environment**

Gender	Male and female students awareness towards environment				Total	
	Yes		No			
	No's	%	No's	%	No's	%
Male	58	64.44	32	35.56	90	100
Female	41	45.56	49	54.44	90	100

Source: Field survey

As shown in Table No. 1 highlights that out of the 90 male student's respondents, 64.44% have awareness regarding the environment and the rest 35.56% have not awareness regarding the environment. Among the 90 female students 45.56% expressed awareness towards environment and 54.44% have not awareness towards environment.

- Table No.2 shows the number and percentages of urban and rural students awareness regarding environment.

**Table No. 2 Urban and rural students awareness regarding environment.**

Locality	Rural and urban students towards environment				Total	
	Yes		No			
	No's	%	No's	%	No's	%
Urban	56	62.22	34	37.78	90	100
Rural	43	47.78	47	52.22	90	100

Source: Field survey

Analyzed data presented in Table No. 1 shows that Out of 90 urban students 62.22% expressed awareness in their environment and 37.78% have not awareness regarding environment and among 90 students 47.78% have awareness, 52.22% have not awareness in their environment.

- Table No.3 shows the number and percentages of students attitude towards environmental education on the basis of gender.

**Table No. 3 Male and female students attitude towards environmental education.**

Gender	Male and female students attitude towards environmental education				Total	
	Positive		Negative			
	No's	%	No's	%	No's	%
Male	69	76.67	21	23.33	90	100
Female	61	67.78	29	32.22	90	100

Source: Field survey

As shown in Table No. 3 highlights that out of 90 male student respondents, 76.67% support the environmental education and 23.33% do not support it. Out of 90 female student respondents 67.78% expressed positive attitude and 32.22% expressed negative attitude.

- Table No.4 shows the number and percentages of students attitude towards environmental education on the basis of area.

**Table No. 4 Rural and urban students attitude towards environmental education.**

Locality	Rural and urban students attitude towards environmental education				Total	
	Positive		Negative			
	No's	%	No's	%	No's	%
Urban	71	78.89	19	21.11	90	100
Rural	59	65.56	31	34.44	90	100

Source: Field survey

Analyzed data presented in Table No. 4 shows that 90 urban students respondents 78.89% are in favour of environmental education in the higher secondary schools while the rest 21.11% are not in favour of it. The table also highlights that among 90 rural students respondents 65.56% have positive attitude and 34.44% have negative attitude towards environmental education.

## 8. MAJOR FINDINGS:

The findings from the present study are grounded as under.

- This study has found that male students showed greater awareness than female higher secondary students in their environment, as boys are more perseverant towards their environment.
- Majority of the urban students showed greater awareness than rural students in environmental awareness.
- Most of the male students are having better attitude than female students regarding environmental education.
- Majority of the urban students expressed healthy attitude than rural students towards environmental education.

## 9. SUGGESTIONS:

- Higher secondary students should take part in various environmental seminars organized by the school.
- Children should contribute significantly in preserving the environment.
- Parents should teach their children the use of dust bins, how to keep their surroundings clean.
- Teachers should provide project based activities to students so that students are close to nature. Environmental issues should be taught by the teacher.
- Teacher should treat environment education as important subject rather than just as a subject for syllabus coverage and examination.
- Teachers must acquaint their students about pros and cons of environmental pollution.
- Government should take initiative to make environmental education a compulsory subject.

## 10. CONCLUSION:

The present study was conducted to find out the level of environmental awareness amongst higher secondary school students in Bongaigaon District, Assam. The overall level of environmental awareness of the students was good. The researcher feels that environmental education has not been given priority in the higher secondary school. No separate environmental education textbook had been prescribed for the higher secondary school students. The major concern should be to provide environmental knowledge and skills, to inculcate healthy attitude combined with the practical applications of that knowledge. Students have to be encouraged to actively participate in the preservation and improvement of the environment. . Environmental education is an important technique through which the goals for awareness can be achieved easily. This is the crucial time for inculcate the environmental awareness among the people particularly among students.

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Automation, Computer Science and Technology Department,  
Kryvyi Rih National University, Ukraine and 'Research Culture Society'.

### An insight into the flow-chart development of fault tolerant MPCR routing energy efficient protocol in WSNs

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**Abstract :** *In this paper, the design & development of routing protocols using 3 improvised algorithms is presented, viz., MPCR algorithms. The MPCR algorithm is an improvised algorithm that is implemented for minimizing the energy required for the transfer of the data packets from the source to the destination in minimal times. Here, we have presented the brief outcomes of the proposed works with simulation results. The results show the efficacy of the methodology that is being developed. This paper also demonstrates the various results obtained for all the test cases along with the necessary observations and explanations in the form of discussions and diagrammatic representations. The paper finally concludes with the overall conclusions of the MPCR work.*

**Keywords :** WSN, Static, Dynamic, Packets, Authentication, Sensor, Node, Distribution, Network, Key, Message Authentication Code Protocol, Security, Routing, Management, Sink, Cryptography, Source, Energy, Router, Attacker, Base Station, Machine condition monitoring, Industrial wireless sensor networks, Cooperative communication, Medium access control, Indoor industrial monitoring, Energy efficiency, Space time block, Stability.

#### 1. INTRODUCTION:

Efficient Fault-Tolerant Routing in IoT Wireless Sensor Networks Based on Bipartite-Flow Graph Modeling. ... Once one or more CHs fail, the faulty CHs cannot forward the sensed data of their serving sensor nodes. As a result, the sink node (gateway) has not sufficient sensed data of the IoT application field. The terminology of fault tolerant relates to a design capable to continue its operation, probably at a lower efficiency level, instead of failing utterly, when some part of the system fails. ... Fault tolerance is one of the critical issues in Wireless Sensor Network (WSN) applications. ... WSNs experience failure problems due to various factors such as power depletion, environmental impact, radio interference, asymmetric communication links, dislocation of sensor node and collision.

Fault tolerance ensures that a system is available for use without any interruption in the presence of faults; thus fault tolerance increases the reliability, availability, and consequently dependability of the system. The most popular approach for fault tolerance is the multipath routing where a set of multiple paths between the source nodes and the sink are determined at the expense of increased energy consumption and traffic generation. Multipath routing provides additional benefits of load balancing and bandwidth aggregation [100].

## 2. MPCR Algorithm:

MPCR : To begin with, we present the MPCR revised algorithm for routing purposes. The work done could be categorized into different phases such as the

- discovery phase,
- request phase,
- routing phase & the
- transmission phase

which are explained one after the other in succession.

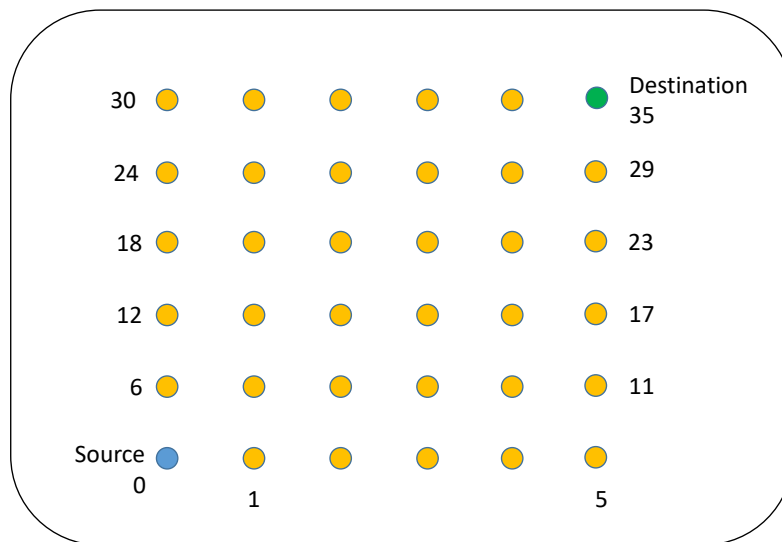
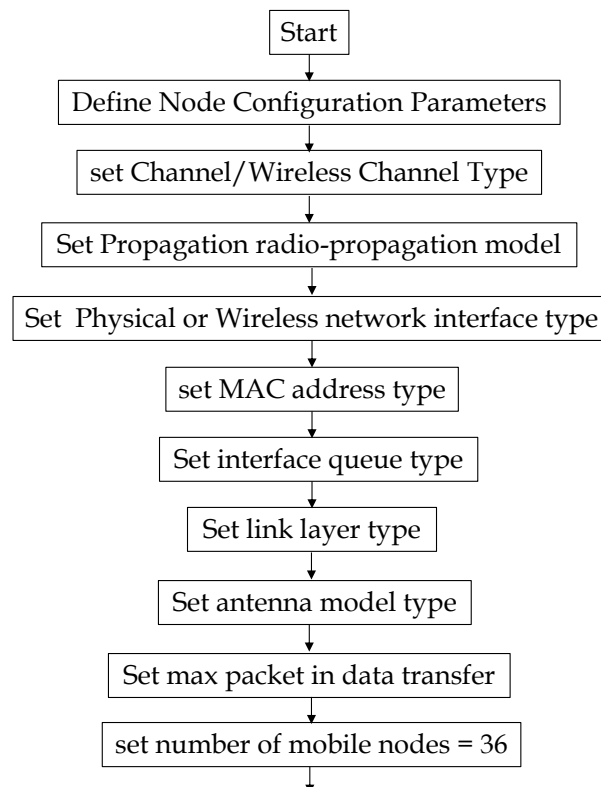


Fig. 1 : Layout of the sensor nodes

The network layer, i.e., the layout of the network nodes such as the sink, source, intermediate nodes is shown in the Fig. 1 along with the flow chart of the MPCR algo as shown in the Fig. 2.





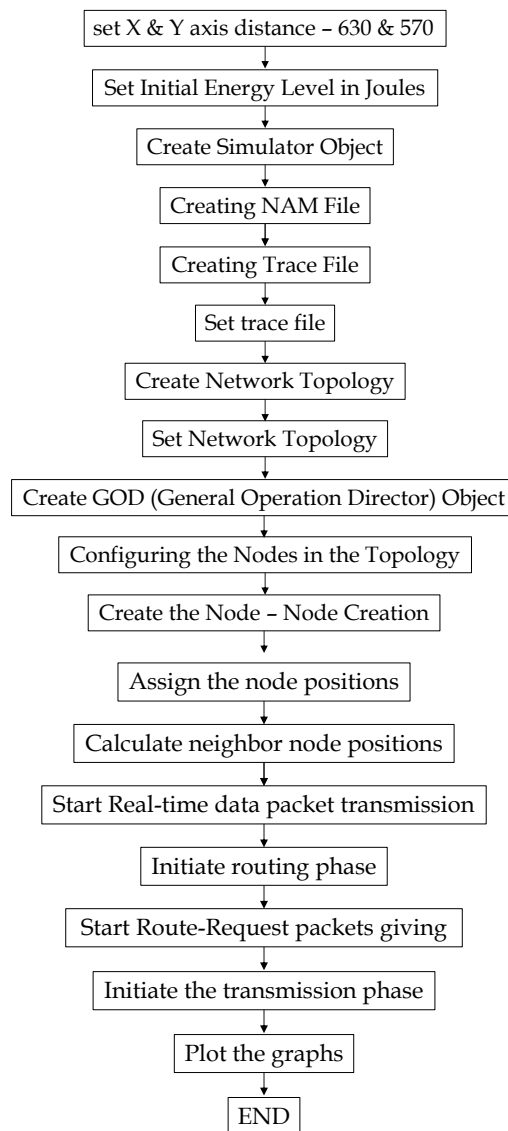


Fig. 2 : Flow chart / data flow diagram of the distributed routing scheme process

The coding (script writing) w.r.t. the wireless sensor network is developed in the NS2 tool by writing .tcl scripts as per the above mentioned flow chart and once it is completed, it is tested for its effectiveness as per the algo steps given in the flow chart. The simulation is run & the results are observed both for the individual parameters as well as for the comparison ones. The results are shown in the Figs. 3 to 10 respectively. The different plots that are obtained are as follows.

- Plot of packet delivery ratio (PDR) as a function of time
- Plot of throughput as a function of time
- Plot of energy consumed by the sensor nodes as a function of time
- Plot of packet drop delay as a function of time
- Plot showing the comparison of packet delivery ratio with the existing ones, PDD is compared with the shortest path algo (green) & the normal mechanism (blue), proposed showing the better results compared to the others as existing systems are not producing much throughputs
- Plot of packet-loss comparison v/s time with the existing systems, proposed (red) showing better results compared to (shortest path – green & the normal system - blue), showing better results as the cooperative mechanisms are being used for the transmission purposes
- Plot of energy consumed v/s time & comparison with the existing systems
- Plot of throughput v/s time & comparison with the existing methods

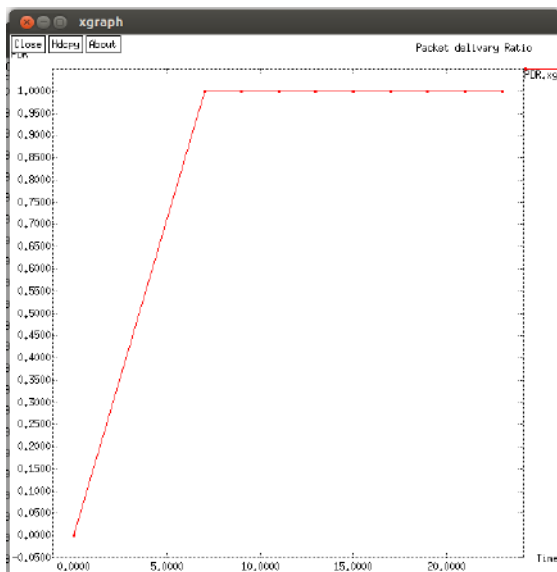


Fig. 3 : Plot of packet delivery ratio (PDR) as a function of time

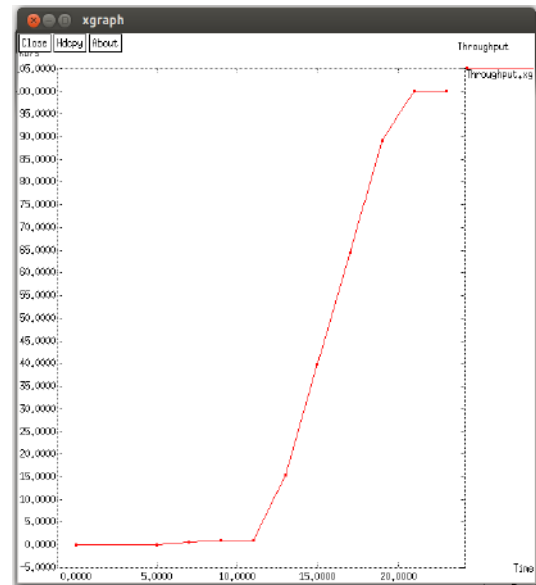


Fig. 4 : Plot of throughput as a function of time

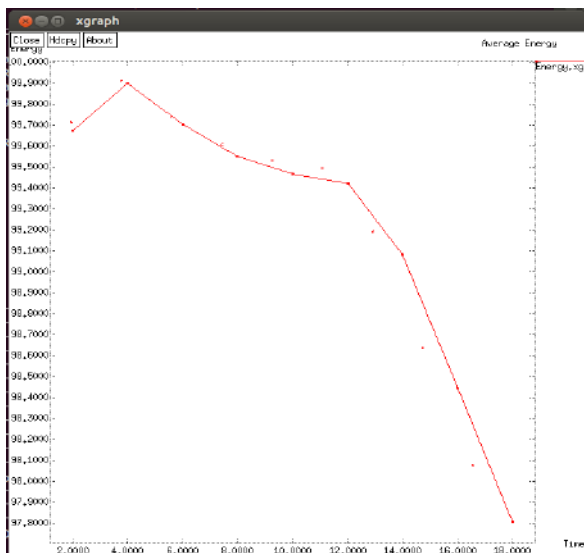


Fig. 5 : Plot of energy consumed by the sensor nodes as a function of time

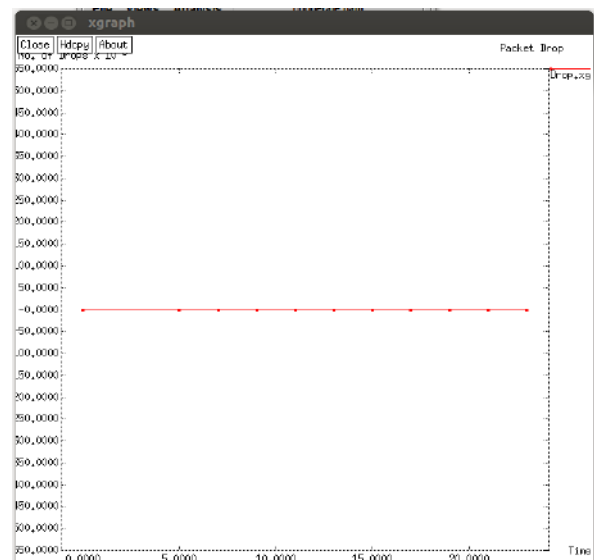


Fig. 6 : Plot of packet drop delay as a function of time

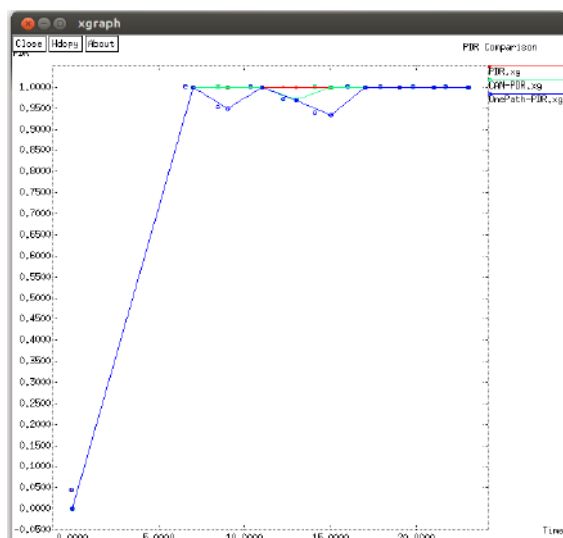


Fig. 7 : Plot showing the comparison of packet delivery ratio with the existing ones, PDD is compared with the shortest path algo (green) & the normal mechanism (blue), proposed showing the better results compared to the others as existing systems are not producing much throughputs

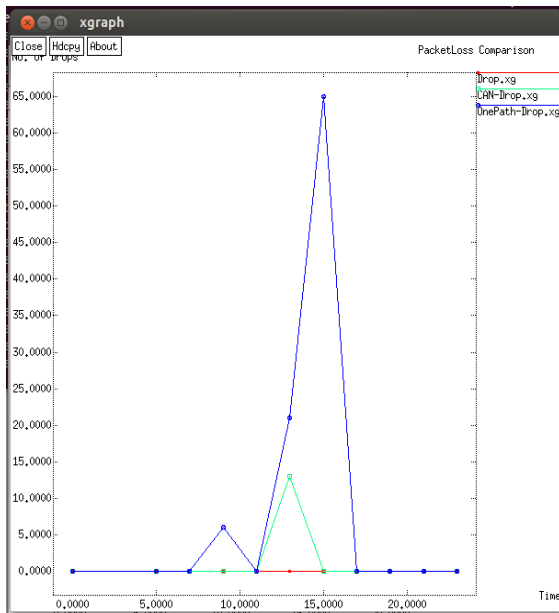


Fig. 8 : Plot of packet-loss comparison v/s time with the existing systems, proposed (red) showing better results compared to (shortest path – green & the normal system - blue), showing better results as the cooperative mechanisms are being used for the transmission purposes.

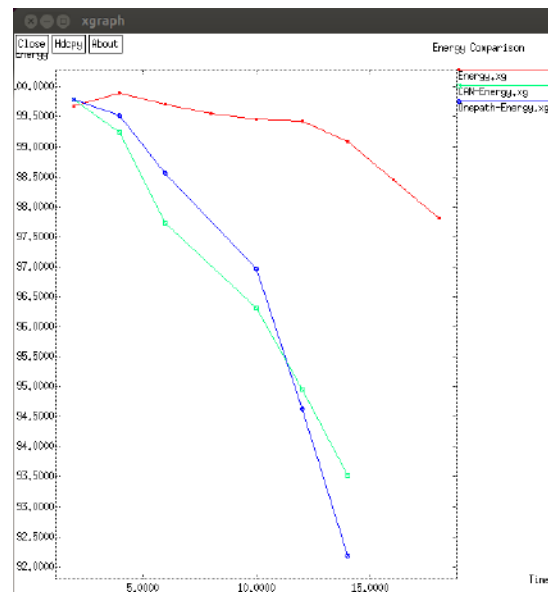


Fig. 9 : Plot of energy consumed v/s time & comparison with the existing systems

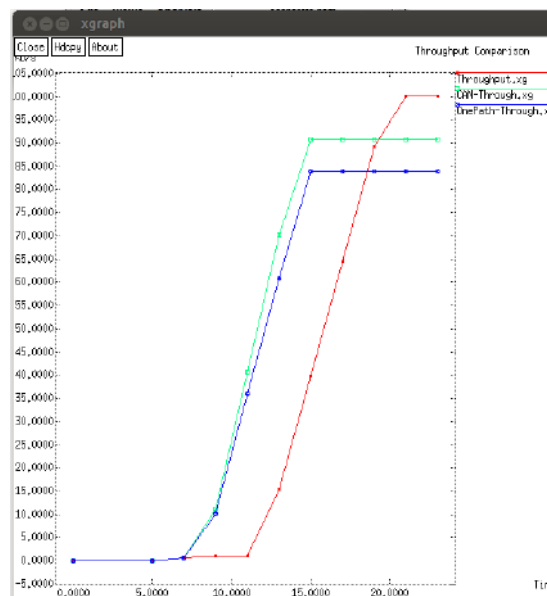


Fig. 10 : Plot of throughput v/s time & comparison with the existing methods

### 3. CONCLUSIONS:

In this research paper, the design & development of a data centric multipath routing protocols in WSNs using MPCR with enhancement in their lifetimes and reduced energies is being presented along with the simulation results. The simulation results show the effectivity of the methodology adopted. Here, an improvised / enhanced version of the MPCR protocol development for the WSNs

and by comparing its performance with existing system by using some rejuvenated & improvised routing security routing protocol schemes is presented. From the results, it can be inferred that after each round, the number of data packets received by the sink increases, thus reducing the power energy consumption, thus providing a better throughput.

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**In-silico approaches to construct chimeric proteins having dimers**

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**Abstract:** Various studies have demonstrated the correlation between the amino acid composition and structure of proteins. This correlation might be the ideal approach to understand the structure of proteins instead of producing them in a wet lab. The generation of chimeric or fusion proteins has revolutionized the field of biotechnology. It is found that these chimeric proteins are important considerations for drug targeting and delivery, but it is a time consuming, laborious, and very costly process. For the construction of recombinant fusion proteins, the final product must be the same as the proposed biologics. Also, the selection of suitable partner proteins, achieving dimerization, reducing the conformation changes, and maintaining the functionality of both partner proteins are the key challenges. This study is an in-silico attempt to achieve these characteristics before transforming the therapeutic proteins in a wet lab. Here, the suitability of the COTH server for achieving the dimer formation for fusion/chimeric proteins was explored. Further, the validity of modeled structures was tested by Ramachandran plots. This study has implications in the formation of stable dimeric recombinant chimera for therapeutic purposes.

### **1. Introduction:**

Determining the protein structure and its function from the amino acid length and composition are the aims of protein bioinformatics. It is assumed that the protein structures can be predicted successfully using the information on the amino acid composition of a protein. The methods of protein bioinformatics are useful for the prediction of subcellular localization, enzyme subclasses, domain boundaries, signal sequences, and unfolded segments in protein sequences with remarkable prediction accuracy (average error of the most successful method is 3.4%) [1]. “Sequence implies the Structure and Structure implies the Function” is the key to protein biology. Due to advancements in sequencing techniques, the amount of available sequences is huge but this information is useless until its transformation into structures. As it is difficult to express these all sequences in a wet lab, further the determination of protein structure by XRD and NMR is highly expensive and time-consuming. Therefore, it is the best way to predict the protein structure in the dry lab. It is also required because the functionality of a protein mainly depends on its native structure. Homology modeling, Threading, or Fold recognition, and *ab initio* methods are routinely used algorithms for protein structure determination based on the sequence information.

The in-silico approaches are very useful and accurate for predicting the structures of simple or small proteins. However, predicting the structures of complex or lengthy proteins is quite tricky and difficult. Further, the modeling of chimeric proteins (protein 1 + protein 2) is a very complex process and needs proper skills. The chimeric proteins having Immunoglobulin base like Etanercept (hup75 TNFR-huIgG1), Abatacept (*Orencia*: CTLA4-Ig), Rilonacept (IL-1R-IL-1R accessory protein-IgG1), AS1409 (IL-12-EDB Fibronectin), Aflibercept (VEGF binding protein-IgG1), Alefacept (CD2-binding portion of LFA-3-IgG1), Romiplostim (Thrombopoietin receptor c-Mpl-IgG1), PRO-542 (CD4-immunoglobulin G2) have promising therapeutic values. Therefore, many R&Ds are working on designing and commercializing chimeric proteins. At the same time, the

dimeric structure of these chimeric proteins is also desirable. This study is an attempt to explore the in-silico approaches to construct chimeric proteins having dimers.

## 2. Materials and Methods :

### 2.1 Amino Acid Sequences

The amino acid sequences of target proteins were obtained from the Uniprot database. Each sequence has a Protein Data Bank (PDB) entry code and a Uniprot id. The selected sequences were analyzed for their sequence similarity using the BLAST program.

**2.2 UniProt** is a freely available protein database that provides comprehensive and high-quality sequence and functional information of given proteins. The UniProt consortium comprises the European Bioinformatics Institute (EBI), the Swiss Institute of Bioinformatics (SIB), and the Protein Information Resource (PIR) (Adapted from Uniprot database, <http://www.uniprot.org>) [2].

**2.3** After getting the right sequences, *in-silico* we required a suitable tool for the generation and prediction of fusion proteins. Several algorithms (tools) are available for protein prediction. I-TASSER was remained in the first position for protein structure prediction according to the CASP (Critical Assessment of protein Structure Prediction) 2006-2012. HHpred was the leading server for template-based protein structure prediction in CASP 2010. For homology modeling, SWISS-MODEL, MODELLER, and YASARA tools are commonly used. Prediction of peptide structures from amino acid sequences is done by PEP-FOLD. QUARK and Bhageerath are used for ab initio protein structure modeling. For folding simulations Abalone is useful. Rossetta is a highly accessible online server having many useful tools. The Foldit program is helpful for pattern-recognition. These tools are mainly used for monomer prediction. By using I-TASSER, we can generate and analyze the single-chain fusion proteins [3]. But, here the main focus of our study is to determine the formation of dimer or homodimer structures. For this, we started our search for suitable tools. PREDDIMER predicts the dimer structure of transmembrane proteins. HOMCOS 1.0 is a server used for the prediction of binding sites and protein pairs of protein-protein interaction. Finally, we found the **COTH (CO-THreader)** server suitable for our study [4].

**COTH (CO-THreader)** server is an online service for the prediction of protein complex structure. COTH predicts the protein complex structures from the primary amino acid sequence by threading based approach. We have submitted fused sequences (FASTA sequence of cytokine without stop codon followed by FASTA sequence of Immunoglobulin domains with stop codon). COTH processed and gave the final structures in form of a **.pdb file**.

**2.4 The Protein Data Bank (.pdb) file format** is a textual file format that provides the three-dimensional structural information, annotation of protein, and nucleic acid structures including atomic coordinates, observed side-chain rotamers, secondary structure assignments, as well as atomic connectivity [5].

**2.5 Pymol** is a structure visualization tool. The .pdb files, generated by Various servers were downloaded and visualized in the Pymol tool [6].

**2.6** We have used the **ExPASy tool ProtParam** for Physico-chemical analyses particularly the amino acid composition of partner proteins.

**2.7 The DrugBank** database is a unique bioinformatics and cheminformatics resource that combines detailed drug (i.e. chemical, pharmacological, and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information. The database contains 7737 drug entries including 1585 FDA-approved small molecule drugs, 158 FDA-approved biotech (protein/peptide) drugs, 89 nutraceuticals, and over 6000 experimental drugs. Additionally, 4281 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries (Adapted from DrugBank database, <http://www.drugbank.ca/>).

### 2.8 Validation of structure

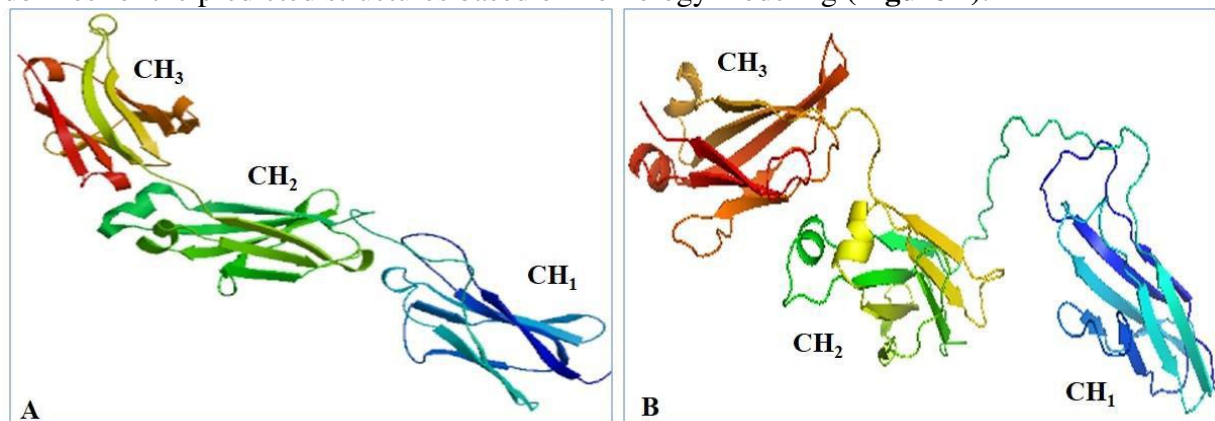
We validated the modeled structures by Ramachandran plot and superimposition of structures.



### 3. Results and Discussion:

#### 3.1 Prediction of single-chain structure

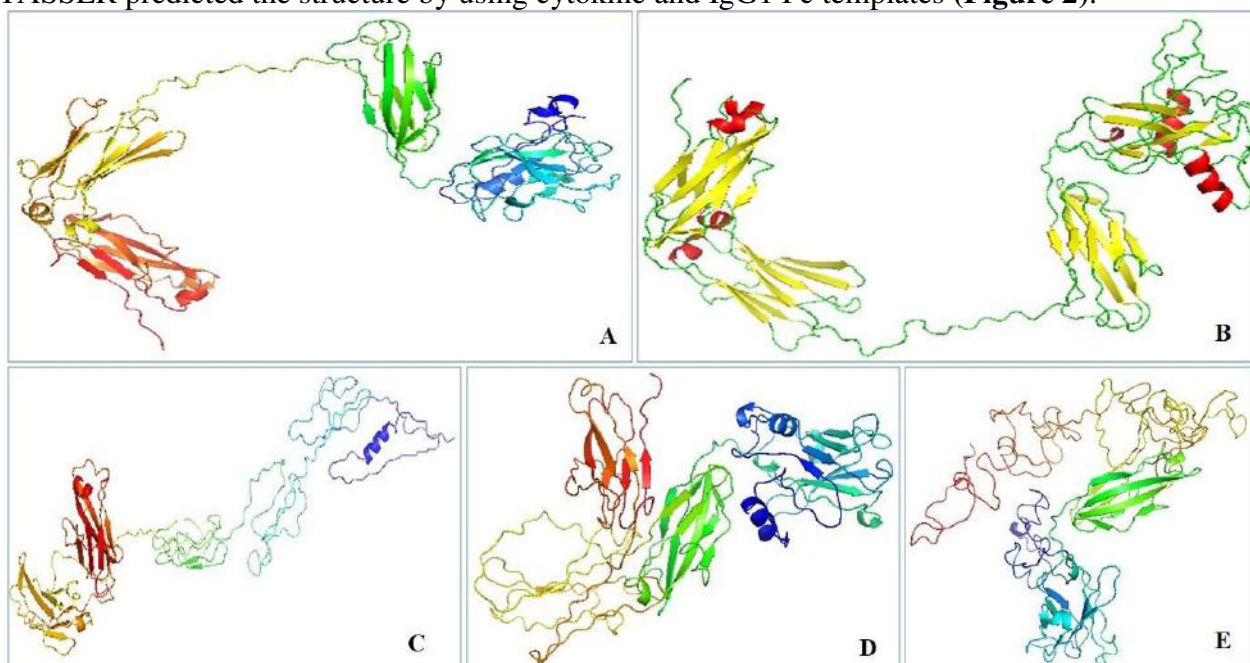
The structure of a single-chain of IgG1 was predicted by various tools like used I-TASSER [3], RaptorX [7], and the Swiss model [8] for single-chain fusion protein prediction. The sequence of IgG1 domains (CH1-CH2-CH3) was submitted to the respective servers. The servers provided .pdb files for the predicted structures based on homology modeling (**Figure 1**).



**Figure 1: Prediction of single-chain structure:** the figure depicts the structure for IgG1 (CH1-CH2-CH3) domains generated by the Swiss model (A) and I-TASSER (B).

#### 3.2 Prediction of single-chain chimeric structure

The sequences of IgG1 Fc and one protein of interest (for example cytokine) were fused and submitted to the various servers for prediction of the chimeric structures. Many servers were not able to give the desired structures due to the unavailability of proper sequences for homology modeling. But I-TASSER successfully provided the chimeric structures by using two different templates based on the submitted sequences. In this case, we fused cytokine with IgG1 Fc and I-TASSER predicted the structure by using cytokine and IgG1 Fc templates (**Figure 2**).

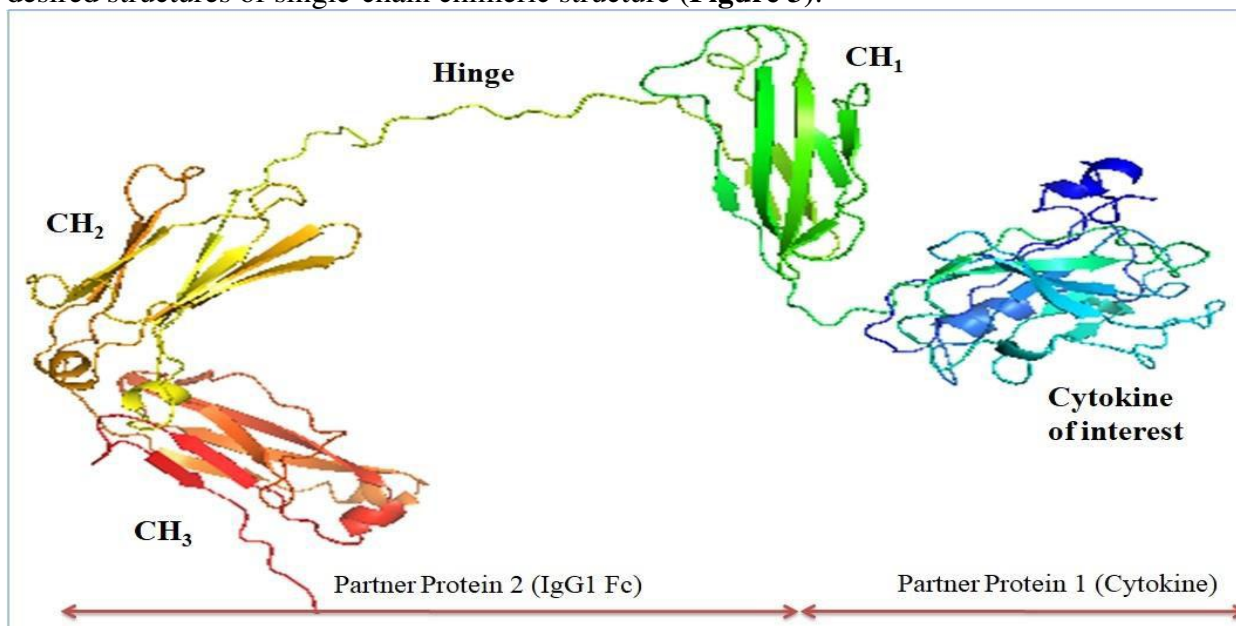


**Figure 2: Prediction of single-chain chimeric structure:** the figure depicts the structure for fused sequence generated by I-TASSER: Model 1 (A) to Model 5 (E).

#### 3.3 Detailed analysis of different models

The above result stated that I-TASSER provided five different modeled structures for one single fused sequence. So here the question arises which is the best suited for our study. As per the

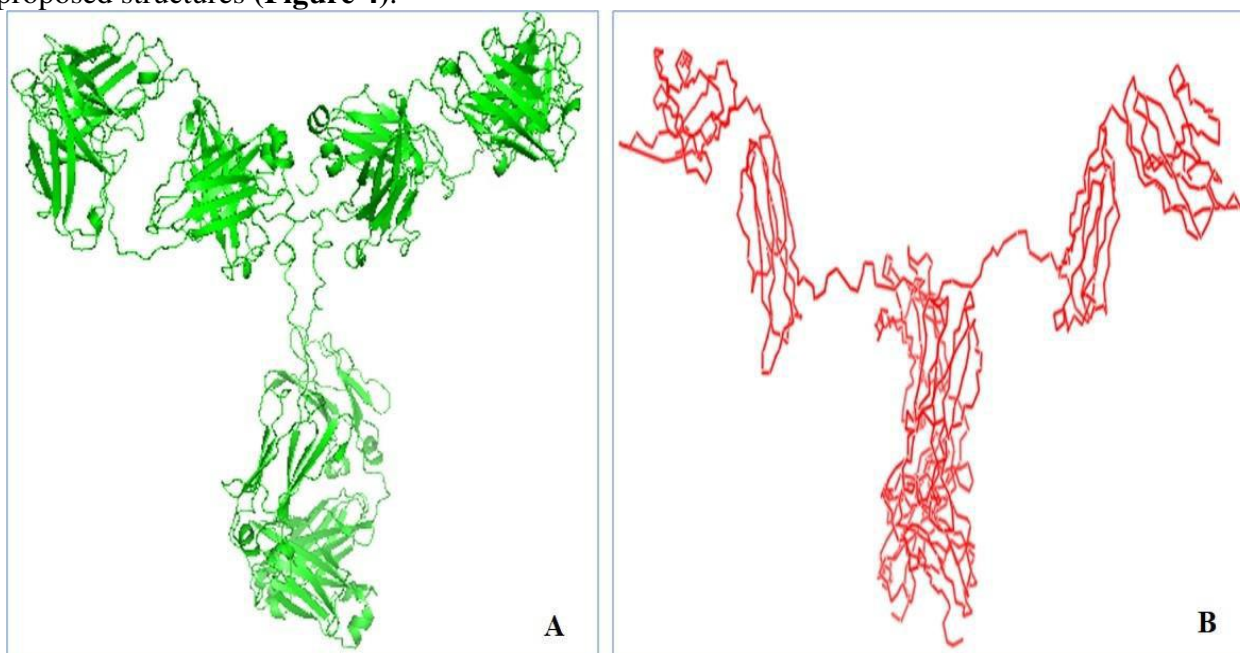
first view, model 1 and model 2 were most closure to the proposed structure. When we critically analyzed the templates used by I-TASSER, it was found that for these two models the template was the same as the input sequence i.e., cytokine and IgG1. Therefore, model 1 and model 2 are the desired structures of single-chain chimeric structure (**Figure 3**).



**Figure 3: Prediction of single-chain chimeric structure:** here model 2 was explored for further studies as it is closure to the proposed molecule.

### 3.4 Prediction of the chimeric structure having dimers

The main objective of this study was to predict the dimeric structures of chimeric proteins. After trying various algorithm, this study establishes COTH as the most suitable server for the prediction of dimeric structures based on homology modeling. COTH also uses different templates based on input sequences. In this study, we used the known structure of IgG1 to compare with the COTH generated structure. It was found that COTH generates the dimeric structure similar to the proposed structures (**Figure 4**).



**Figure 4: Prediction of the chimeric structure having dimer:** here the known structure of IgG1 (A) was used to compare with the COTH generated model (B).

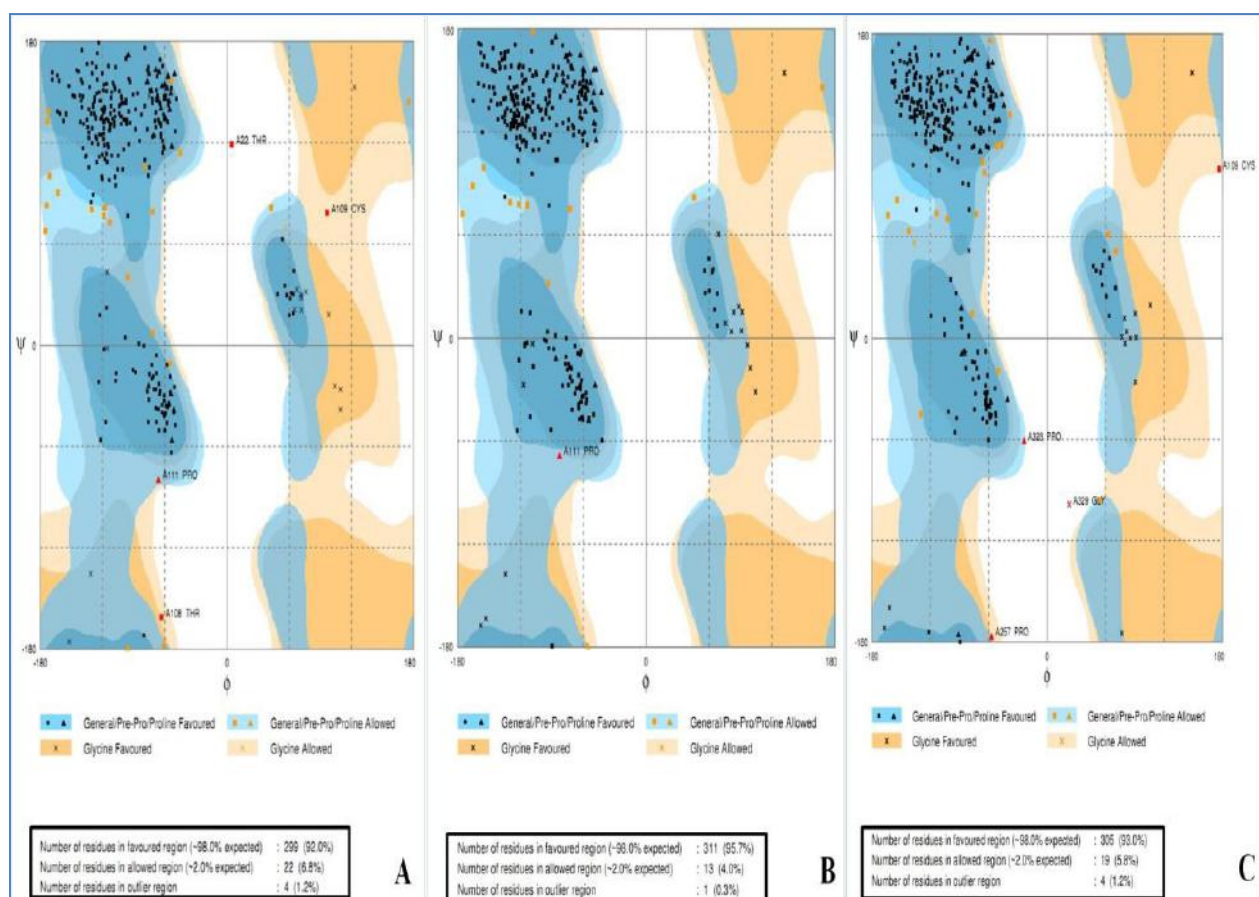


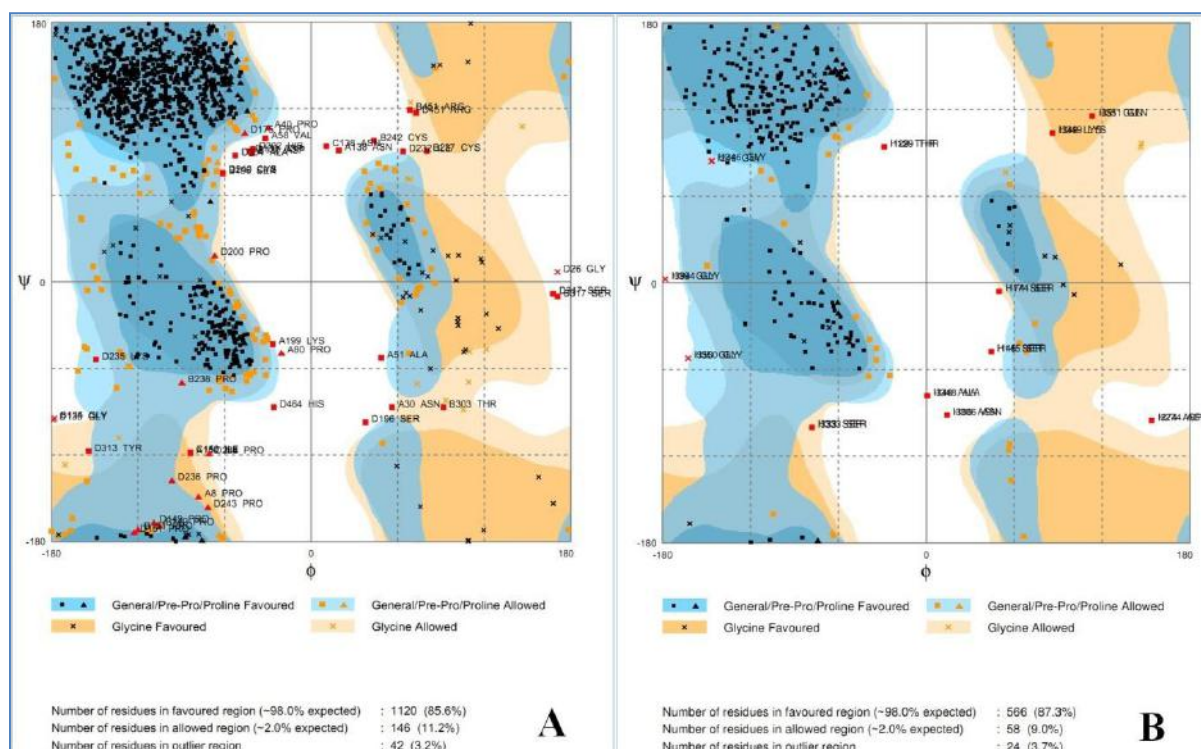
### 3.5 Structural Validation

To test the validity of predicted models, the Ramachandran plot was generated by Rampage [9] and Molprobit [10]. The residues in the Preferred Region, Allowed Regions, and Outliers were counted and compared. For example, the structure of the Fc region of IgG1 (CH1-CH2-CH3) was submitted and the Ramachandran plot was generated. This Ramachandran plot was compared with the Ramachandran plot of models 1 and 2 generated by I-TASSER. As the original aim of the study to determine, the feasibility of the in-silico approach to make the dimeric structure and test the validity of these structures. For example, the structure for IgG1 whole (with VH and without any light chain) was generated by COTH and its Ramachandran plot was compared with the Ramachandran plot of original IgG1. The overall results suggest that the structures generated by I-TASSER and COTH are valid and favorable.

**Table 1: Comparison of Ramachandran plots**

Residues in	Original IgG1 Fc	Model 1	Model 2	Whole IgG1 Original	Predicted IgG1 (No light chain)
Preferred Region	299 (92.0%)	311 (95.7%)	305 (93.0%)	1120 (85.6%)	566 (87.3%)
Allowed Regions	22 (6.8%)	13 (4.0%)	19 (5.8%)	146 (11.2%)	58 (9.0%)
Outliers	4 (1.2%)	1 (0.3%)	4 (1.2%)	42 (3.2%)	24 (3.7%)





#### 4. Conclusion:

As per our understanding and knowledge, we are the first group that is trying to explore the in-silico approach for constructing functional chimeric proteins having dimers. We have reported that the length of chimeric proteins and amino acid composition (particularly, hydrophobic content, cysteine content, and its disulfide bond formation property) are essential for homodimer formation [11]. We also demonstrated the feasibility of linkers for achieving the dimer formation of chimeric proteins [12]. This study is useful in the evaluation of therapeutic proteins particularly, the dimerization of chimeric proteins in-silico. before going to make any therapeutic structure, it is better to look for its properties including dimer formation capacity, to obtain the desired efficacy.

#### Acknowledgment

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**Automation, Computer Science and Technology Department,  
Kryvyi Rih National University, Ukraine and 'Research Culture Society'.**

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## **An outline of an Electronic resources among State university libraries of Gujarat**

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**Abstract:** *The study examines the perception and use of Electronic resources (e-resources) among users of selected eight State university libraries of Gujarat. The well-structured questionnaires were distributed among users (faculty, research scholar and students). In each university 300 questionnaires were distributed among five selected disciplines (Arts, Commerce, Education, Science and Law), hence the total 2400 questionnaires were distributed among eight State University libraries. The analyses revealed that the users of state university libraries were satisfied with the online resources provided to them, they prefer it most because of its easy and convenient availability, multidimensional interaction, easy to preserve and independence infrastructure.*

**Keywords:** *E-Resources, Electronic resources, Online resources, Gujarat, State universities, State University libraries, State University libraries of Gujarat.*

### **1. Introduction:**

Nowadays usually all the individuals use to access internet for various daily chores such as e-mail, job search, knowledge update, daily news, access various digital format for their research work, academic news etc. ICT is now the most widely accepted concept in the world. On the other hand, the meaning of information technology is the blending of different digital products whether its processing processes and collecting, storing, transmitting data etc. It covers all aspects of arts or science of processing data to produce data. IT has transforming the human society to knowledge society where information is the mainstay and life-blood of both individuals and for academic organizations. In the last few decades ICT has changed the way in teaching, learning and research activities in higher education. ICT has helped to overcome the barriers of time and space and reduced time gap between the producer of information and its consumption by the end user. University library, as a sub-system of higher education, should act as a trend-setter in adopting ICT in its activities. Challenges to the traditional library activities and this inspires the necessity for university libraries to adopt the ICT based information technologies. It offers efficient and effective library co-operation activities includes resource sharing networks, provides value added services and initiates capacity building programs for library staff and users. The present study is an attempt to overview and report the way in which the university libraries in Gujarat responded the changing information environment and developed library infrastructure to use online resources. Electronic resources (ER) are more development than the traditional



resources. They are dominating in the research activities and the users have realized the importance of it. Further online resources can give users efficient, effective and easy access to the information. The libraries are moving towards e-resources to e-services, which is easy and more accessible for the users. Electronic resources, particularly included online databases, e-journals, e-books, e-reports etc, have become major elements of any university library's collection.

**State Universities of Gujarat:** In simple words, “University” presents a major contribution in the development of human resources. It is the centre of learning for higher education, provides facilities and infrastructure research and specialization. The University established or incorporated by or under a Central Act, a Provincial Act or a State Act, and includes any such institution as may, in consultation with the University concerned, be recognized by the Commission in accordance with the regulations made in this behalf under this Act. (UGC report 1956). A state university is a university established or incorporated by a state act. State universities are public universities run by the state government of each of the states and territories of India, and are usually established by a local legislative assembly act. The UGC publishes and regularly updates the lists of state universities. As of 9 February 2017, the UGC lists 358 state universities. ([www.ugc.ac.in](http://www.ugc.ac.in)). The State Universities are established by the Act of the State Legislature concerned and are funded by the State Government.

## 2. Literature Review:

Previous studies help the researcher to formulate, research design using appropriate tools for the successful completion of the study. Habiba, Umme & Salma Chowdhury (2012) this study reveals that, a majority of the users of DUL use e-resources for their learning purpose and users are generally satisfied with the existing e-resources. Wijetunge, Pradeepa (2015) according to the study, it is perceived that the internet is most effective method to obtain desire information and easy to understand. The study reveals that the E-resources were new to them and few of them have never used it. It was recommended to provide adequate training to them and also the infrastructure facility like computer, internet connection make them available in the library for the easy access to E-resources. Tella, A., Dare, O., Adebisi, O., & Lawal, A. (2018) the findings demonstrate that LIS undergraduate students use e-books more compare to print books. The major problem encountered by the students with e-books is the difficulties reading on the computers or internet, followed by the cost of e-book reader. Bhairu P. B. and Shamprasad M. Pujar (2016) the study found that the Knowledge of e-resources and training impacts information seeking behavior and empowers users to understand in an effective way. Anil Kumar Siwach, Satish Kumar Malik (2018) the study indicates that e-journals and free internet resources are the most used e-resources. The libraries should focus more on promoting the e-resources and increasing the training programs in order to have optimum use of e-resources.

## 3. Objectives of the study:

The objective of the present study includes:

- To study the perception of Electronic resources among users of State university libraries of Gujarat.
- To study use of online resources among users such as students, research scholar and faculty members.
- Enhance usage patterns and sources used to access online resources.
- To study the concept and need of various type of Electronic resources.
- To identify problems faced by the users while accessing Electronic Resources.
- To suggest measures for improvement of existing electronic resources and services related to it.

## 4. Methodology:

There are different types of State universities (Public and Private) as well as specific subject oriented universities such as Swarnim Sports university, Shree Somnath Sanskrit university etc. To fulfil the purpose



of the present study specific subject oriented universities were dropped. Thus, for the study purpose data has been collected from the below selected State university libraries:

- Gujarat University (GU)
- Hemchandracharya North Gujarat University (HNGU)
- Krantiguru Shyamji Krishna Verma Kachchh University (KSKVKU)
- Maharaja Krishna kumarsinji Bhavnagar University (MKBU)
- Maharaja Sayajirao University of Baroda (MSU)
- Sardar Patel University (SPU)
- Saurashtra University (SU)
- Veer Narmad South Gujarat university (VNSGU)

From the selected State universities common Faculty/School/discipline has been chosen for the study. The selected five common Faculty or School or disciplines are Art, Commerce, Education, Science and Law. The structured questionnaire designed to obtain the data from the State university library users. The tools and techniques used have their roots in mathematics & statistics. The primary technique used for analysis is percentage. The data was collected during the period of 2016 to 2018 and has been organized in tabular form, and a suitable calculation has been done to draw the conclusions.

## 5. Data Analysis:

### 5.1 General Information of State universities:

**Table 1:** Selected State universities of Gujarat

State University	Year	Place	Website
GU	1949	Ahmedabad	<a href="http://www.gujaratuniversity.org.in">www.gujaratuniversity.org.in</a>
HNGU	1986	Patan	<a href="http://www.ngu.ac.in">www.ngu.ac.in</a>
KSKVKU	2004	Kachchh-Bhuj	<a href="http://www.kskvku.digitaluniversity.ac">www.kskvku.digitaluniversity.ac</a>
MKBU	1978	Bhavnagar	<a href="http://www.mkbhavuni.edu.in">www.mkbhavuni.edu.in</a>
MSU	1949	Vadodara	<a href="http://www.msubaroda.ac.in">www.msubaroda.ac.in</a>
SP	1955	Anand	<a href="http://www.spuvvn.edu">www.spuvvn.edu</a>
SU	1968	Junagadh	<a href="http://www.saurashtrauniversity.edu">www.saurashtrauniversity.edu</a>
VNSGU	1965	Surat	<a href="http://www.vnsgu.ac.in">www.vnsgu.ac.in</a>

The above table shows the establishment year of the university and where it is located. It is revealed that the all the State universities were located at different district of Gujarat.

**5.2 The Response:** To get an overview of the study information was required from the potential users of State university libraries such as from faculty, research scholars and students. The same has been presented in the below table.

**Table 2:** Response

Details	GU	HNGU	KSKVKU	MKBU	MSU	SP	SU	VNSGU
<b>Students</b>	180	147	146	150	175	188	158	186
<b>Research scholars</b>	46	36	37	37	43	42	35	37
<b>Faculty members</b>	45	36	39	39	46	37	33	31
<b>Total</b>	<b>271</b>	<b>219</b>	<b>222</b>	<b>226</b>	<b>264</b>	<b>267</b>	<b>226</b>	<b>254</b>

The above table indicates that the response received from various State university libraries. It that with 271 (67.75%) with 271 (67.75%) from GU followed by HNGU with 219 (54.75%), KSKVKU with 222 (55.5%), MKBU with 226 (56.5%), MSU with 264 (66%), SP with 267 (66.75%), SU with 228 (57%), VNSGU with 254 (63.5%).

**5.3 Frequency of visit to Library:** In this section details regarding how often do they visit to library to avail various library resources and services, regarding to this various response are given in below table.

**Table 3:** Frequency – Faculty

Details	GU			HNGU			KSKVKU			MKBU			MSU			SP			SU			VNSGU		
	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C
Students	82	77	21	68	50	29	72	47	27	69	55	26	84	57	34	84	68	36	78	45	35	75	66	45
Research scholars	22	17	7	16	11	9	23	7	7	21	10	6	27	10	6	28	8	6	22	7	6	24	8	5
Faculty members	20	17	8	11	15	0	11	18	0	17	12	0	14	22	0	10	19	8	10	17	8	9	15	7
Total	124	111	36	95	76	48	106	72	44	107	77	42	125	89	50	122	95	50	122	69	49	108	89	57

A – Daily, B – Weekly & C – Fortnightly/rarely

The above table shows that users use to visit library to fulfil their academic purpose. Accordingly, to respondent's data collected and analysed, it is found that majority of users use to visit library daily such as from GU with 124 (41.33%) followed by HNGU with 95 (31.66%), KSKVKU with 106 (35.33%), MKBU with 107(35.66%), MSU with 125 (41.66%), SP with 110 (36.66%), SU with 122 (40.66%), VNSGU with 108 (36%).

**5.4 Awareness about E-resources:** For the maximum utilization of Electronic resources, it is very important that the users should be aware of it. Skills are the pre-requisite for the effective usage of online resources and therefore users were asked whether they are aware of the e-resources provided to them.

**Table 4: Awareness about E-resources**

Details	GU		HNGU		KSKVKU		MKBU		MSU		SP		SU		VNSGU	
	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Students	168	12	135	10	132	14	138	12	162	13	173	15	139	19	169	17
Research scholars	43	3	32	4	33	4	34	3	40	3	38	4	31	4	32	5
Faculty members	42	3	29	7	35	4	34	5	43	3	32	5	29	4	26	6
Total	253	18	196	21	200	22	206	20	245	19	243	24	199	27	227	28

The question was asked regarding the knowledge of Electronic resources and accordingly the options were listed. From the above table it is found that the majority of users were aware of the online resources provided by the State university libraries such as GU with 253 (63.25%), followed by HNGU with 196 (49%), KSKVKU with 200 (50%), MKBU with 206 (51.5%), MSU with 245 (61.25%), SP with 243 (60.75%), SU with 199 (49.75%), VNSGU with 227 (56.75%).

**5.5 Preferred sources:** The various digital formats are available in online resources, due to which they become first preference among users. An effective, easy and fast mode of communication between users is an added advantage for the preference of e-resources. The question was asked to respondents the most preferable source of information whether Electronic Resources or printed or both format, what are the preferences.

**Table 5: Preferred sources:**

Details	GU			HNGU			KSKVKU			MKBU			MSU			SP			SU			VNSGU		
	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C
Students	89	4	4	7	3	3	7	3	3	8	3	2	9	4	3	9	4	4	7	4	3	8	5	4
		6	5	5	5	7	6	7	3	7	5	8	6	1	8	5	7	6	8	2	7	9	2	6
Research scholars	20	1	1	1	1	8	1	1	7	1	1	8	2	1	1	1	1	1	1	1	1	2	1	4
		4	2	7	1		9	1		7	2		0	1	2	9	2	1	4	1	0	0	3	
Faculty members	20	1	1	1	1	1	2	1	9	1	9	1	2	1	1	1	1	9	1	1	9	1	9	8
		2	3	6	0	0	0	0		9		1	1	1	4	8	0		3	1		5		
Total				1			1			1			1			1			1			1		
	12	7	7	0	5	5	1	5	4	2	5	4	3	6	6	3	6	6	0	6	5	2	7	5
	9	2	0	8	6	5	5	8	9	3	6	7	7	3	4	2	9	6	5	4	6	4	4	8

A – Electronic resources, B – Print resources & C – Both resources

In this section the question was asked to respondents the most preferable source of information whether Electronic Resources or printed format or both the resources they prefer. The table reveals the data that the majority of them prefer online resource due to it features such as easy, convenient to access, available before print, anywhere anytime available etc. The Electronic resources were preferred in GU with 129 (32.25%), followed by HNGU with 108 (27%), KSKVKU with 115 (28.75%), MKBU with 123 (30.75%), MSU with 137 (34.25%), SP with 132 (33%), SU with 105 (26.25%), VNSGU with 124 (31%).

**5.6 Access Issues:** The number issue come while accessing Electronic Resources. The respondents were requested to furnish the details and the same is presented in below table.

**Table 6: Access issue**

Details	GU			HNGU			KSKVKU			MKBU			MSU			SP			SU			VNSGU		
	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C
Students	98	38	44	83	25	39	83	27	36	76	27	47	89	32	54	98	34	56	86	30	42	10	37	43
Research scholars	21	8	15	18	8	10	18	8	11	19	7	11	19	9	15	22	9	11	17	7	11	21	7	9
Faculty members	22	7	16	15	6	15	19	9	11	22	7	10	24	10	12	18	7	12	18	5	9	15	6	11
Total	141	53	75	116	39	64	120	44	58	117	41	68	132	51	81	138	50	79	121	42	62	144	50	63

A - Slow Internet connections/download speed, B - Limited terminals/insufficient system configuration, C - Insufficient time & training/resources

The table data shows that various issues faced by the users while accessing the online resources and were listed accordingly such as GU with 141 (35.25%), followed by HNGU with 116 (29%), KSKVKU with 120 (30%), MKBU with 117 (29.25%), MSU with 132 (33%), SP with 138 (33%), SU with 121 (30.25%), VNSGU with 142 (35.5%). Hence, the major problem during the access was slow internet or slow downloading speed.

## 6. Major Findings:

Major findings of the study are as below:

- From the selected State universities, Gujarat University (GU) and Maharaja Sayajirao University of Baroda (MSU) were the oldest among all.
- All the State universities were located at various districts of Gujarat.
- The findings show that the majority of respondents were from Gujarat University with 67.75%.
- The study highlights that majority of users visit their respective university libraries daily.
- Majority of users are aware of online resources provided to them in the State University.
- Electronic resources were the highly preferred resources among all the respondent categories.
- The study reveals that the all the categories were aware of the Electronic resources usage and they used it for different purposes such as faculty members and research scholar use it for academic work, whereas, student's respondents use it for knowledge purpose.
- Slow internet connection or slow download speed was the major drawback in the study.

## 7. Conclusion:

Earlier it was not possible to pursue research with easy availability of materials and needed resources. The changing technology has made things easy, accessible and convenient. Now its became easy to get up-to-date information with the latest trends. The present study is an effort to get an overview of Electronic resources usage among users of State university libraries. The current obstacles identified in the study were similar to those obstacles which existed almost a decade earlier, such as insufficient system or its configuration, library budget etc. Electronic resources provide an effective means for students, research scholars, and faculty members to fulfil academic purpose.

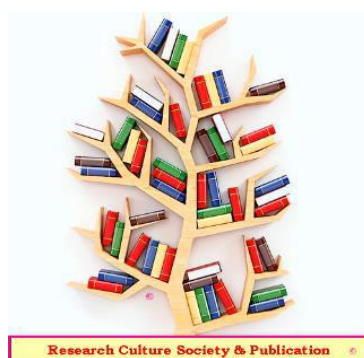
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