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

What Governs the Nature of Fouling in Forward Osmosis (FO) and Reverse Osmosis (RO)? A Molecular Dynamics Study

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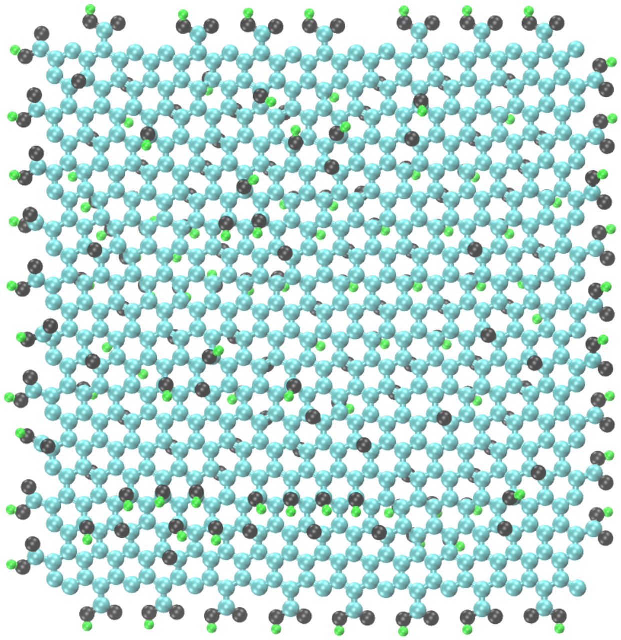
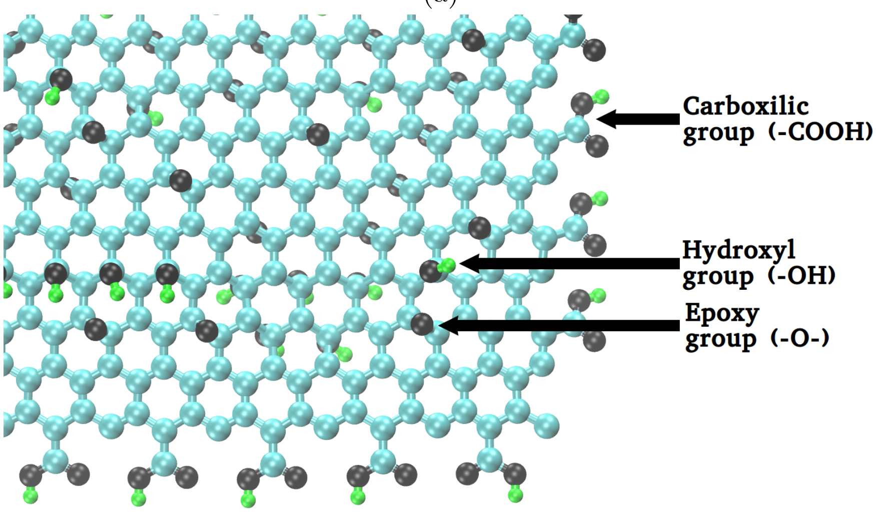
GO nanosheet



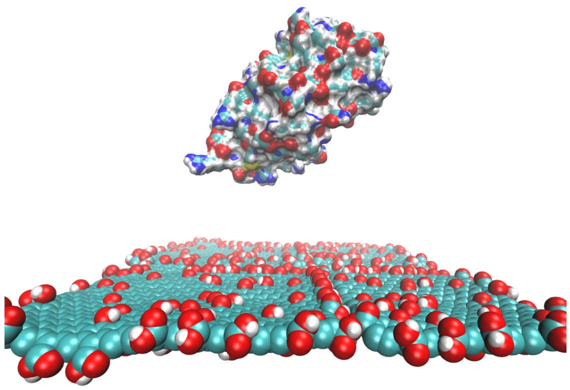
(a)



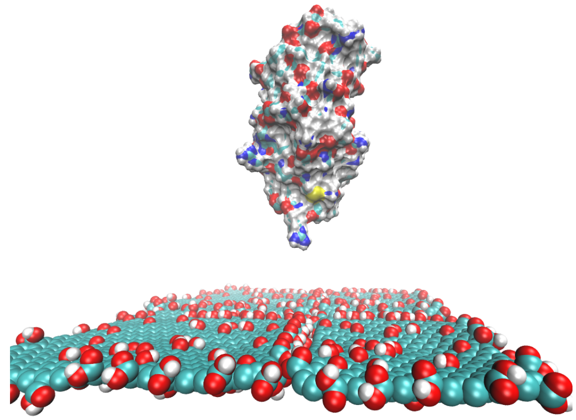
(b)

Figure S1: (a) GO nanosheet. (b) 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.

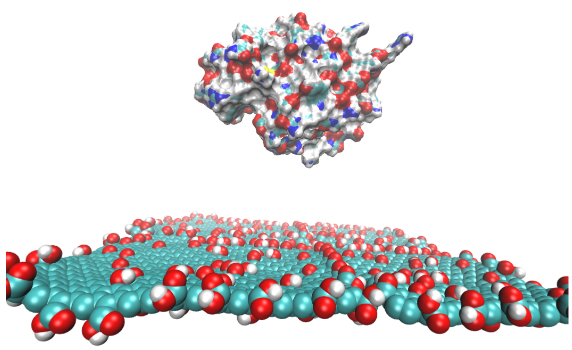
Different initial orientation



(a)



(b)



(c)

Figure S2: Three initial configuration with different protein orientation relative to the surface (a) Orientation I(O1) (b) Orientation II(O2) (c) Oreintation III(O3). Membrane surface is shown in Vdw and protein is shown in surf representation respectively.

Angle between protein and GO surface

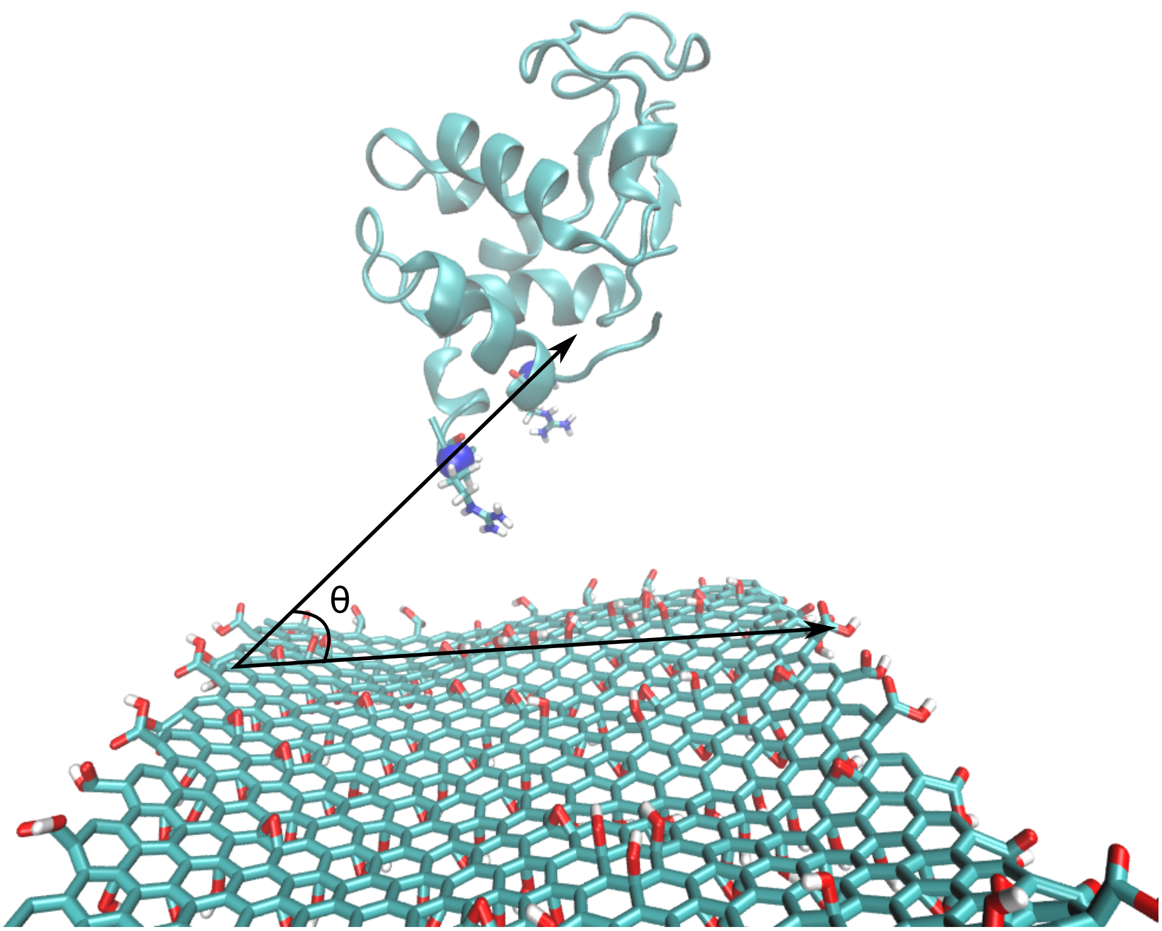


Figure S3: Pictorial representation of angle between the protein and GO surface. GO surface and key residues are shown in licorice representation. Aplha carbons (blue color) and rest of the protein are shown in VDW and New Cartoon representation respectively.

Time evolution of distance

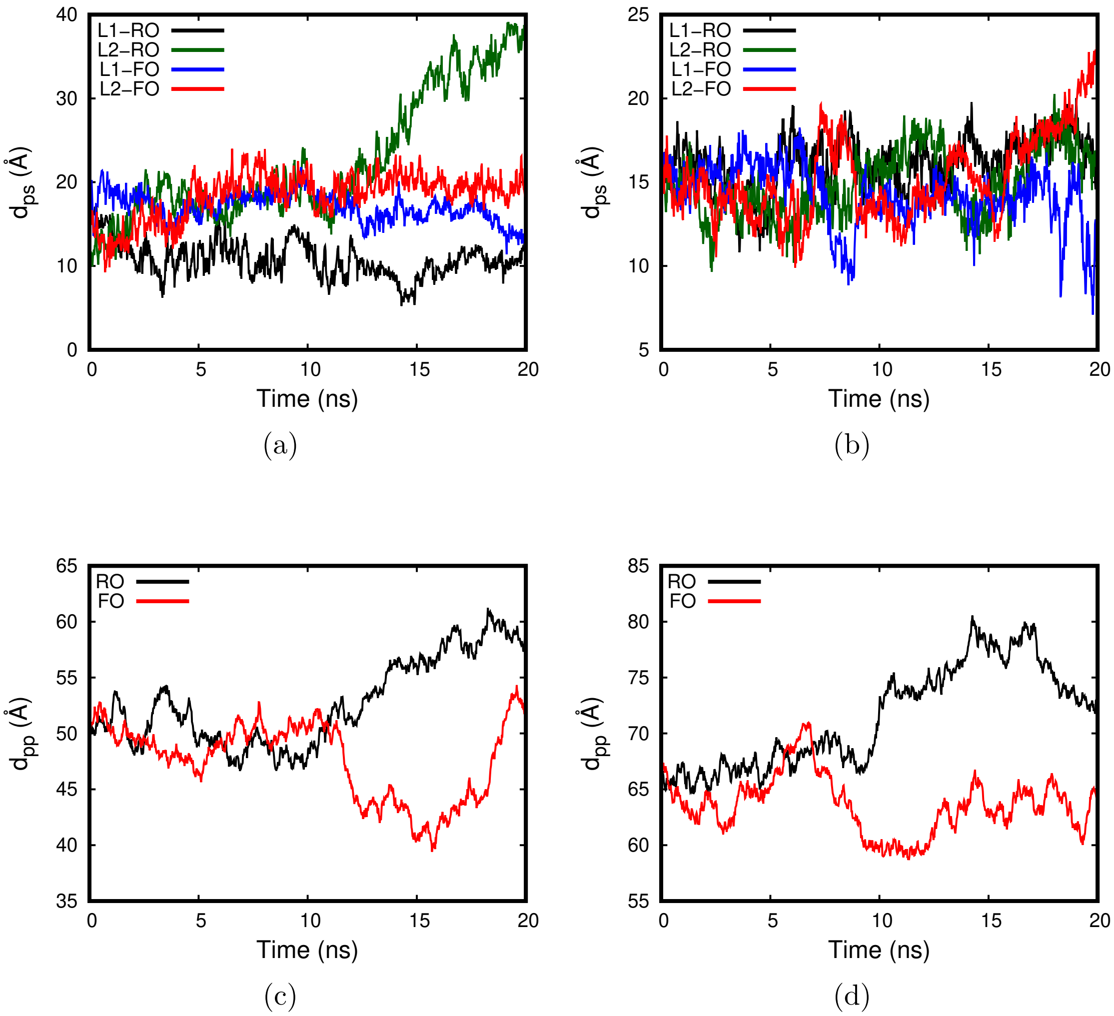


Figure S4: Time evolution of distance between membrane and protein for (a) O2 (b) O3. Time evolution of distance between between L1 and L2 for (c) O2 (d) O3.

Time evolution of Interaction energy

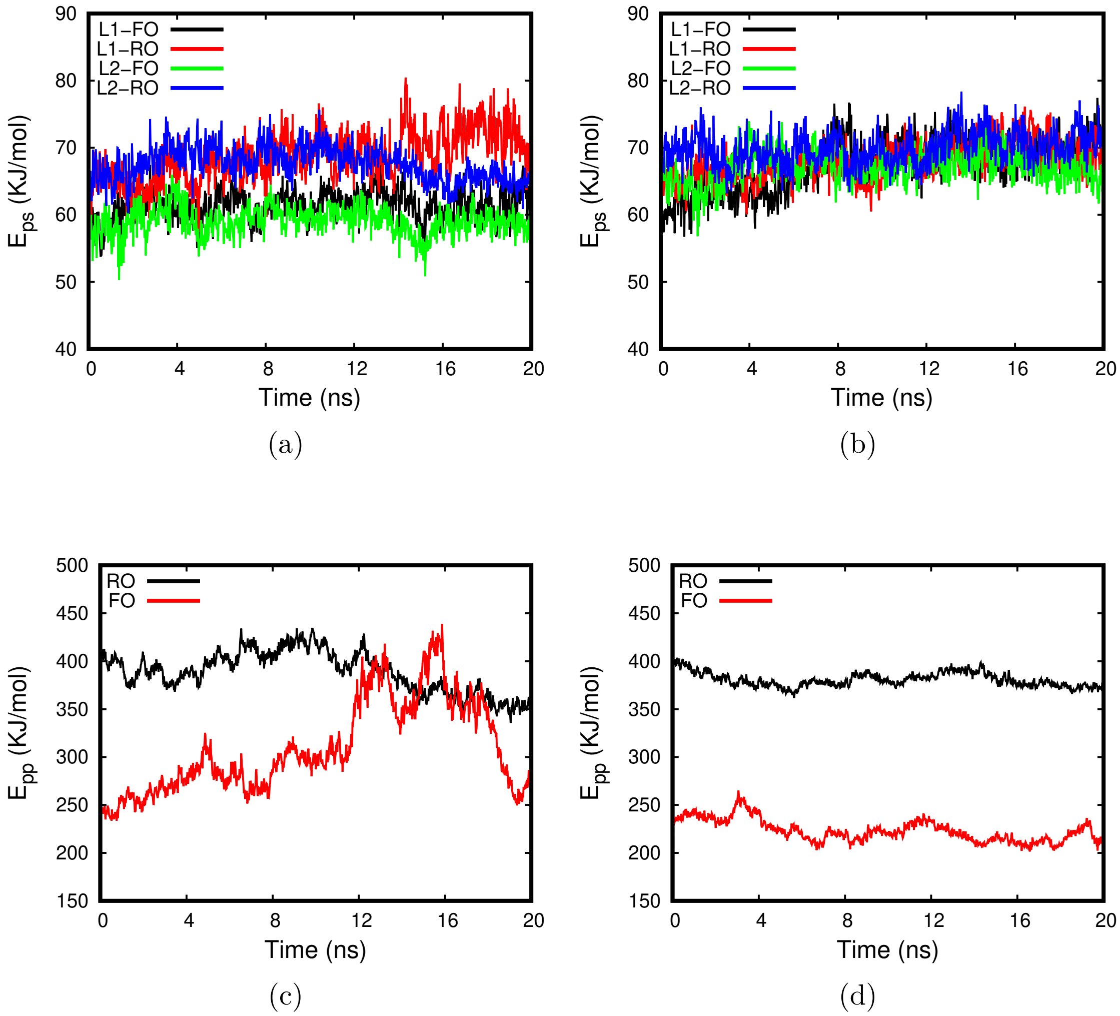
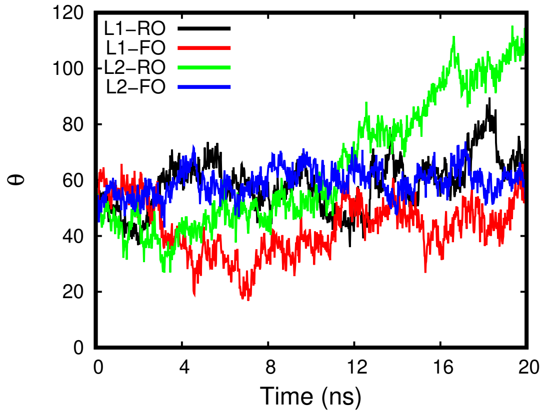
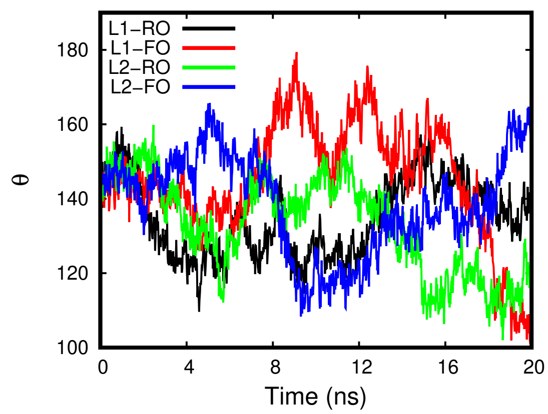


Figure S5: Time evolution of interaction energy between membrane and protein for (a) O2 (b) O3. Time evolution of interaction energy between L1 and L2 for (c) O2 (d) O3.

Time evolution of orientation



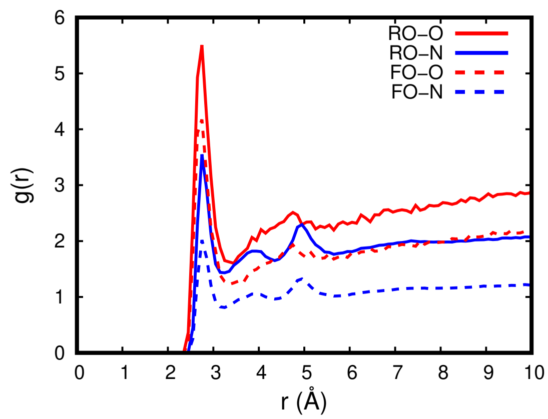
(a)



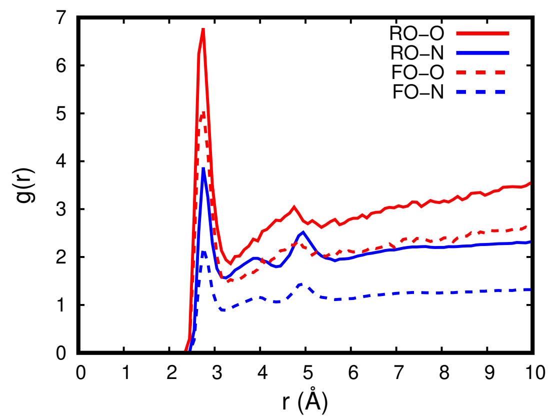
(b)

Figure S6: Temporal evolution of protein orientation relative to the membrane surface for (a)O2 (b)O3

g(r) between protein and water molecules



(a)



(b)

Figure S7: RDF between (oxygen(L1)-oxygen(water) and nitrogen(L1)-oxygen(water) shown in red and blue color respectively for (a) O2 (b) O3 for RO(solid lines) and FO(dashed lines).

g(r) between protein and ions

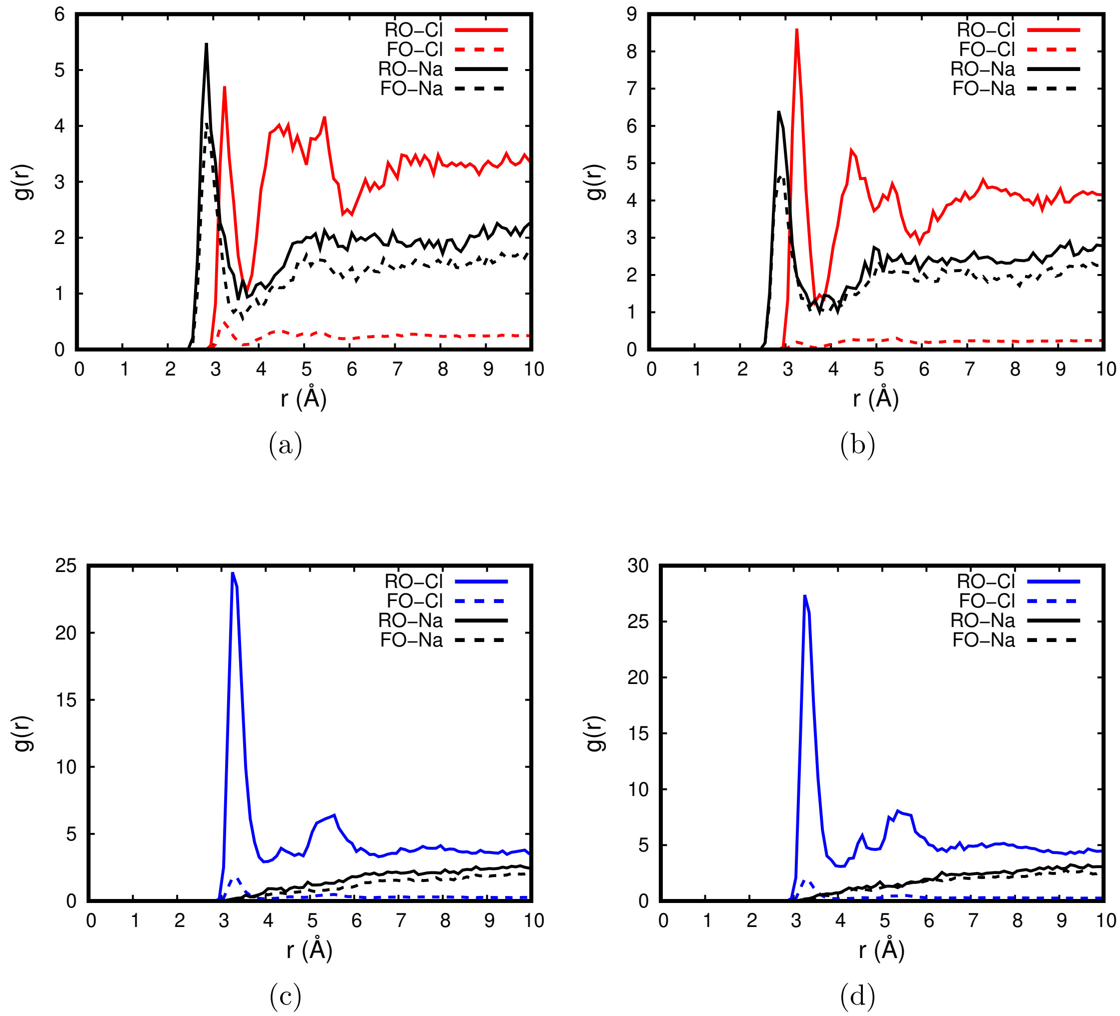


Figure S8: RDF between oxygen(L1)-chloride(ions) and oxygen(L1)-sodium(ions) shown in red and black respectively for (a) O2 (b) O3. RDF between nitrogen(L1)-chloride(ions) and nitrogen(L1)-sodium(ions) shown in blue and black color respectively for (c) O2 (d) O3 for RO(solid lines) and FO(dashed lines).

Force field and parameters

OPLS-AA force field is employed in the simulations which has a functinal form as follows:

$$U_{total} = U_{bonds} + U_{angles} + U_{dihedrals} + U_{vdW} + U_{coulomb} \tag{1}$$

The first three terms in the equation above represents the bonded interactions, which are given as:

$$U_{bonds} = \sum_{bonds} k_r(r_i - r_{eq})^2 \tag{2}$$

$$U_{angle} = \sum_{angles} k_\theta(\theta_i - \theta_{eq})^2 \tag{3}$$

$$U_{torsion} = \sum_i \frac{V_1^i}{2}[1 + \cos(\phi_i + f_{i1})] + \frac{V_2^i}{2}[1 - \cos(2\phi_i + f_{i2})] + \frac{V_3^i}{2}[1 + \cos(3\phi_i + f_{i3})] \tag{4}$$

eqs 2 and 3 represents potential for bond stretching and angle bending, where (k_r, k_θ) are force constants, (r_i, θ_i) are instantaneous bond length and angle respectively and (r_{eq}, θ_{eq}) are equilibrium bond lengths and bond angles respectively for the corresponding cases. Eq 4 is for the torsional energy contribution, where (V_1, V_2, V_3) are coefficients of Fourier series, ϕ_i is the dihedral angle and (f_1, f_2, f_3) are phase angles.

The nonbonded interactions are modeled with coulomb's law and Lennard-Jones potential for electrostatic and Van der Wal's contribution as follows:

$$U_{vdW} = \sum_i \sum_{j>i} 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] \tag{5}$$

$$U_{coulomb} = \sum_i \sum_{j>i} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \tag{6}$$

ϵ_{ij} in eq 5 is depth of the potential well, σ_{ij} is the distance between the two atoms at which the inter-particle potential becomes zero and r_{ij} is the distance between two atoms. The combination rules used for different atom types are $\sigma_{ij} = (\sigma_{ii}\sigma_{jj})^{\frac{1}{2}}$ and $\epsilon_{ij} = (\epsilon_{ii}\epsilon_{jj})^{\frac{1}{2}}$. In eq 6 (q_i, q_j) are partial charges on ith and jth atom respectively, ϵ_0 is dielectric constant of the medium between charges and r_{ij} is the distance between the atoms.

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