Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Effect of Ionic environment on Membrane Fouling: A Molecular Dynamics Study

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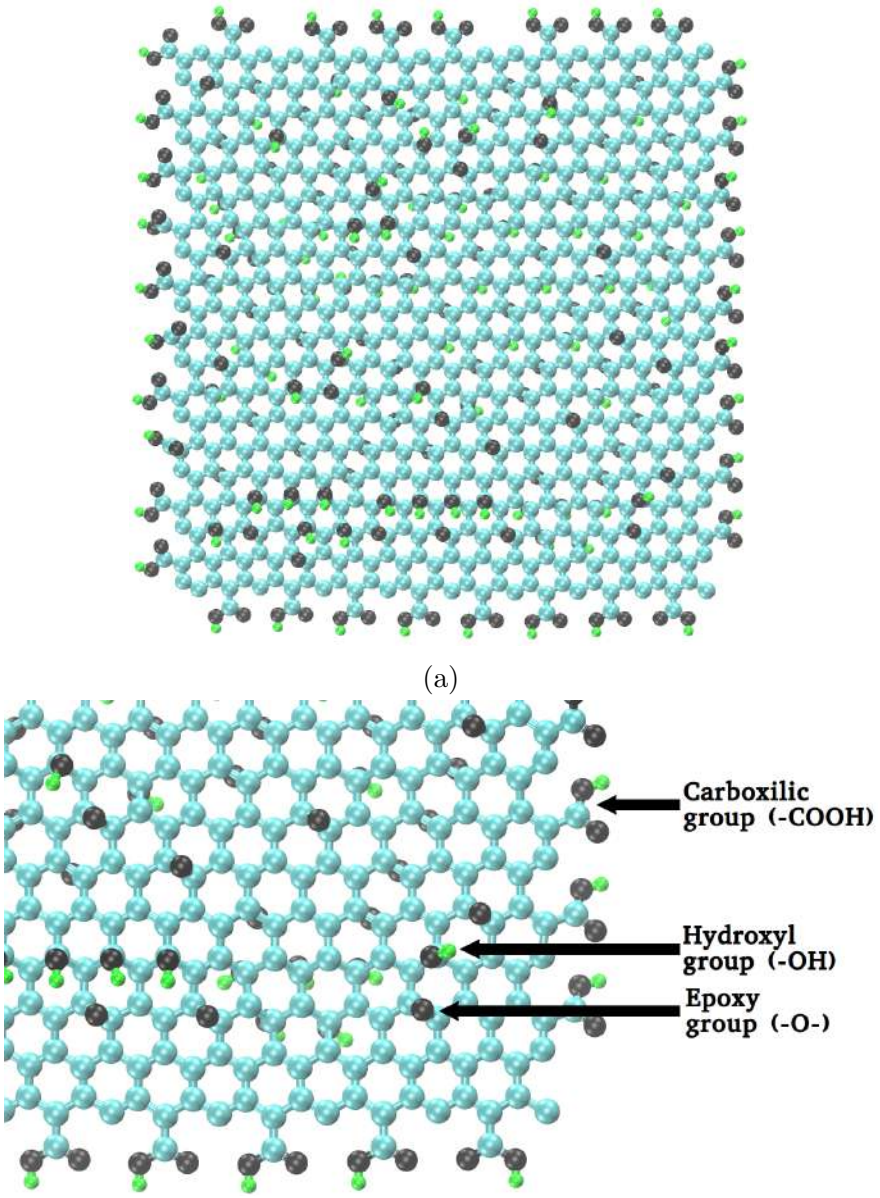
GO nanosheet



(a)

(b)

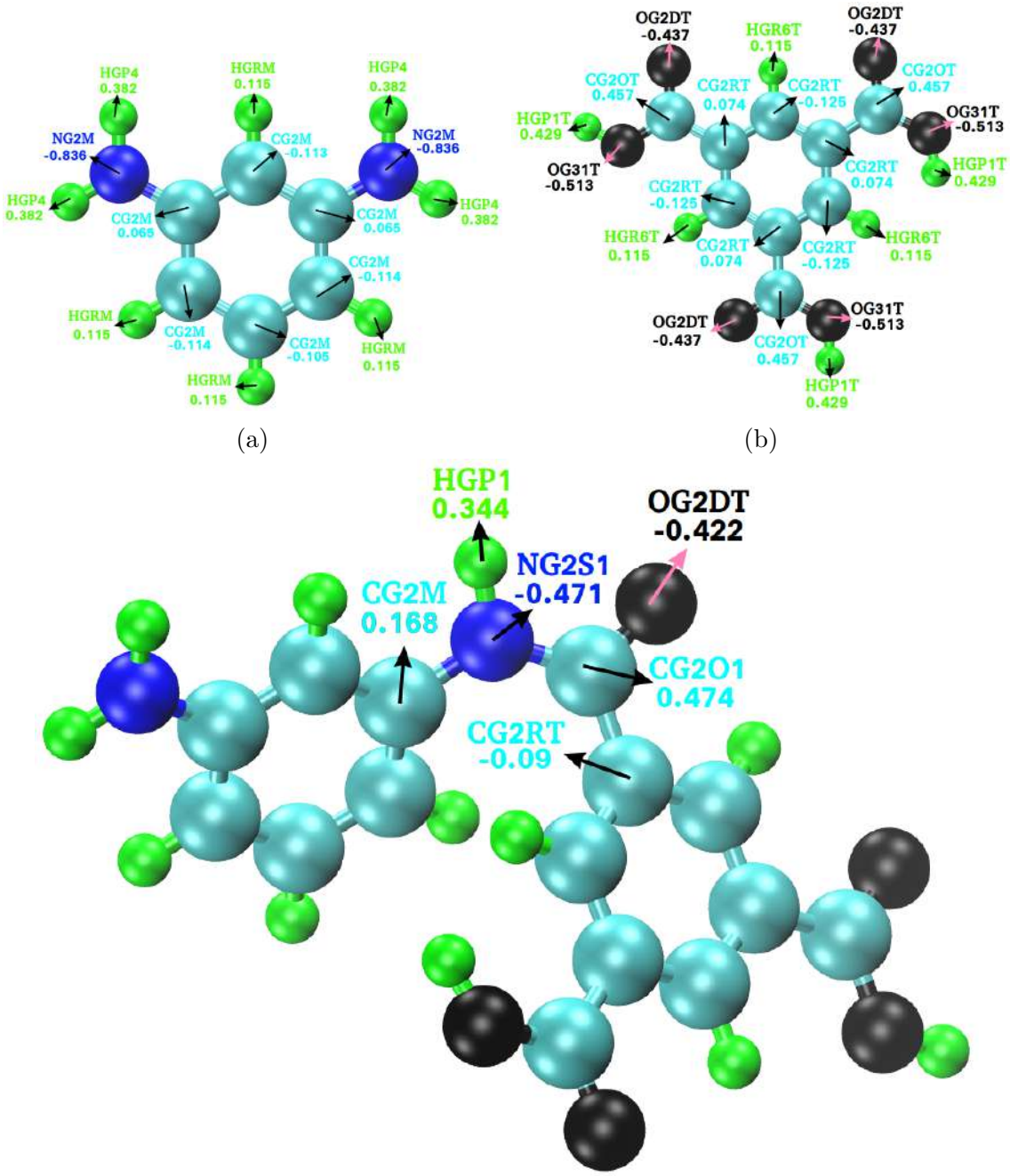
Figure S1: (a) GO nanosheet. (b) The distribution of functional groups on GO nanosheet. The green color is for hydrogen atoms, the black color is for oxygen atoms and the cyan color is for carbon atoms.

Partial charges and other parameters for GO

Table S1: Nonbonded potential parameters and charges for atoms of GO.

atom	σ (Å)	ϵ (kcal/mol)	charge (q)
C(C——C)	1.908	0.053	0
C(C—OH)	1.908	0.053	+0.2
C(C═O)	2.105	0.105	+0.52
O(C——O)	1.627	0.139	-0.4
O(O——H)	1.751	0.170	-0.683
O(O═C)	0.210	1.661	-0.44
O(C—OH)	1.684	0.170	-0.53
H(C—OH)	0.0	0.0	+0.45
H(O——H)	0.0	0.0	+0.418

Polyamide



(a) (b)

(c)

Figure S2: Monomers and atomtypes of (a) MPD (b) TMO and (c) amide linkage between an MPD and TMO monomer.

Functional Groups on Graphene Oxide

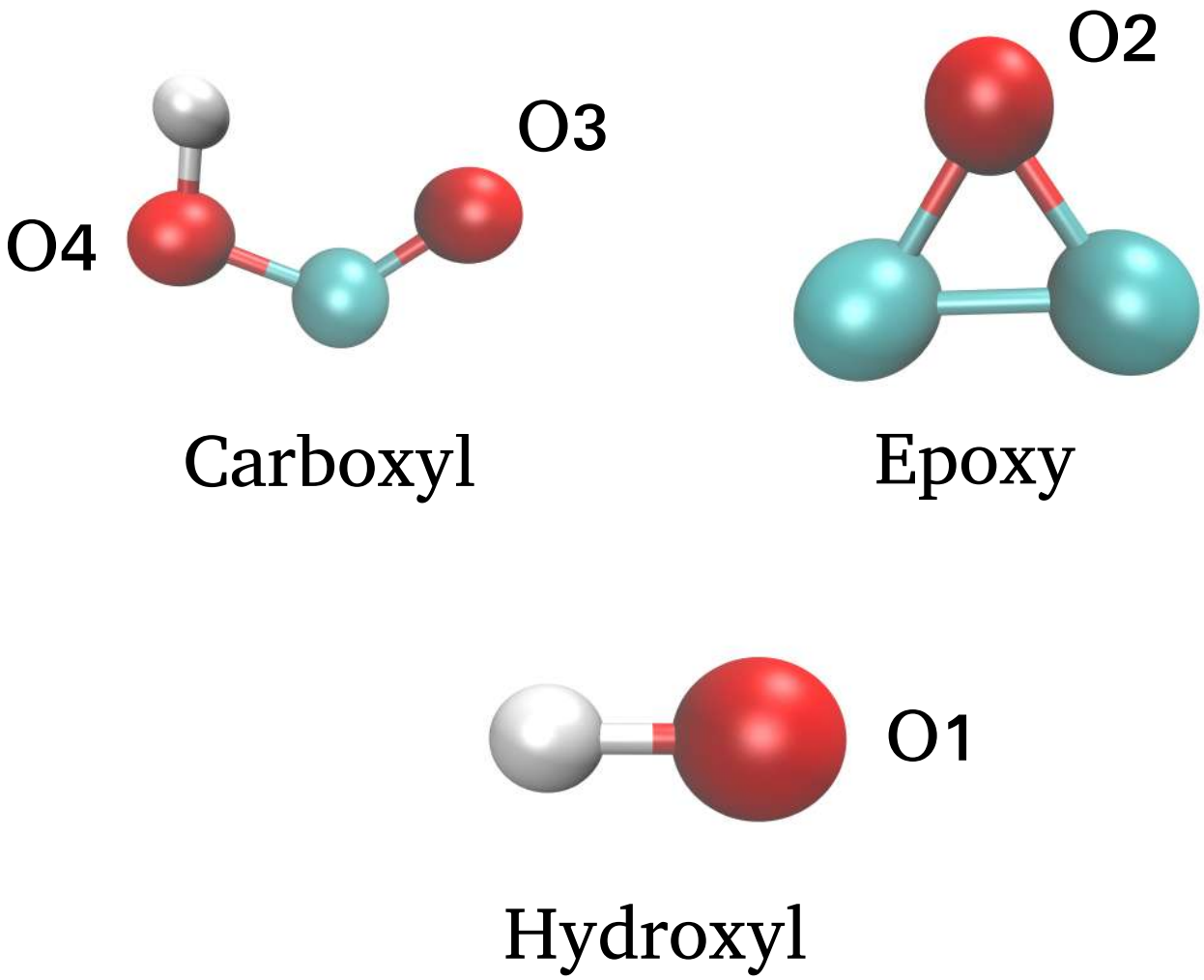
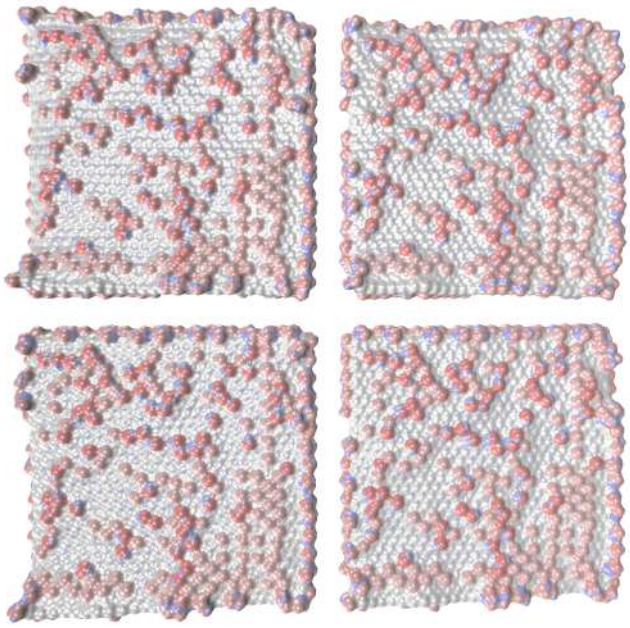
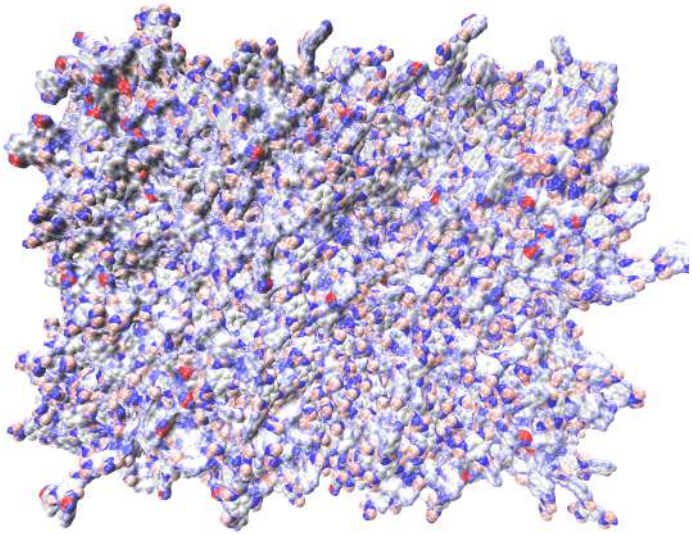


Figure S3: Different functional groups present on the graphene oxide surface and the atom types of oxygen atom on them.

Surface Charge Distribution



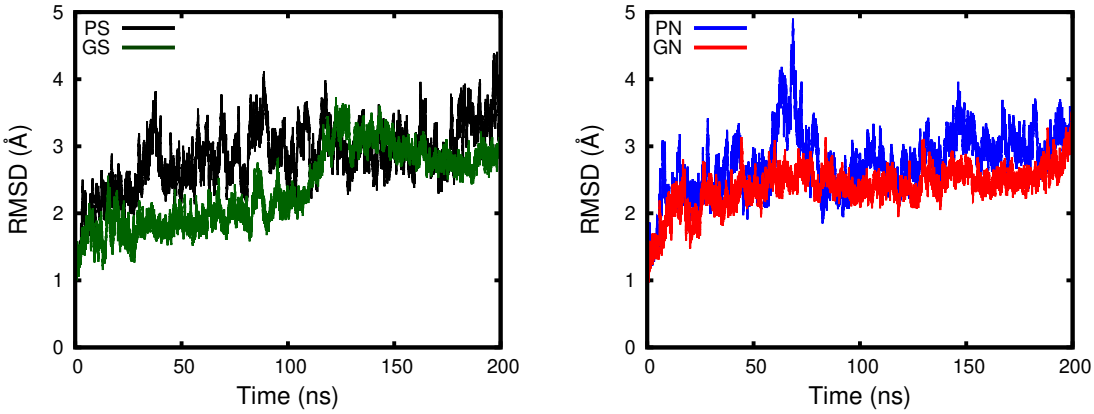
(a)



(b)

Figure S4: Charge distribution on the surfaces of the two membranes (a) Graphene Oxide (b) Polyamide. The blue, red and white color represents positive, negative and neutral charges.

Structural Evolution of Protein



(a) (b)

Figure S5: Time evolution of RMSD of backbone alpha carbon atoms of protein for (a) excess ions systems and (b) without excess ion systems .

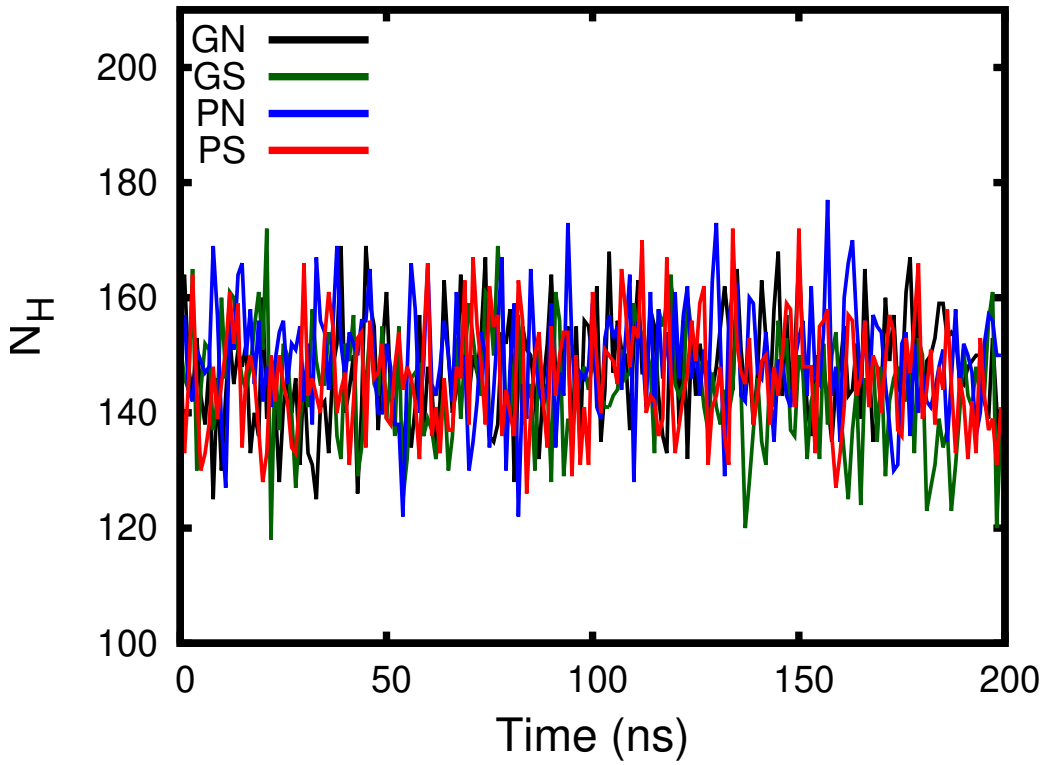


Figure S6: Time evolution of the number of hydrogen bonds in protein for all the systems .