Electronic Supplementary Material (ESI) for RSC Advances.

Fullerene Translocation through Peroxidized Lipid Membranes

Gulsah Gul and Nazar Ileri-Ercan*

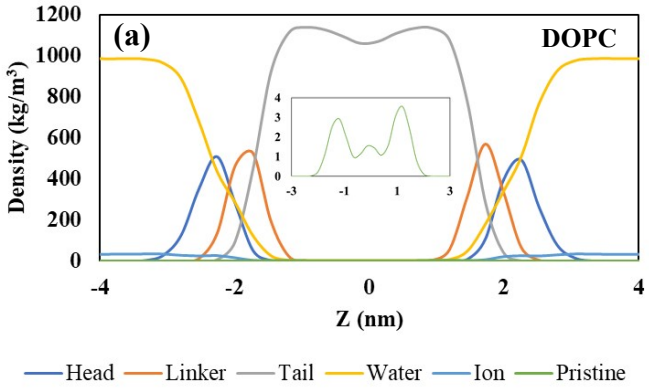
Department of Chemical Engineering, Bogazici University, Istanbul, Turkey

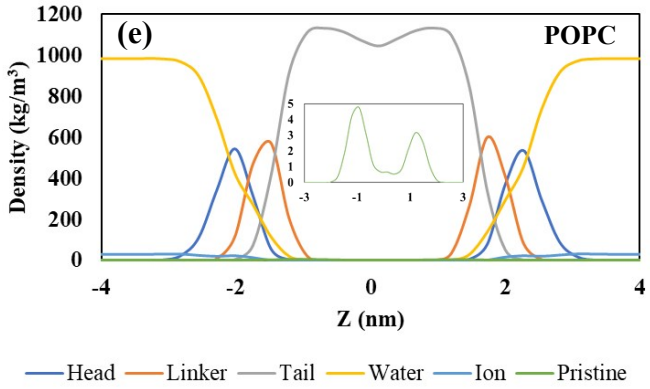
SUPPORTING INFORMATION

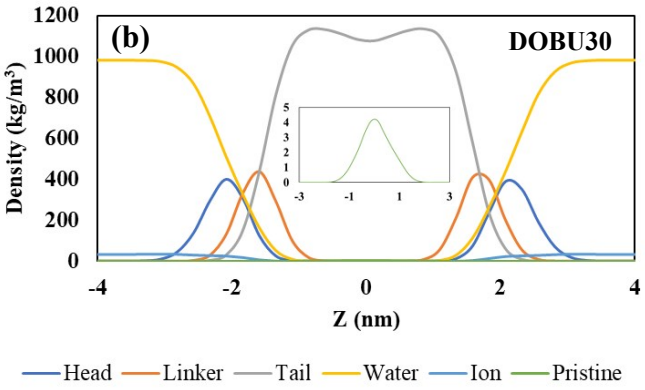
Table S1. List of the simulated systems. Here P denotes pristine fullerenes while J denotes janus fullerenes. Third column represents the regular PC number (either DOPC or POPC) while fourth column shows the oxidized number of lipids (either DOBU or POBU) according to the membrane model. Salt concentration is determined as 0.15 M and ion numbers are calculated based on the simulated box volumes. The total simulation time including equilibration exceeds 400 μs.

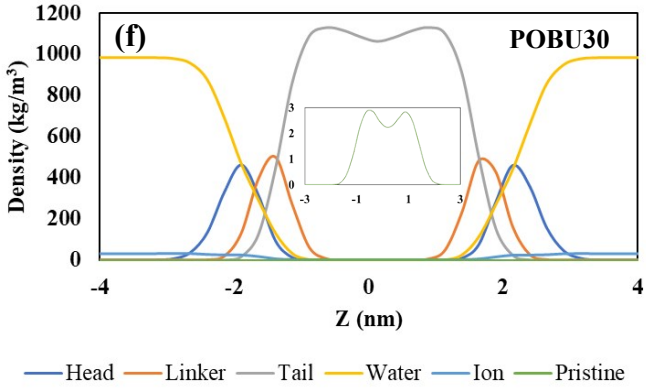
Membrane	No of Molecules						Simulation Time (μs)	No
	Fullerene	DOPC/POPC	DOBU/POBU	Water	Na^+	Cl^-		
DOPC	no	512	-	12312	204	204	10	1
	1P	512	-	12312	204	204	10	2
	1J	512	-	12312	204	204	10	3
	10P	512	-	12312	204	204	10	4
	10J	512	-	12312	204	204	10	5
DOBU30	no	358	154	12312	208	208	10	6
	1P	358	154	12312	208	208	10	7
	1J	358	154	12312	208	208	10	8
	10P	358	154	12312	208	208	10	9
	10J	358	154	12312	208	208	10	10
DOBU70	no	154	358	12312	210	210	10	11
	1P	154	358	12312	210	210	10	12
	1J	154	358	12312	210	210	10	13
	10P	154	358	12312	210	210	10	14
	10J	154	358	12312	210	210	10	15
DOBU	no	-	512	12312	212	212	10	16
	1P	-	512	12312	212	212	10	17
	1J	-	512	12312	212	212	10	18
	10P	-	512	12312	212	212	10	19
	10J	-	512	12312	212	212	10	20
POPC	no	512	-	12312	200	200	10	21
	1P	512	-	12312	200	200	10	22

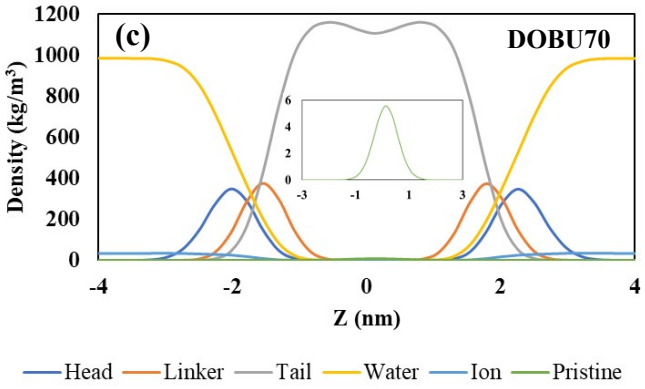
	1J	512	-	12312	200	200	10	23
	10P	512	-	12312	200	200	10	24
	10J	512	-	12312	200	200	10	25
POBU30	no	358	154	12312	201	201	10	26
	1P	358	154	12312	201	201	10	27
	1J	358	154	12312	201	201	10	28
	10P	358	154	12312	201	201	10	29
	10J	358	154	12312	201	201	10	30
POBU70	no	154	358	12312	202	202	10	31
	1P	154	358	12312	202	202	10	32
	1J	154	358	12312	202	202	10	33
	10P	154	358	12312	202	202	10	34
	10J	154	358	12312	202	202	10	35
POBU	no	-	512	12312	204	204	10	36
	1P	-	512	12312	204	204	10	37
	1J	-	512	12312	204	204	10	38
	10P	-	512	12312	204	204	10	39
	10J	-	512	12312	204	204	10	40

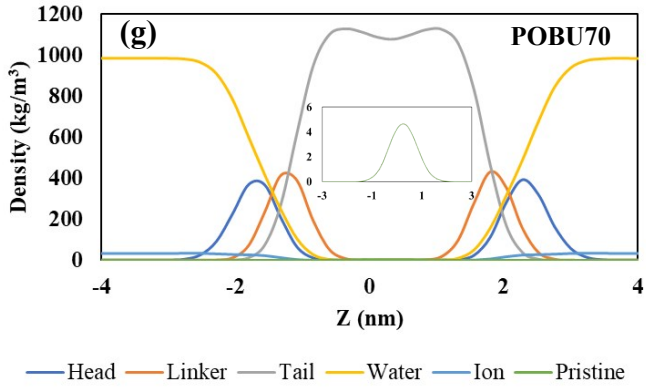

(a)
DOPC
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine

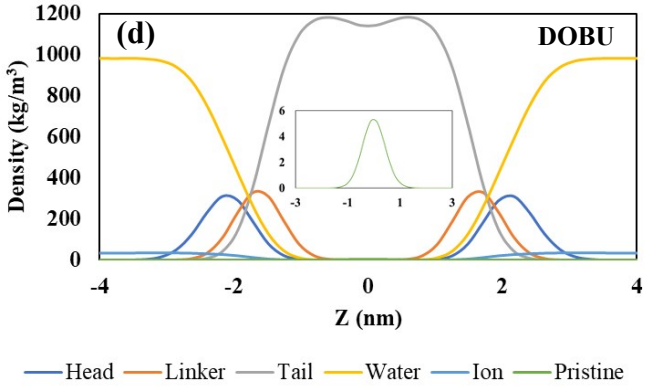

(e)
POPC
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine


(b)
DOBU30
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine


(f)
POBU30
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine


(c)
DOBU70
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine


(g)
POBU70
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine


(d)
DOBU
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine

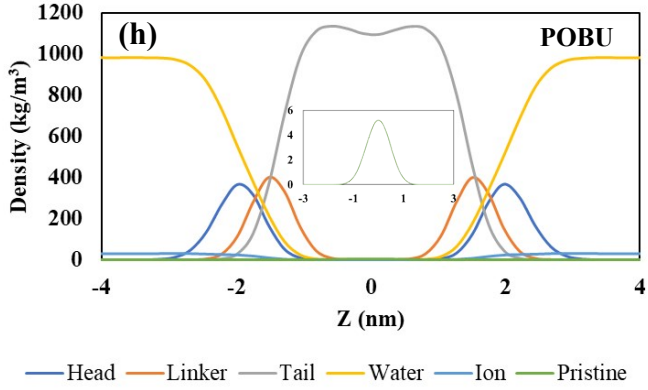
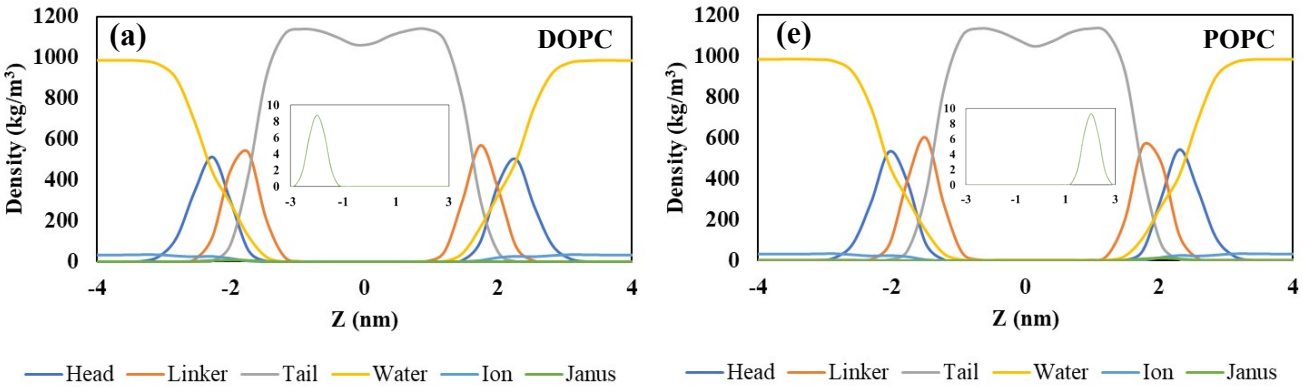

(h)
POBU
Density (kg/m³)
Z (nm)
Head
Linker
Tail
Water
Ion
Pristine

Figure S1. Density distribution profiles of lipid head (NC3 & PO4 beads), linker (GL1 & GL2 beads), and tail groups together with water, ion and pristine fullerenes (enlarged in insets), **(a-d)** for DOPC and its oxidized forms, **(e-h)** for POPC and its oxidized forms at fullerene to lipid ratio of F/L =1/512.


(a)
DOPC
Density (kg/m3)
1200
1000
800
600
400
200
0
-4
-2
0
2
4
Z (nm)
10
8
6
4
2
0
-3
-1
1
3
Head
Linker
Tail
Water
Ion
Janus
(e)
POPC
Density (kg/m3)
1200
1000
800
600
400
200
0
-4
-2
0
2
4
Z (nm)
10
8
6
4
2
0
-3
-1
1
3
Head
Linker
Tail
Water
Ion
Janus

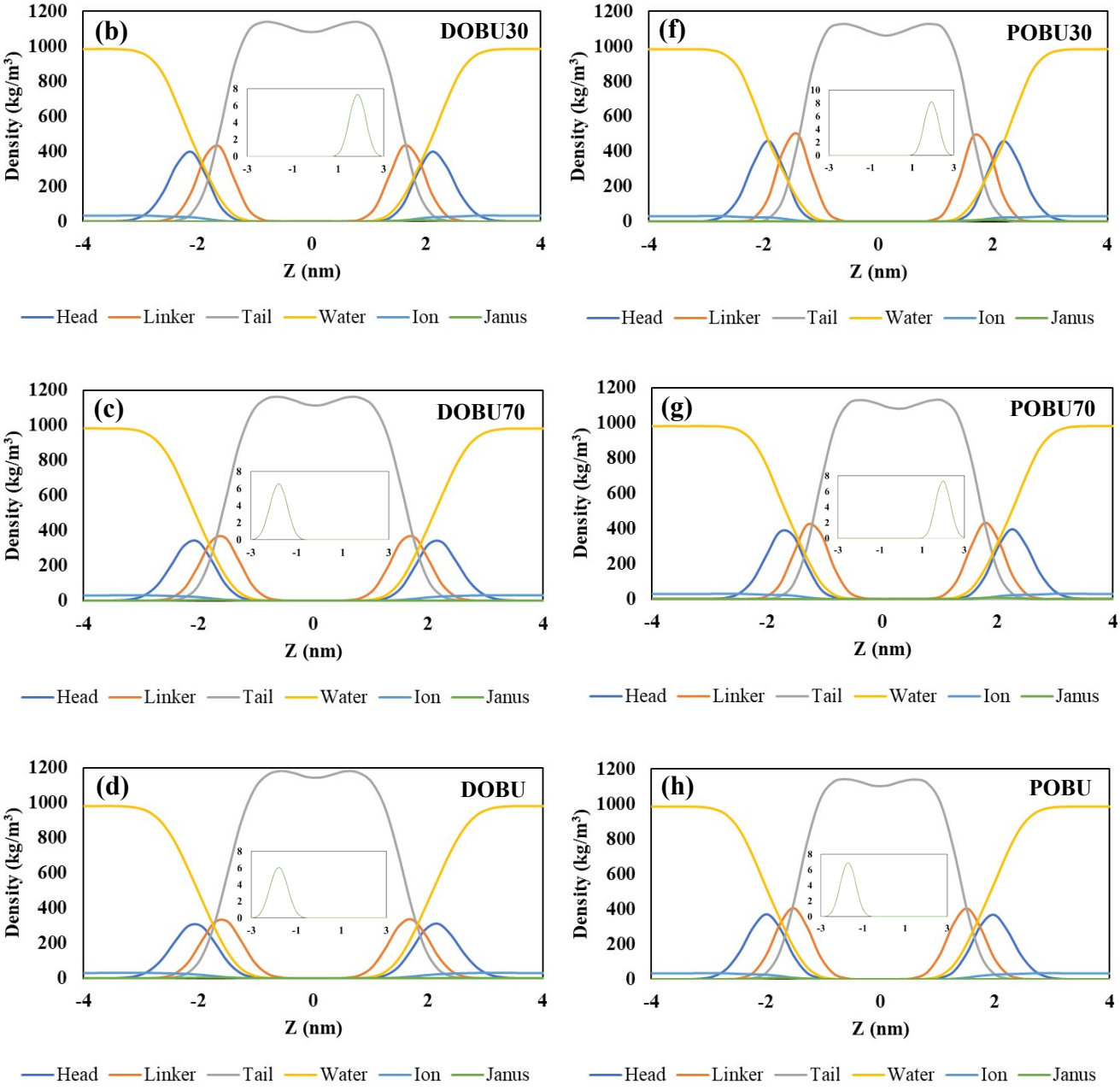


Figure S2. Density distribution profiles of lipid head (NC3 & PO4 beads), linker (GL1 & GL2 beads), and tail groups together with water, ion and janus fullerenes (enlarged in insets), **(a-d)** for DOPC and its oxidized forms, **(e-h)** for POPC and its oxidized forms at fullerene to lipid ratio of F/L =1/512.

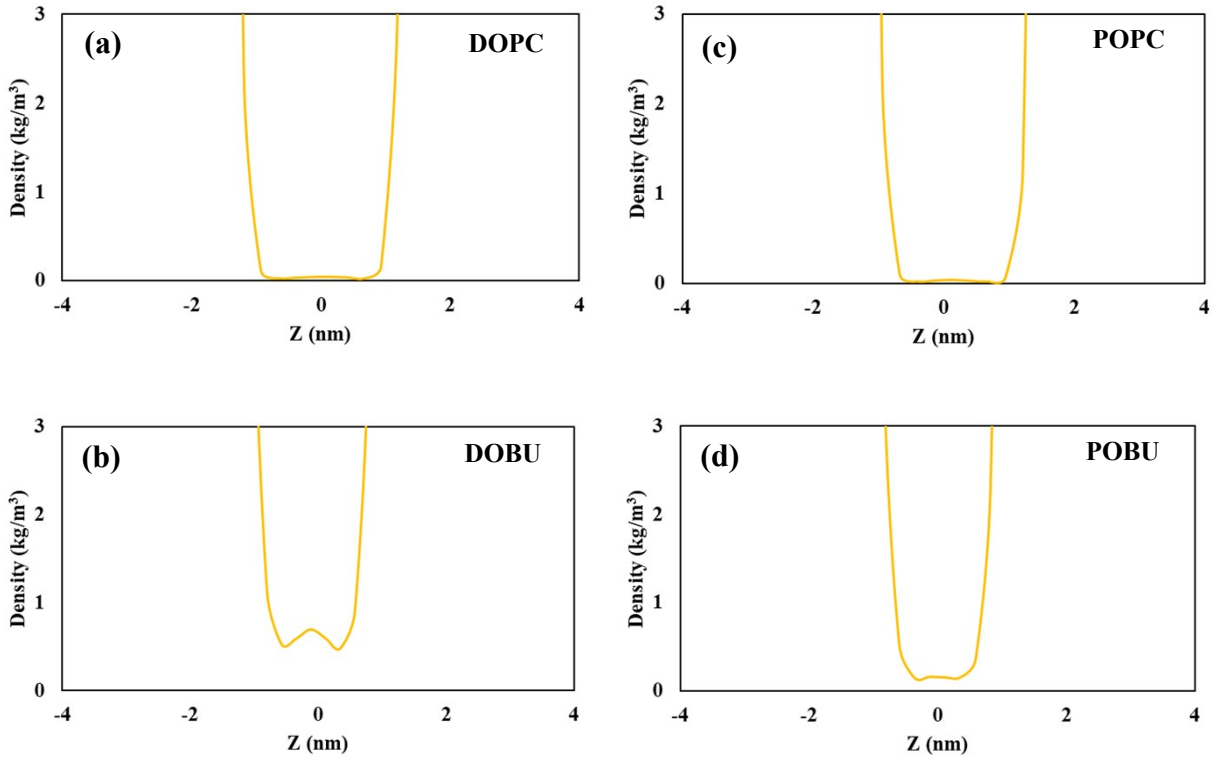


Figure S3. Enlarged density distribution profiles of water **(a-b)** for DOPC and its oxidized form (DOBU), **(c-d)** for POPC and its oxidized form (POBU) at pristine fullerene to lipid ratio of F/L =10/512.

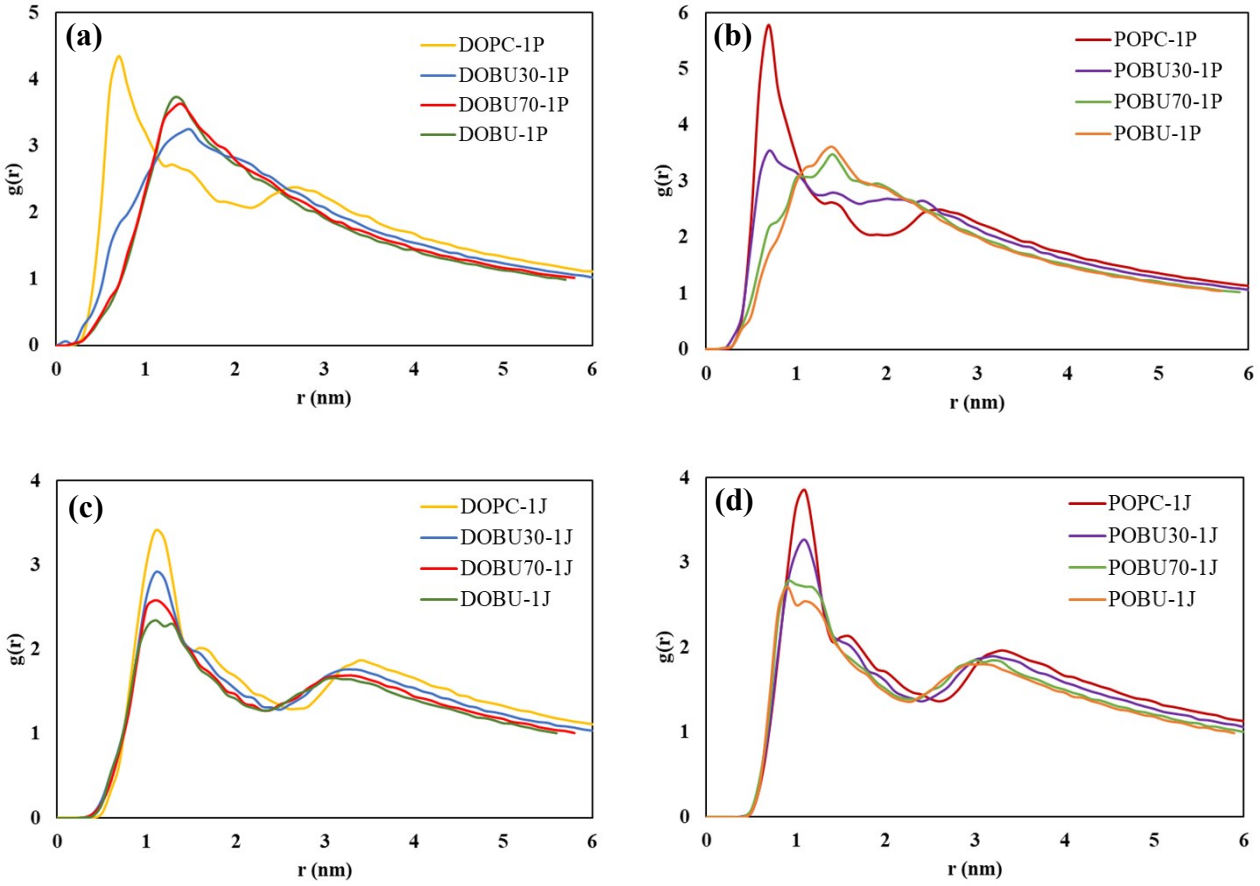


Figure S4. Membrane-Fullerene COM radial distribution functions for **(a-b)** pristine fullerenes, **(c-d)** janus fullerenes at fullerene-to-lipid ratio of 1/512.

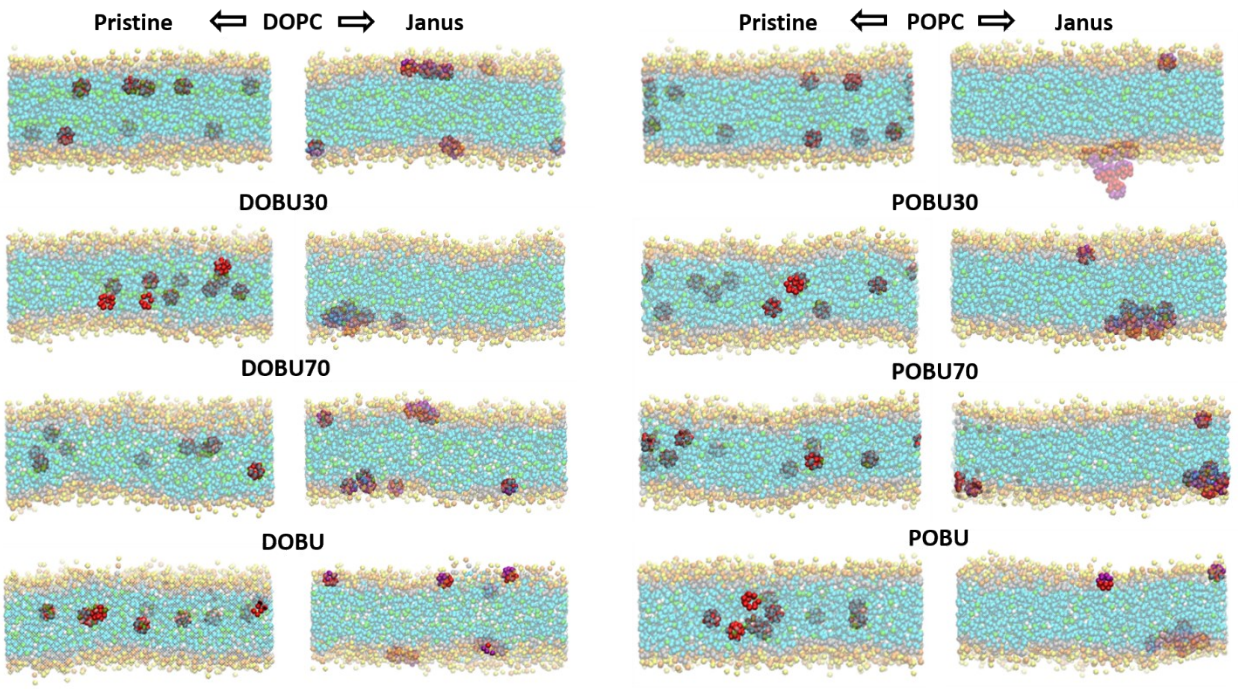


Figure S5. Last configurations (side view) obtained after 10 μs simulation time at fullerene-to-lipid (F/L) ratio of 10/512.