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Electronic Properties of Ethylene Glycol and Styrene Glycol: DFT Calculation

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Abstract: ***In this paper we worked on a theoretical study of Ethylene glycol and styrene glycol Which is based on density functional theory, implement in computational program SIESTA with use of general gradient approximation (GGA) of Perdew, Burke and Emzerhof (PBE) scheme for an account of exchange co-relation effect to obtain density of state , projected density of state and charge density.***
Keywords: Density functional theory, SIESTA, Density of state .Projected density of state ,charge density .

I. INTRODUCTION

Ethylene glycol is developed in 1859 by a french chemist Charle -A dolphe Wurtz. The glycol is a type of the compound which is containing two hydroxyl groups. Ethylene Glycol is used for the industrial and commercial purpose. Ethylene glycol is also used as the cooling and an anti-freezing.

II. METHODOLOGY

DFT calculation permit prediction and the calculation of material actions on the basis of a quantum a mechanical deliberation without the obligatory high order parameter such as fundamental properties . All calculation is executed by using the Spanish Initiative for Electronic Simulations with Thousand of Atoms (SIESTA) code. All calculation is an original method and its computer program implementation method in the local density (LDA) and generalization gradient (GGA)approximation of Perdew, Burke and Emzerhof (PBE) .In a calculation the pseudo-potentials of H,C and O were taken from SIESTA web page . After a final optimization the Mesh-Cuttoff and Kgrid in Ethylene glycol is 100 Ry , 8x8x1 and in a styrene glycol is 400 Ry,11x11x1.

III. RESULT AND DISCUSSION

A. V Molecular Geometry Optimization

Fig 1 Shows an optimized structural of ethylene glycol and styrene glycol Table 1 and 2 contain an optimize parameters bond lengths and bond angles of Ethylene glycol and styrene glycol. The H – O bond lengths 1.09 Å is close to the standard H - O bond lengths [11,12].

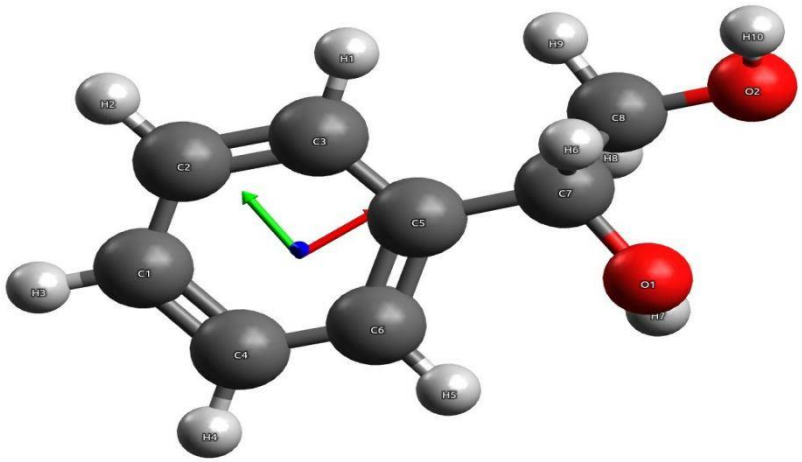


Fig. 1 (a)

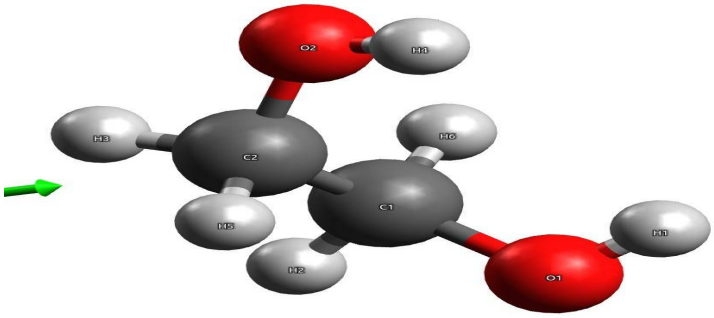


Fig 1 (b)

Fig. 1 Optimized geometry (a) Styrene glycol (b) Ethylene glycol

Tabel 1. Optimize parameters (bond length and bond angel) of Styrene glycol

Parameter	Bond length	Parameter	Bond Angel
H1- O1	1.00306	C4-C1-H3	120.2822
O2-H10	1.00415	C2-C1-H3	119.9697
C3-H1	1.09425	C2-C3-C4	119.7479
H4-C4	1.09433	C1-C2-H2	119.6618
H5-C6	1.09645	C1-C2-C3	120.1212
C2-H2	1.09776	C3-C2-H2	120.2170
H3-C1	1.10023	C2-C3-C5	120.8071
H8-C8	1.12297	C2-C3-H1	118.9890
C7-H6	1.12366	C5-C3-H1	120.2035
C8-H9	1.12733	C1-C4-H4	119.6161
C1-C2	1.41111	C6-C4-H4	119.8839
C4-C1	1.41577	C1-C4-C6	120.4999
C2-C3	1.42097	C3-C5-C6	118.4930
C4-C6	1.42158	C6-C5-C7	121.7173
C8-O2	1.42528	C3-C5-C7	119.7861
C6-C5	1.42711	C4-C6-H5	118.7662
C7-O1	1.42718	C4-C6-C5	120.3294
C5-C3	1.42897	C5-C6-H5	120.9043
C5-C7	1.54834	C5-C7-C8	111.7884
C8-C7	1.55247	C8-C7-O1	110.1200
		C8-C7-H6	107.5941
		C5-C7-O1	112.4009
		C5-C7-H6	107.6742
		O1-C7-H6	106.9986
		H8-C8-H9	106.5936
		O2-C8-H8	108.6028
		C7-C8-H8	109.5810
		O2-C8-H9	109.9673
		C7-C8-H9	111.5903
		C7-C8-O2	110.3912
		C7-O1-H7	108.1003
		C8-O2-H10	106.7405

Tabel.4 Optimize parameters (bond angle and bond length) of Ethylene glycol

Parameter	Bond length	Parameter	Bond Angel
O1-H1	0.907078	O1-C1-H2	101.7525
O1-C1	1.44359	C2-C1-O1	114.9203
H4-O2	0.967566	O1-C1-H6	109.1739
H5-C2	1.12946	C2-C1-H2	109.2910
H2-C1	1.12946	H2-C1-H6	110.8056
C2-O2	1.41276	C2-C1-H6	110.5830
C1-H6	1.12141	C1-C2-H5	108.8829
C2-H3	1.11046	H3-C2--H5	108.9978
C1-C2	1.52332	O2-C2-H5	114.2311

C1-C2-H3	3104.8361
C1-C2-O2	116.1108
O2-C2-H3	102.9945
C1-O1-H1	110.9350
C2-O2-H4	114.4200

IV. ELECTRONIC PROPERTIES

The DOS gives the number of allowed electron (or holes) states per volume at a given energy .When DOS is high,it means that many states are available at different energy level .When DOS is zero there will be no states at any particular energy level .Hence, the resultant DOS curve is obtained due to s-p hybridization .Gap between the lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (LUMO) is called HOMO-LUMO gap.HOMO -LUMO gap of styrene glycol is ~4.7 eV and ~3.9 eV in ethylene glycol.

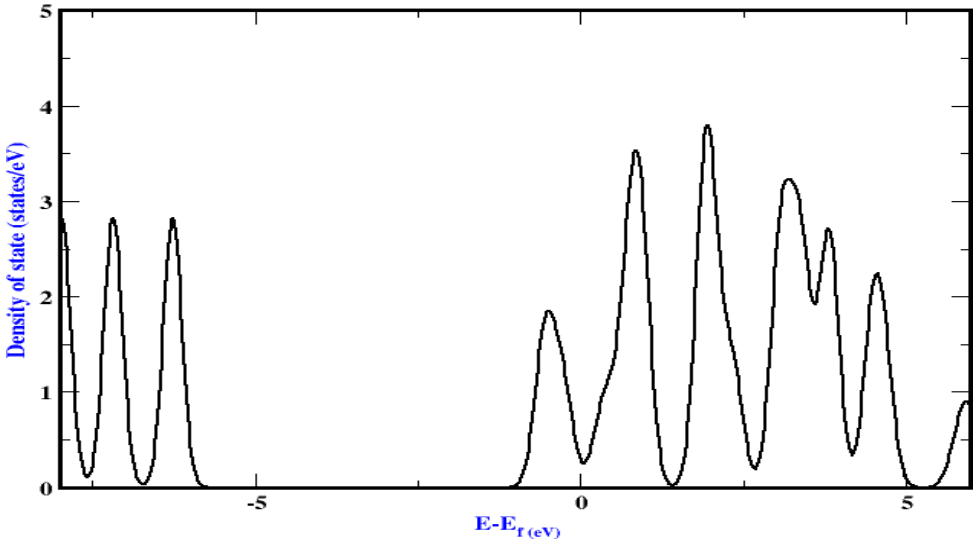


Fig . 2 (c)

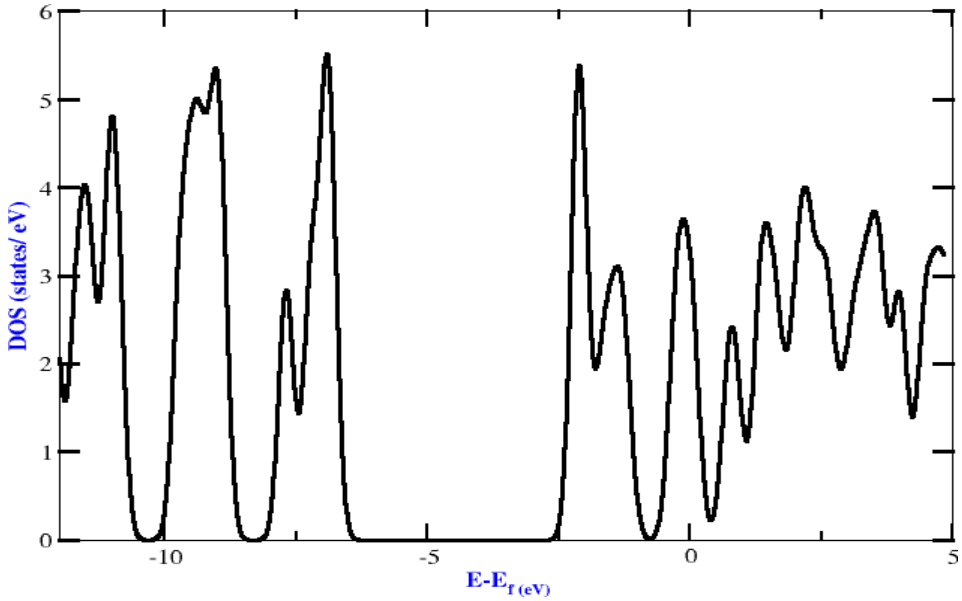


Fig .2 (d)

Fig.2 Density of state 2(c) Styrene glycol 2(d) Ethylene glycol

In projected density of state of EG (Ethylene glycol) and SG (styrene glycol), 0 eV represents the Fermi level ,aloft of a conduction band and beneath of a valence band is Fermi level. Valence band is formed at the below level of the HOMO the energy state and the conduction band is formed at the above LUMO .In the frontier the molecular orbital theory, HOMO-LUMO is collectively called as a frontier orbital . They can be used to speculate the strength , a stability and a color of transition metal complexes.

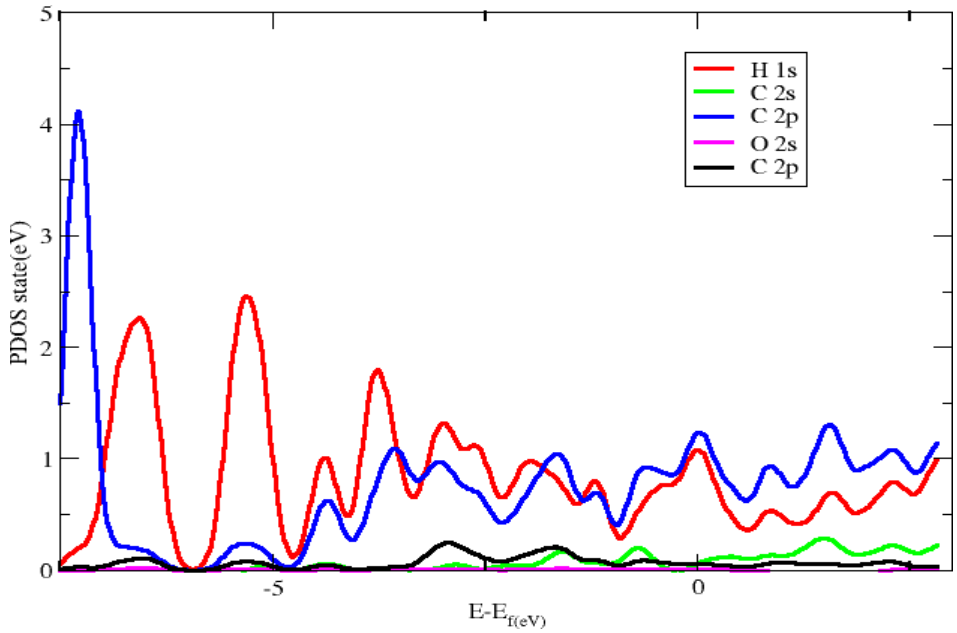


Fig.3 (e)

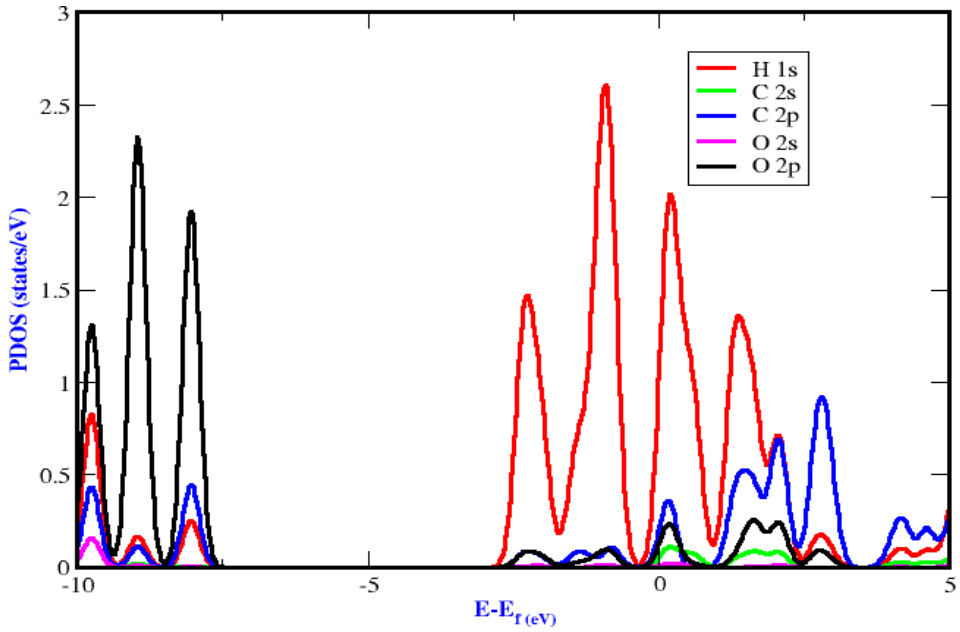


Fig.3 (f)

Fig.3 Project density of state (e) Styrene glycol (f) Ethylene glycol

Fermi Energy of SG and EG

Materials	styrene glycol	Ethylene glycol
Fermi Energy (eV)	-5.179	-1.785

The charge density investigates the nature of the chemical bond, this nature predicts by the concentric circle and distorted dumb-bell shape. Ethylene glycol and the styrene glycol both are highly ionic and partially covalent. Color code values of a charge density are shown in a fig .4

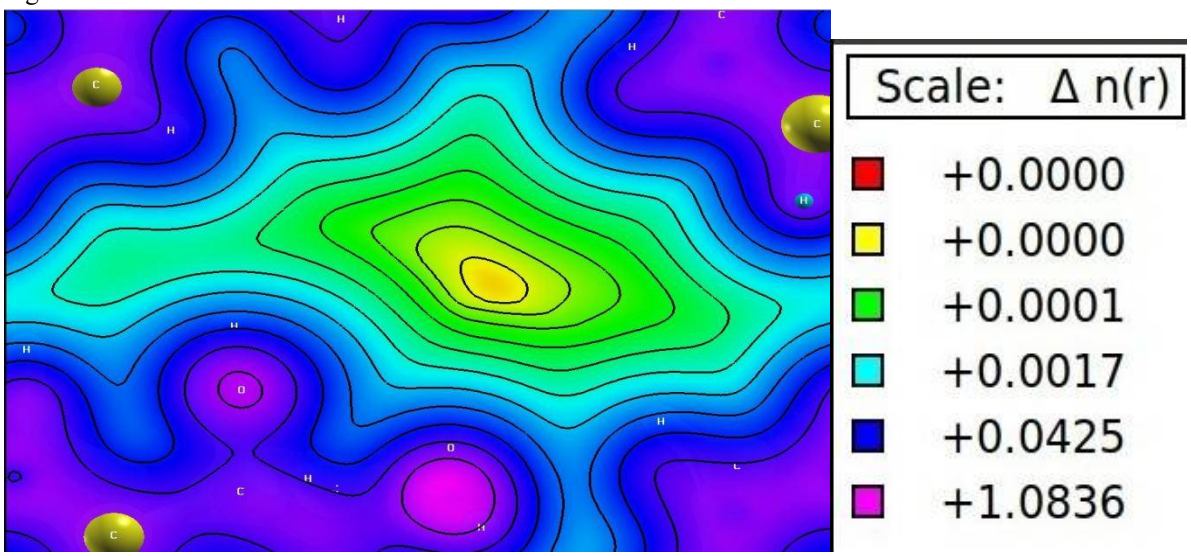
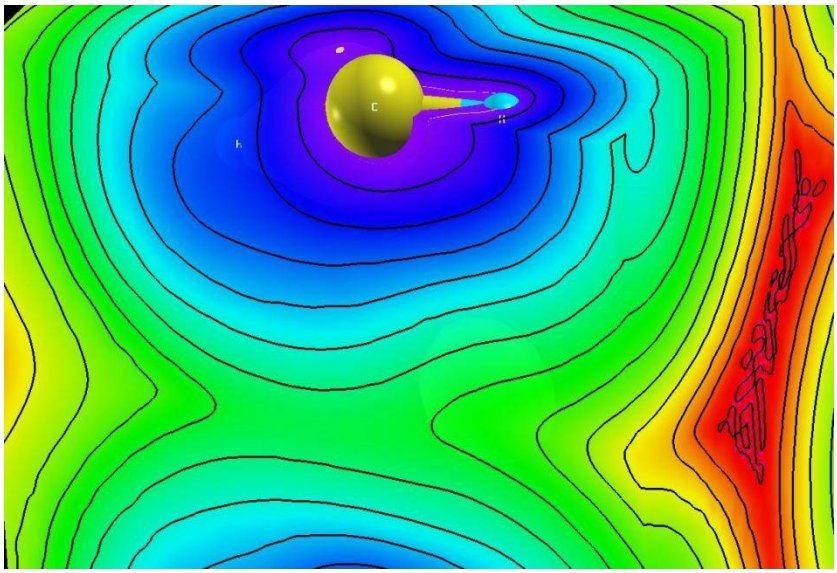


Fig . 4(g) Fig . 4(g')



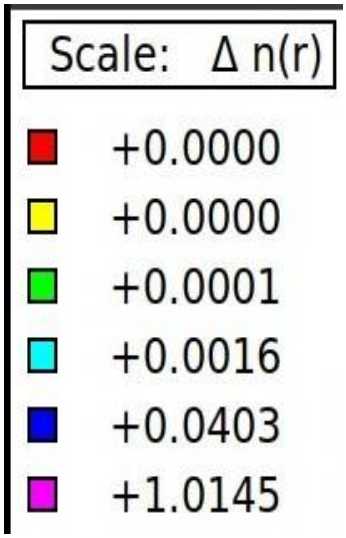


Fig 4 .(h) Fig. 4(h')

Fig. 4 Charge density 4(g) styrene glycol 4(h) Ethylene glycol

V. CONCLUSION

In the analysis of Ethylene glycol and a styrene glycol by using a density functional theory The PDOS(Projected density of state) has explain a strong s-p hybridization and the density of state conducting in nature for both Ethylene glycol and a styrene glycol. The charge density exhibits highly ionic and partially covalent.

VI. ACKNOWLEDGEMENT

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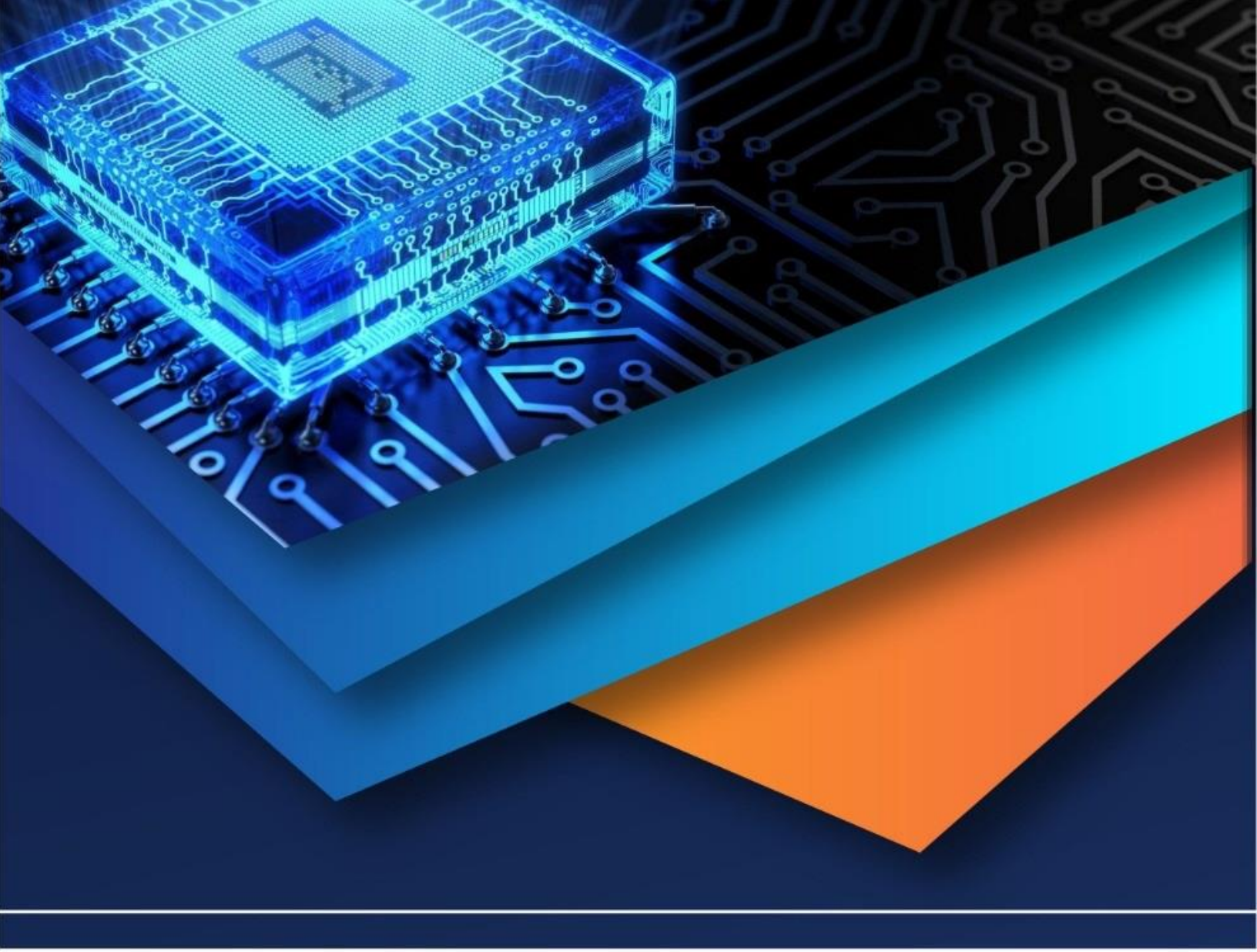

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