Investigation of electrostatic force and dipole moment effects on movement and dancing of Chains in DPPC and DMPC

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ABSTRACT

An understanding of static properties of membrane is an essential prelude to the study of movement of molecules within the membrane. In this investigation any molecule has been theoretically investigated through the quantum mechanical calculations.According to the results obtained, the structural optimization of the isolated Dipalmitoylphosphatidylcholine (DPPC) and Dimyristoylphosphatidylcholine (DMPC) in the gas phase, at the Hartree-Fock level of theory, apply to STO-3G,3-21G, 6-31G and 6-31G basis sets. The most important dihedral angle of these molecules was chosen and the energy, dipole moment, and atomic charges of 14 important atoms were scanned within 180 degrees rotation and sites that have most changes were determined and any rotated molecule was separately placed in 19 solvents (The method is HF/6-31G* model) and the dielectric effect of the surrounding was analyzed. Quantum chemical solvent effect theories describe the electronic structure of a molecular subsystem embedded in a solvent or other molecular environment.The solvent effect on the stability of DPPC & DMPC molecules, dipole moment, and the charge on some atoms of those molecules are discussed using Onsager model.*

INTRODUCTION

One of the great challenges in biophysics is understanding the basic principles that govern lipid bilayer mixtures. Lipid bilayers, or membranes, govern and mediate various biologically relevant processes on the cellular level. Transfer of ions through membranes and function of enzymes attached to membranes provide two examples of these situations [1]. Biological membranes are an essential part of life processes in living organisms. Membrane function goes beyond its obvious role as a physical barrier to contribute to important life processes. Membranes are semipermeable, highly selective barriers containing ion channels and pumps to modulate and maintain balance as required. These channels and pumps are involved in signal transduction and response to stimuli from the environment. In addition, important energy conversion and storage processes take place at the membrane level. Consequently, a fundamental understanding of bilayers and membrane proteins from the atomic point of view is of great biochemical, biophysical, and medical interest [2]. Function of membrane proteins within a complex heterogeneous environment differs markedly from the aqueous medium of globular proteins.

Significant progress has been made toward understanding some of the key characteristics of both lipids and membrane proteins which determine the favorable energetics of this environment[3]. Many physical and biochemical properties of lipid bilayers are important to the bilayer's fundamental role as the basis of biological membranes. These properties are now commonly investigated by atomistic molecular dynamics (MD) simulation and Quantum Mechanics(QM)[4].

Membranes are asymmetric structures. The choline-containing phospholipids are localed mainly in the outer molecular layer [7].This asymmetric distribution is maintained by an ATP-dependent protein which specifically translocates phosphatidylethanolamine (and phosphatidylserine) to the inside of the plasma membrane[5].All major lipids in membranes contain

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both hydrophobic and hydrophilic regions and therefore, they are termed amphipathic. Dipalmitoylphosphatidylcholine (DPPC) and dimyristoylphosphatidylcholine (DMPC) are taken as phospholipids with an equal polar heads and with the difference in the length of hydrocarbon chains[6,7]. These two molecules have saturated fatty acid tail groups[8].

On a molecular level it has been of interest to explore to what extent PC head groups differ with respect to molecular conformation, lateral interactions, and dipole arrangements and how these features affect the properties and topology of the membrane surface. [9, 10]

DPPC and DMPC are important phospholipids in cell bilayer, then investigation of interaction between peptides and bilayer of these molecule is very important[11]. The main component that is responsible for considerable lowering of the interfacial tension is DPPC which accounts for 50%-70% of the PC[12]. DPPC has gel to liquid crystalline transition temperature(Tm) of 41.5 degree of centigrade and at a physiological tempeture of 37 degree of centigrade; it is in an ordered gel state [13].

These two molecules are zwitterionic having a negative charge on the phosphate group and a positive charge on the amin. The hydrocarbon chain of DPPC is 16 and DMPC is 14 carbons long (Fig.1), then the solvent effects on these molecules are important [2, 14].

In this work, we have used of the Ab-initio calculations to determine minimum energy conformations of the dimyristoyl phsphatidylchline and Dipalmitoyl-phosphatidylcholine and have performed calculations according to the continuum solvating model by Onsager [15].

2. Computational Method

All calculations have done by ab initio at the Hartree-Fock (HF) level of theory Gaussian 98 package. Four basis sets have used, namely the STO-3G 3-21G, 6-31G and 6-31G*.

First, the geometry of DPPC,DMPC have full optimized at the RHF/ 6-31G*, 6-31G, 3-21G and STO-3G levels of the theory in the gas phase. The most important dihedral angle of these molecules (DPPC and DMPC) is chosen and the energy, dipole moment, and atomic charges of 15 important atoms have scanned within 180 degrees rotation. In this manner after the optimization of total molecules, important dihedral angle of these molecules has rotated 15 degrees at every time.

The effects of the solvent polarization are described in terms of proper QM operators to be added to the Hamiltonian of the isolated system. Then, the salvation calculations have performed using Onsager [18] method at HF/6-31G*. For Onsager model, it does require values of volume (a0) of the molecule and the dielectric (ε) of solvent. The volume of DPPC and DMPC molecules was obtained using the “volume” keyword.

The Onsager-SCRF was that it permitted one to directly exploit almost all of the computational facilities of the Gaussian packages. For this reason, and for its very limited computational cost, it is still in use by people not requiring an accurate description of solvation effects but just a guess or a qualitative correction to the values obtained for the isolated molecule. Users must be aware of the limitations of

the approach, of the unphysical deformation of the solute charge distribution it may induce, and of other shortcomings specific of the approach, such as the lack of solvation for solutes with zero permanent dipole.

In the Onsager method, the solute molecule is placed in a spherical cavity of radius a_0 surrounded by a continuum with constant dielectric properties.[9] A dipole in the molecule will induce a dipole in the medium, and the electric field applied by the solvent dipole will in turn in interact with the molecular dipole leading to net stabilization

The molecular geometrics have obtained via HF/6-31G* level optimization in the gas phase and have rotated and then any one separately have been placed in the 19 solvents. The solvents is Water(ε =78.39),DiMethylSulfoxide (ε = 46.7), NitroMethane(ε =38.2) ,Acetonitrile (ε =36.64) ,Methanol (ε =32.63), Ethanol(ε =24.55) ,Acetone(ε =20.7) ,DiChloroEthane (ε =10.36), DiChloroMethane (ε =8.93) ,TetraHydroFuran(ε =7.58) ,Aniline(ε =6.89), ChloroBenzene(ε =5.621) ,Chloroform (ε = 4.9) ,Ether Diethyl Ether(ε = 4.335), Toluene(ε =2.379),Benzene(ε =2.247) ,Carbon Tetrachloride (ε =2.228), CycloHexane (ε =2.023) and Heptane(ε =1.92).The total energy of solute and solvent, which depends on the dielectric constant and also dipole moment of solute, induces a dipole moment of opposite direction in the surrounding medium [16].

3. Result and discussion

Dipalmitoylphosphatidylcholine (DPPC) and dimyristoylphosphatidylcholine (DMPC) molecules have been chosen as starting structures for gas phase (Fig1).

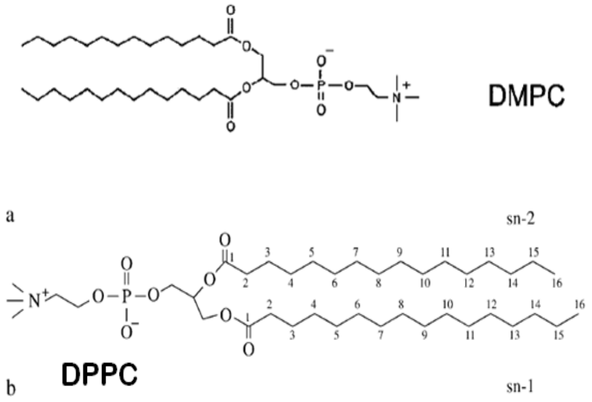


Fig1: DPPC and DMPC molecule

The DPPC and DMPC zwitterionic are found to be unstable in the gas phase when have optimized at HF/3-21G, 6-31G and 6-31G* level [17].The obtained results from optimization and stabilization parameters are shown in table1.

Table 1.Conformational energy of DPPC and DMPC obtained by geometry optimization for basis set 6-31G*, 6-31G, 3-21G, STO-3G levels

basis set	**E/Kcal.mol^{-1}**	
	DPPC	**DMPC**
Sto-3G	-1583811.262	-148406.112
3-21G	-1594584.634	-149458.505
6-31G	-1602682.003	-1505418.2
6-31G*	-1603386.341	-1505422.1

According observed results are obtained, minimum energy is related to 6-31G* the basis set. Therefore we selected basis set 6-31G* for other calculation in this work.

The most important dihedral angle of these molecules (DPPC and DMPC) are chosen in by optimization of total molecules (Fig.2a,2b), then important dihedral angle of these molecules are rotated every time 15 degrees. Alteration of dipole moments and energies of these rotations are shown in Fig.3. A communicating is between dipole moment with energy and rotation angle. First, angle of most important dihedral is 60 degree that every time increase 15 degree (Table2). The minimized energy of DMPC and DPPC are about 60 degree and other minimized energy is about 150 degree.

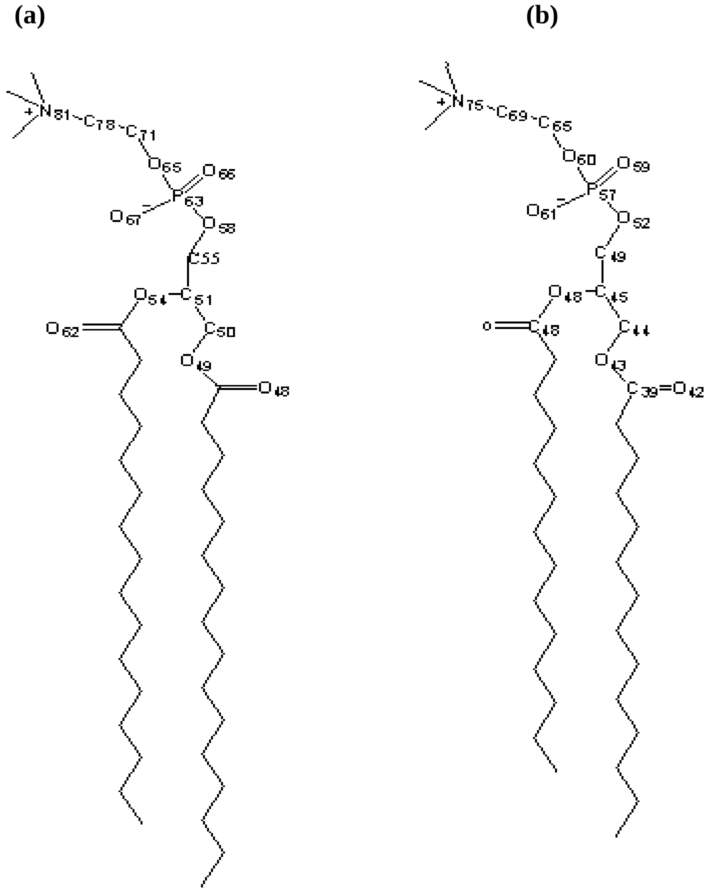


Fig.2. Atom numbering of **a)** DPPC **b)** DMPC.

In Fig.3 is observed a minimum energy that coordinates with maximum dipole moment. Comfortably, it can correspond to relation between dipole moment and energy with rotation angle.

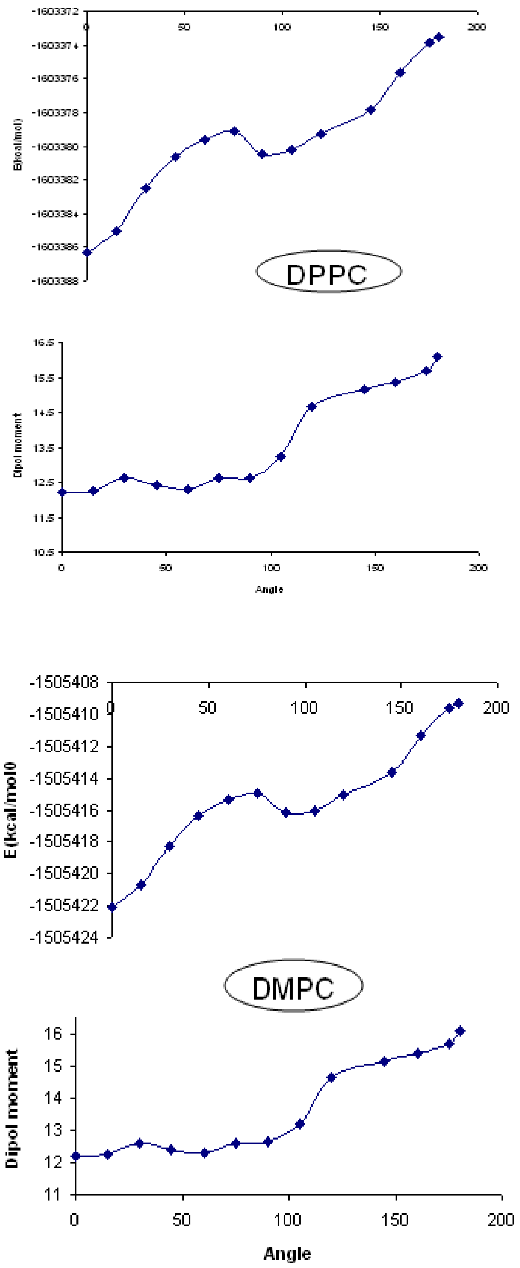


Fig.3. Energy and Dipole moment versus Angle.

Consequently in maximum dipole moment, DMPC and DPPC molecule are the permanent state. Alteration of angle and atomic charge of these rotations are shown in Fig.4. The maximum charge on phosphorus (P57 in DMPC, P63 in DPPC) is in 105 degree that coordinates with angle hybridation.

In DPPC P63 decreases the charge in 160 degree that synchronous O67 has an increased charge. it has been observed increased partial charge in minimum state for O48 and a severe deduction in O66 that causes energy evacuation that similar electroscope sheet charge is transferred to tail. The same result is observed for DMPC.

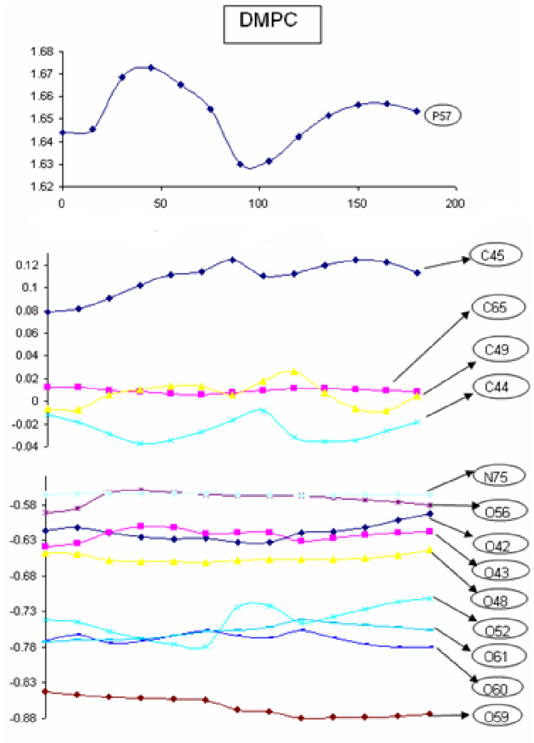
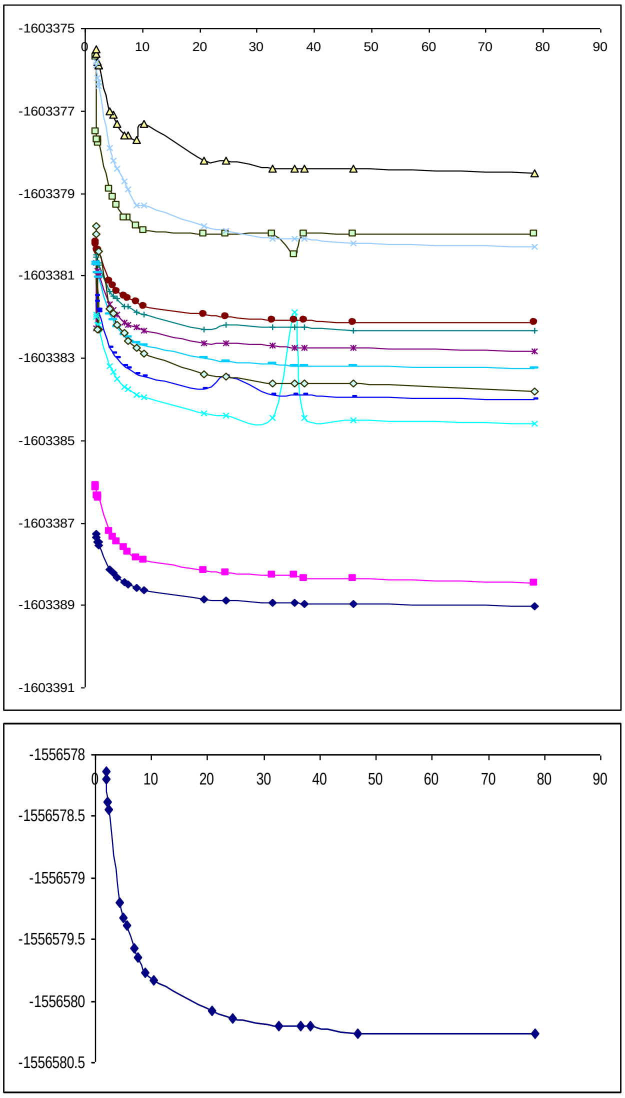


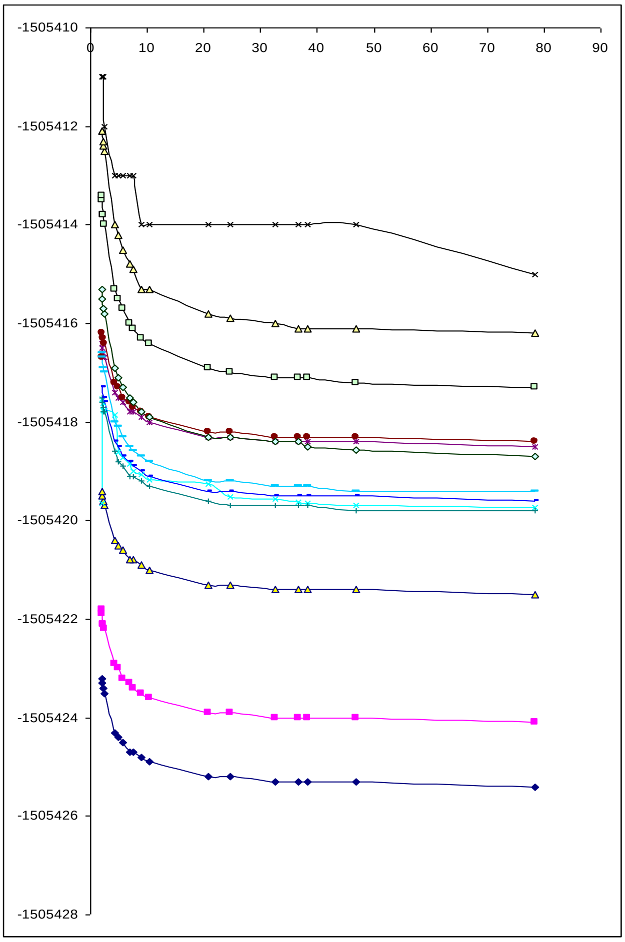
Fig.4. Atomic charge versus Angle.

Most chemical reactions and biological process take place in solutions. The use of the SCRF model in quantum-chemical theory requires that the shape and volume of the solute molecule must be defined uniquely for any set of compounds. A number of approaches to calculate these characteristics are known, but no non-empirical methods for their estimation have been developed. However, from the results of model calculations it may be concluded that the simple model assuming a spherical or an ellipsoidal shape of the cavity for the solute molecule is probably satisfactory for comparatively small and rigid molecules [19].

We present a quantum-chemical analysis of the solvent effect on stability of molecule, dipole moment and by corresponding to atomic charge of some selected atoms of DPPC and DMPC molecule (Table3). The molecular geometrics are obtained via HF/6-31G* level optimization in the gas phase and then important dihedral angle of these molecules have rotated every time 15 degrees and every time, the volume of DPPC and DMPC molecules have obtained using the “volume” keyword. Any one of rotated molecule separately placed in the 19 solvents (keyword, scrf=dipole). Regular alterations have observed concerning energy versus dielectric constant. With increasing of dielectric constant of solvents, stability of 13 AO values of DPPC and DMPC increase (Fig.5).



(a)



(b)

Fig.5. Energy (kcal/mol) versus Dielectric constant for 13 A0 values **a)** DPPC **b)** DMPC.

The computed solvent-dependent acceptor and donor charge distributions for some atoms in each medium are shown on Fig.6.As it was expected, where the charges of the many atoms (C45, C49, C44, O42, O48, O59 of DMPC and C51, C55, C50, O48, O54, O66 of DPPC) are increasing when the dielectric constant is increasing. But the charges of many atoms (P57, C65, N75, O56, O43, O52, O61, O60 of DMPC and P63, C71, N81, O62, O49, O57, O67, O65 of DPPC) are decreasing when the dielectric constant (D) is increasing.

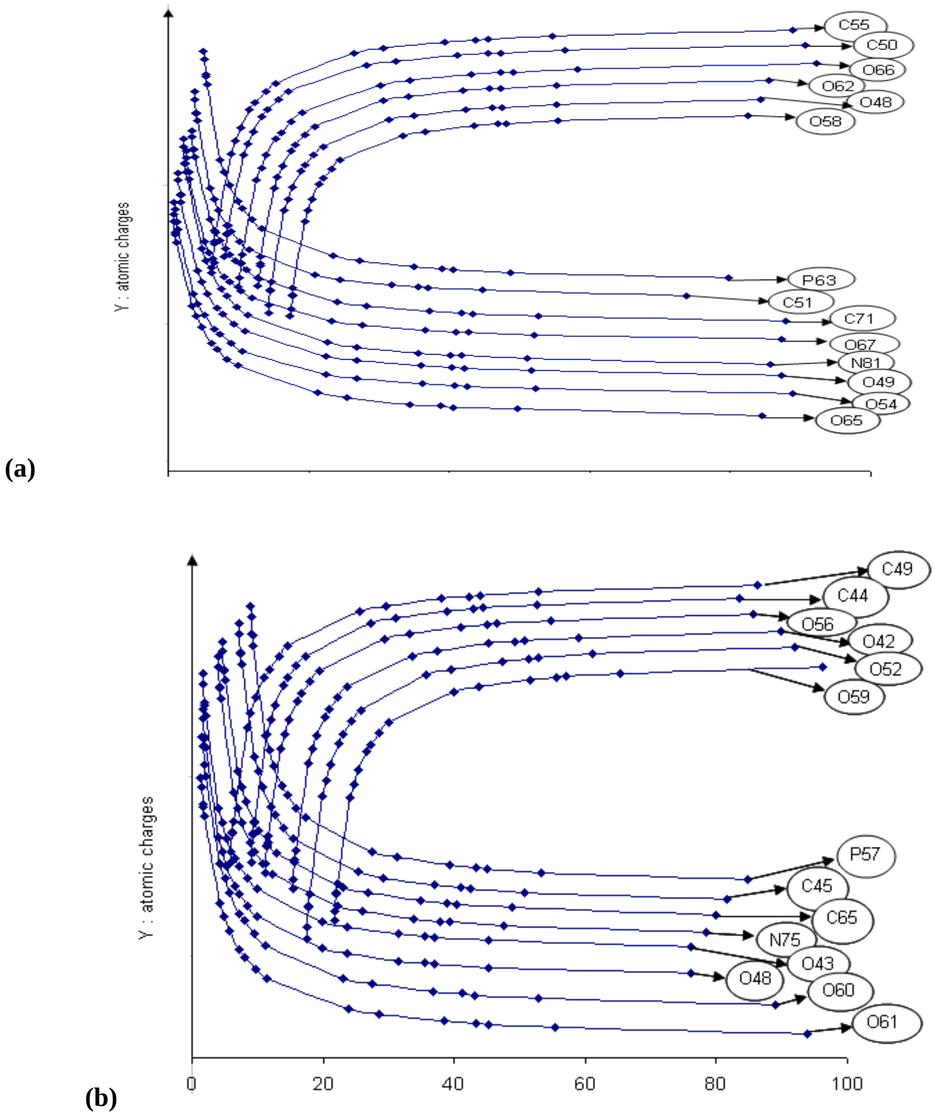


Fig.6. Dielectric constant versus Atomic charge of **(a)** DPPC (**b)** DMPC.

Table 2. Different rotations in most dihedral angle of DPPC and DMPC.

DPPC													
Rotation	0	15	30	45	60	75	90	105	120	145	160	175	180
Angle	60	75	90	105	120	135	150	165	179.9264	-165.0748	150.0753	-135.0739	-120.076
DMPC													
Rotation	0	15	30	45	60	75	90	105	120	145	160	175	180
Angle	60	75	90	105	120	135	150	165	179.9345	-165.0669	-150.0664	-135.0664	-120.0655

Table3. Dielectric constant, Dipole moment and Energies for 12 Rot of DPPC and DMPC.

DPPC

Rotation ε		**15**	**30**	**45**	**60**	**75**	**90**	**105**	**120**	**135**	**150**	**165**	**180**
78.39	**Dipole-moment**	15.295	15.4539	15.8024	15.0285	15.0225	14.9055	15.6035	17.0125	18.487	18.1936	18.3026	20.0203
	E	-1603388.5	-1556580.3	-1603384.6	-1603382.8	-1603382.1	-1603382.3	-1603384	-1603383.3	-1603383.8	-1603380	-1603378.5	-1603380.3
46.8	**Dipole-moment**	15.246	15.4062	15.7462	14.9848	14.9851	14.8727	15.5667	16.9771	18.4343	18.1502	18.2628	19.9572
	E	-1603388.3	-1556580.3	-1603384.5	-1603382.8	-1603382.1	-1603382.3	-1603384	-1603383.2	-1603383.6	-1603380	-1603378.4	-1603380.2
38.2	**Dipole-moment**	15.2193	15.3802	15.7156	14.9611	14.9647	14.8548	15.5466	16.9577	18.4056	18.1266	18.2411	19.9229
	E	-1603388.3	-1556580.2	-1603384.5	-1603382.8	-1603382.1	-1603382.3	-1603383.9	-1603383.2	-1603383.6	-1603380	-1603378.4	-1603380.1
36.64	**Dipole-moment**	15.2131	15.3742	15.7085	14.9555	14.9599	14.8507	15.542	16.9532	18.399	18.1211	18.236	19.9149
	E	-1603388.3	-1556580.2	-1603381.9	-1603382.8	-1603382.1	-1603382.3	-1603383.9	-1603383.2	-1603383.6	-1603380.5	-1603378.4	-1603380.1

32.63	**Dipole-moment**	15.1945	15.3561	15.6872	14.9389	14.9457	14.8382	15.528	16.9397	18.3789	18.1046	18.2209	19.8909
	E	-1603388.3	-1556580.2	-1603384.5	-1603382.7	-1603382.1	-1603382.3	-1603383.9	-1603383.1	-1603383.6	-1603380	-1603378.4	-1603380.1
24.55	**Dipole-moment**	15.1392	15.3023	15.6238	14.8896	14.9034	14.8011	15.4863	16.8995	18.3194	18.0555	18.1757	19.8197
	E	-1603388.2	-1556580.1	-1603384.4	-1603382.6	-1603382	-1603382.2	-1603383.5	-1603383.1	-1603383.5	-1603380	-1603378.2	-1603379.9
20.7	**Dipole-moment**	15.0983	15.2624	15.577	14.8531	14.872	14.7735	15.4555	16.8697	18.2753	18.0191	18.1423	19.767
	E	-1603388.2	-1556580.1	-1603384.3	-1603382.6	-1603381.9	-1603382.3	-1603383.8	-1603383	-1603383.4	-1603380	-1603378.2	-1603379.8
10.36	**Dipole-moment**	14.8495	15.0203	15.2932	14.6311	14.6808	14.6054	15.267	16.6875	18.0069	17.7969	17.9378	19.4467
	E	-1603387.9	-1556579.8	-1603383.9	-1603382.3	-1603381.8	-1603381.9	-1603383.5	-1603382.7	-1603382.9	-1603379.9	-1603377.3	-1603379.3
8.93	**Dipole-moment**	14.7739	14.9466	15.2071	14.5635	14.6224	14.554	15.2094	16.6317	17.9251	17.729	17.8751	19.3493
	E	-1603387.8	-1556579.8	-1603383.9	-1603382.3	-1603381.6	-1603381.9	-1603383.4	-1603382.6	-1603382.8	-1603379.8	-1603377.7	-1603379.3

7.58	**Dipole-moment**	14.679	14.8541	15.0993	14.4786	14.549	14.4893	15.1369	16.5614	17.8224	17.6435	17.7963	19.227
	E	-1603387.7	-1556579.6	-1603383.8	-1603382.2	-1603381.6	-1603381.8	-1603383.3	-1603382.5	-1603382.6	-1603379.6	-1603377.6	-1603378.9
6.89	**Dipole-moment**	14.6177	14.7945	15.0299	14.4238	14.5015	14.4474	15.0901	16.5159	17.756	17.5883	17.7453	19.1482
	E	-1603387.6	-1556579.6	-1603383.7	-1603382.1	-1603381.5	-1603381.8	-1603383.2	-1603382.4	-1603382.4	-1603379.6	-1603377.6	-1603378.7
5.621	**Dipole-moment**	14.4712	14.6517	14.864	14.2925	14.3876	14.3467	14.9775	16.4064	17.597	17.4555	17.6226	18.9593
	E	-1603387.5	-1556579.4	-1603383.5	-1603381.9	-1603381.4	-1603381.6	-1603383	-1603382.3	-1603382.2	-1603379.3	-1603377.3	-1603378.4
4.9	**Dipole-moment**	14.3592	14.5426	14.7376	14.1922	14.3004	14.2695	14.8911	16.3224	17.4754	17.3536	17.5283	18.815
	E	-1603387.3	-1556579.3	-1603383.3	-1603381.8	-1603381.3	-1603381.5	-1603382.9	-1603382.1	-1603381.9	-1603379.1	-1603377.1	-1603378.2
4.335	**Dipole-moment**	14.2499	14.436	14.6145	14.0941	14.2149	14.1937	14.8065	16.2399	17.3564	17.2538	17.4359	18.6741
	E	-1603387.2	-1556579.2	-1603383.2	-1603381.7	-1603381.1	-1603381.4	-1603382.8	-1603381.9	-1603381.8	-1603378.9	-1603377	-1603377.9

2.379	**Dipole-moment**	13.5787	13.7811	13.8635	13.4896	13.6851	13.7217	14.28	15.7243	16.6223	16.6327	16.8585	17.8081
	E	-1603386.4	-1556578.4	-1603382.3	-1603381	-1603380.4	-1603380.8	-1603381.9	-1603381.1	-1603380.4	-1603377.8	-1603375.9	-1603376.4
2.247	**Dipole-moment**	13.5031	13.7074	13.7796	13.4214	13.625	13.6678	14.22	15.6653	16.5393	16.5619	16.7925	17.7106
	E	-1603386.3	-1556578.4	-1603382.2	-1603380.9	-1603380.4	-1603380.7	-1603381.8	-1603380.9	-1603382.3	-1603377.7	-1603375.9	-1603376.3
2.228	**Dipole-moment**	13.4917	13.6963	13.7669	13.4111	13.6159	13.6597	14.211	15.6564	16.5268	16.5513	16.7825	17.6959
	E	-1603386.3	-1556578.4	-1603382.2	-1603380.9	-1603380.4	-1603380.7	-1603381.8	-1603380.9	-1603382.3	-1603377.7	-1603375.8	-1603376.2
2.023	**Dipole-moment**	13.3592	13.5668	13.62	13.2913	13.51	13.5647	14.1053	15.5523	16.3809	16.4266	16.6661	17.5248
	E	-1603386.1	-1556578.2	-1603382	-1603382.3	-1603380.3	-1603380.6	-1603381.6	-1603380.8	-1603380	-1603377.5	-1603375.6	-1603375.9
1.99	**Dipole-moment**	13.2853	13.4946	13.5382	13.2244	13.4508	13.5116	14.0462	15.494	16.2995	16.3569	16.6009	17.4293
	E	-1603386.1	-1556578.1	-1603381.9	-1603380.7	-1603380.2	-1603380.5	-1603381.5	-1603380.7	-1603379.8	-1603375.7	-1603375.5	-1603375.8

DMPC

Rotation		30	45	60	75	90	105	120	135	150	165	180
ε												
78.39	Dipole-moment	15.0472	14.9915	14.6579	15.1193	14.8771	15.2871	17.0061	17.7067	18.3733	19.0782	18.8395
	E	-1505421.5	-1505419.7	-1505418.5	-1505418.4	-1505419.8	-1505419.6	-1505419.4	-1505418.7	-1505417.3	-1505416.2	-1505415
46.8	Dipole-moment	15.0094	14.9508	14.6211	15.08	14.8426	15.256	16.9708	17.6682	18.3268	19.0244	18.798
	E	-1505421.4	-1505419.7	-1505418.4	-1505418.3	-1505419.8	-1505419.5	-1505419.4	-1505418.6	-1505417.2	-1505416.1	-1505414
38.2	Dipole-moment	14.9888	14.9287	14.601	15.0586	14.8238	15.239	16.9516	17.6472	18.3014	18.9951	18.7753
	E	-1505421.4	-1505419.7	-1505418.4	-1505418.3	-1505419.7	-1505419.5	-1505419.3	-1505418.5	-1505417.1	-1505416.1	-1505414
36.64	Dipole-moment	14.984	14.9235	14.5963	15.0537	14.8194	15.235	16.9472	17.6423	18.2955	18.9883	18.77
	E	-1505421.4	-1505419.6	-1505418.4	-1505418.3	-1505419.7	-1505419.5	-1505419.3	-1505418.4	-1505417.1	-1505416.1	-1505414
32.63	Dipole-moment	14.9696	14.908	14.5823	15.0387	14.8062	15.2232	16.9337	17.6277	18.2778	18.9679	18.7542
	E	-1505421.4	-1505419.6	-1505418.4	-1505418.3	-1505419.7	-1505419.5	-1505419.3	-1505418.4	-1505417.1	-1505416	-1505414

24.55	**Dipole-moment**	14.9268	14.862	14.5406	14.9944	14.7671	15.1879	16.8938	17.584	18.2252	18.9071	18.7071
	E	-1505421.3	-1505419.5	-1505418.3	-1505418.2	-1505419.7	-1505419.4	-1505419.2	-1505418.3	-1505417	-1505415.9	-1505414
20.7	**Dipole-moment**	14.8951	14.8279	14.5097	14.9615	14.7382	15.1617	16.8642	17.5516	18.1861	18.8621	18.6722
	E	-1505421.3	-1505419.3	-1505418.3	-1505418.2	-1505419.6	-1505419.4	-1505419.2	-1505418.3	-1505416.9	-1505415.8	-1505414
10.36	**Dipole-moment**	14.7017	14.6204	14.3213	14.7612	14.5613	15.0015	16.683	17.3537	17.9482	18.588	18.4589
	E	-1505421	-1505419.2	-1505418	-1505417.9	-1505419.3	-1505419.1	-1505418.8	-1505417.9	-1505416.4	-1505415.3	-1505414
8.93	**Dipole-moment**	14.6426	14.5571	14.2637	14.7001	14.5072	14.9524	16.6275	17.2931	17.9482	18.5044	18.3935
	E	-1505420.9	-1505419.1	-1505417.9	-1505417.8	-1505419.2	-1505419	-1505418.7	-1505417.8	-1505416.3	-1505415.3	-1505414
7.58	**Dipole-moment**	14.5683	14.4776	14.1914	14.6233	14.4392	14.8906	16.5576	17.2169	17.8755	19.0782	18.3113
	E	-1505420.8	-1505419	-1505417.8	-1505417.7	-1505419.1	-1505418.9	-1505418.6	-1505417.6	-1505416.1	-1505414.9	-1505413
6.89	**Dipole-moment**	14.5203	14.4262	14.1446	14.5736	14.3951	14.8506	16.5123	17.1675	17.7841	18.3316	18.2581
	E	-1505420.8	-1505418.8	-1505417.8	-1505417.6	-1505419.1	-1505418.8	-1505418.5	-1505417.5	-1505416	-1505414.8	-1505413

5.621	**Dipole-moment**	14.405	14.303	14.0324	14.4546	14.2895	14.7543	16.4035	17.0488	17.725	18.169	18.1301
	E	-1505420.6	-1505418.7	-1505417.6	-1505417.5	-1505418.9	-1505418.7	-1505418.3	-1505417.3	-1505415.7	-1505414.5	-1505413
4.9	**Dipole-moment**	14.3167	14.2087	13.9464	14.3634	14.2084	14.6803	16.3199	16.9577	17.4745	18.0446	18.0318
	E	-1505420.5	-1505418.6	-1505417.5	-1505417.3	-1505418.8	-1505418.5	-1505418.1	-1505417.1	-1505415.5	-1505414.2	-1505413
4.335	**Dipole-moment**	14.2301	14.1165	13.8622	14.2741	14.1289	14.6077	16.2378	16.8682	17.368	17.9229	17.9354
	E	-1505420.4	-1505417.9	-1505417.4	-1505417.2	-1505418.6	-1505418.4	-1505418	-1505416.9	-1505415.3	-1505414	-1505413
2.379	**Dipole-moment**	13.6934	13.546	13.3399	13.7217	13.6346	14.1533	15.7249	16.3101	16.7071	17.1711	17.3336
	E	-1505419.7	-1505417.8	-1505416.7	-1505416.4	-1505417.8	-1505417.6	-1505417	-1505415.8	-1505414	-1505412.5	-1505412
2.247	**Dipole-moment**	13.6324	13.4814	13.2805	13.6591	13.5783	14.1013	15.6662	16.2462	16.632	17.086	17.2649
	E	-1505419.6	-1505417.8	-1505416.6	-1505416.3	-1505417.8	-1505417.5	-1505416.9	-1505415.7	-1505413.8	-1505412.4	-1505411
2.228	**Dipole-moment**	13.6231	13.4716	13.2716	13.6496	13.5698	14.0934	15.6573	16.2366	16.6206	17.0732	17.2544
	E	-1505419.6	-1505417.6	-1505416.6	-1505416.3	-1505417.7	-1505417.5	-1505416.9	-1505415.7	-1505413.8	-1505412.3	-1505411

2.023	**Dipole-moment**	13.5158	13.3581	13.1671	13.5394	13.4706	14.0016	15.5538	16.1241	16.4884	16.9236	17.1332
	E	-1505419.5	-1505417.5	-1505416.5	-1505416.2	-1505417.6	-1505417.3	-1505416.7	-1505415.5	-1505413.5	-1505412.1	-1505411
1.99	**Dipole-moment**	13.4558	13.2946	13.1088	13.4778	13.4151	13.9501	15.4957	16.0611	16.4145	16.8401	17.0653
	E	-1505419.4	-1505419.6	-1505416.4	-1505416.7	-1505417.5	-1505417.3	-1505416.6	-1505415.3	-1505413.4	-1505412.1	-1505411

Conclusion

We have compared DMPC & DPPC molecules in membrane to electroscope that using external charges on the ball of electroscope can regulate handicap distance of angle between two sheet of electroscope. The role of this ball is the same role of phosphorus in the membrane molecules and the hydrocarbons chines have the same role of electroscope sheet. Hydrophobic and hydrophilic forces of charges accruing on metal ions at the time that effect on membrane create one charge induction in the phosphorus atom. This charge induction effects on the hydrocarbons chains and cause particular dynamic movement of phospholipids. This dynamic movement causes to enter and exit material to or of cytoplasm membrane. Our exertion in this investigation is determined agents such as atom partially charges on dipole moment and dielectric constant in angle between chain-phosphorus-chain that results this notation.

1-A communicating is between dipole moment with energy and rotation angle

2-The most P charge was in 105 degree that coordinates with angle hybridation

3-Synchronus to induction charges in phosphorus is observed addition charge in oxygen

4-Coordination between O62, O49, C50, and N81 in DPPC totally can comfortably with studies consider charge theory dynamic stochastic behavior.

5-Two regions of dielectric constant values are identified (1<D<10) and (10<D<80). As it is expected, with increasing of dielectric constant of solvents and stability of DPPC and DMPC are increased also atomic charge of the some atoms were increased versus to increase of dielectric constant but a some atoms were decreased. Whit plot of the calculated energies, dipole moment and atomic charge of selected atoms of DPPC and DMPC as a function of 1/D, we have linear equations and it is a good result. We propose for future is founding a empirical communicating between effect of solvent and membrane molecule.

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