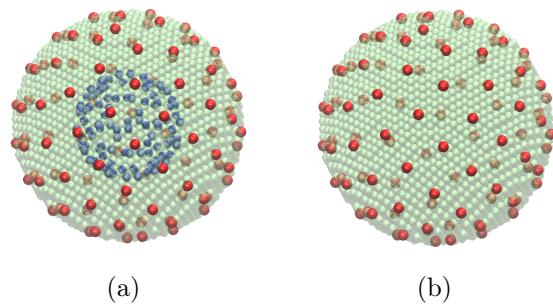


# Dipolar Nanoparticle Interacting with a Lipid Membrane

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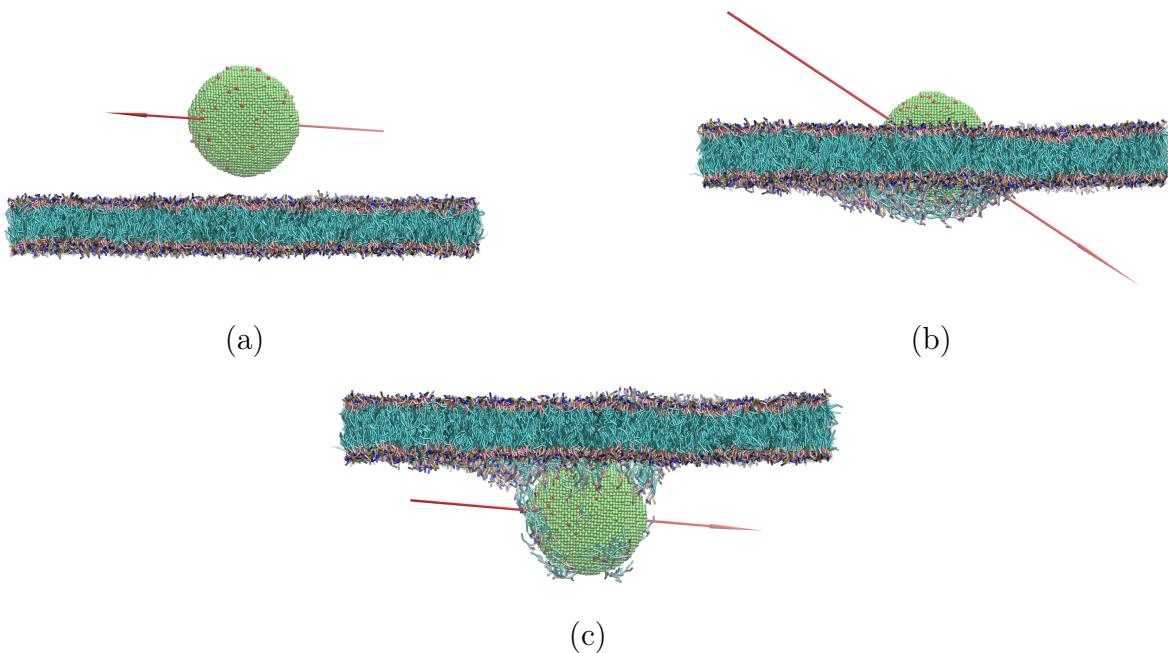
E-mail: rabdolvahab@iust.ac.ir



(a)

(b)

Figure S1: Nanoparticles (a) with and (b) without electric dipole. Red beads represent electrons, while blue beads inside nanoparticle denote positively charged atoms.



(a)

(b)

(c)

Figure S2: Nanoparticle with electric dipole (red arrow) at different stages, (a) when nanoparticle reaches membrane surface, (b) when nanoparticle is in center of membrane, and (c) when the nanoparticle moves out from center of membrane.

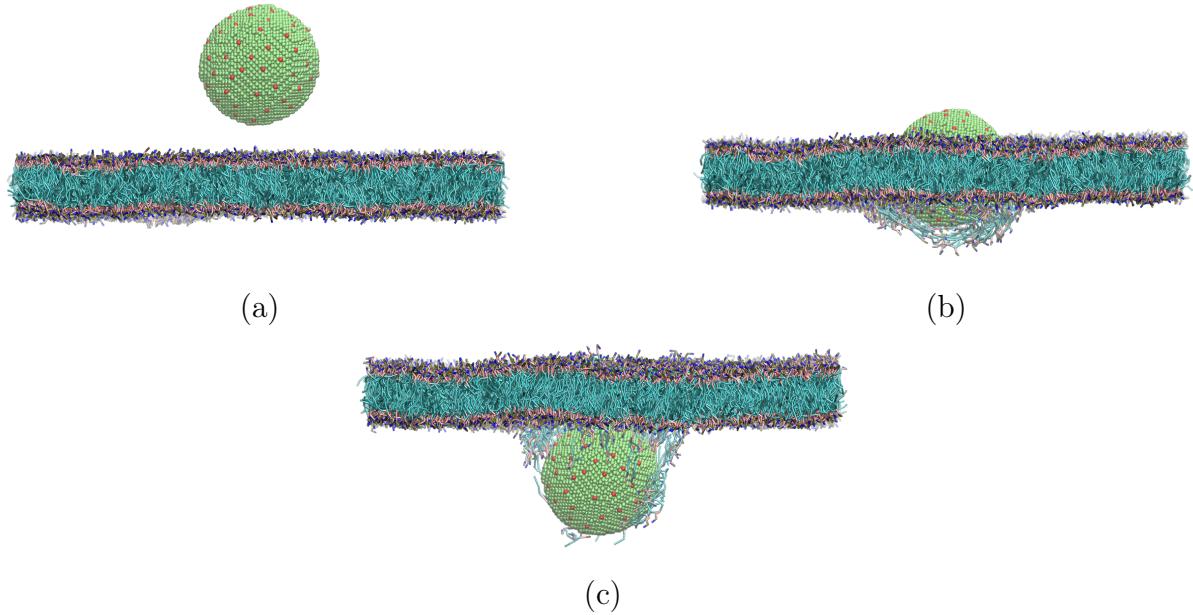


Figure S3: Nanoparticle without electric dipole at different stages, (a) when nanoparticle reaches membrane surface, (b) when nanoparticle is in center of membrane, and (c) when the nanoparticle moves out of membrane from center of membrane.

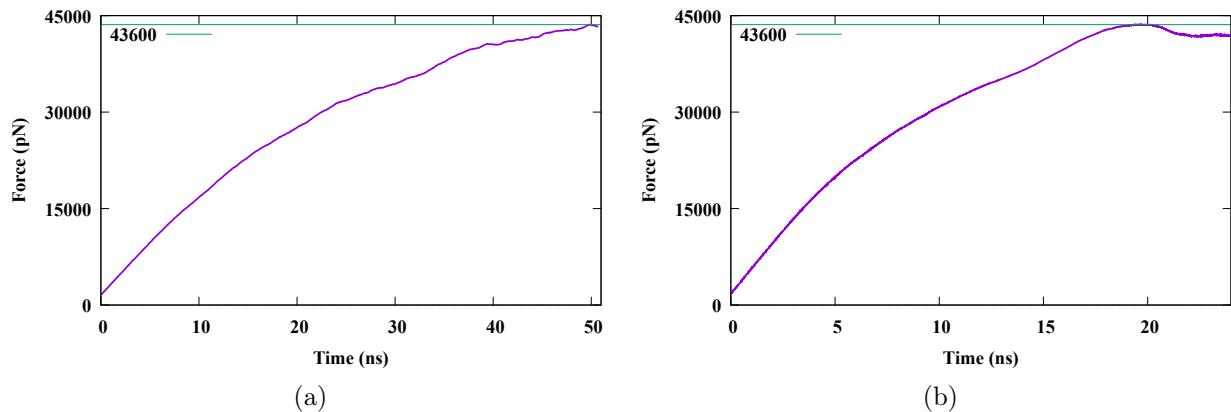


Figure S4: SMD force profile comparision of (a) system with dimensions of  $50 \times 50 \times 34 \text{ nm}^3$  and pull rate of  $625 \times 10^{-8}$  and (b) system with dimensions of  $40 \times 40 \times 34 \text{ nm}^3$  and pull rate of  $125 \times 10^{-7}$ .

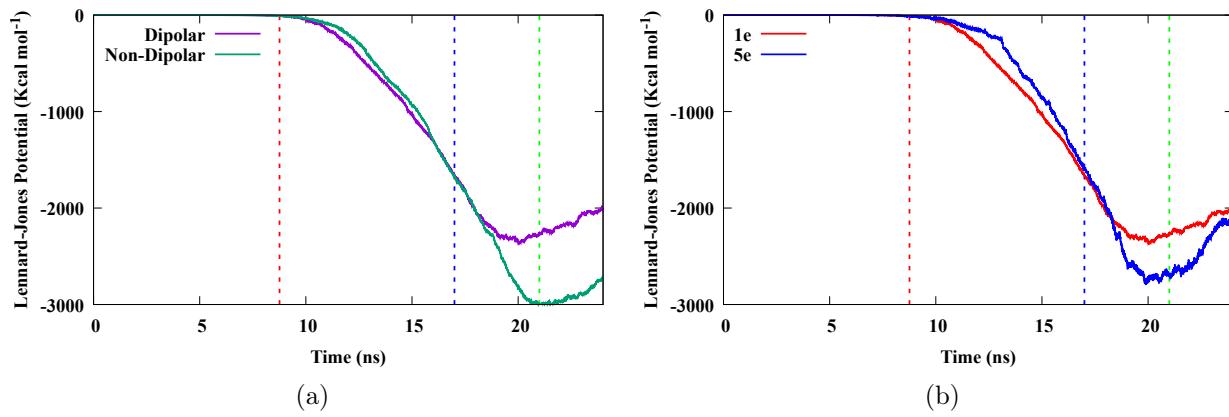
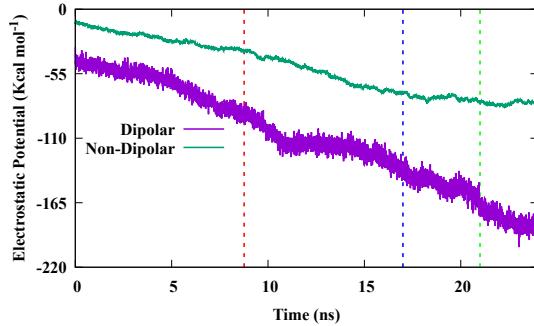
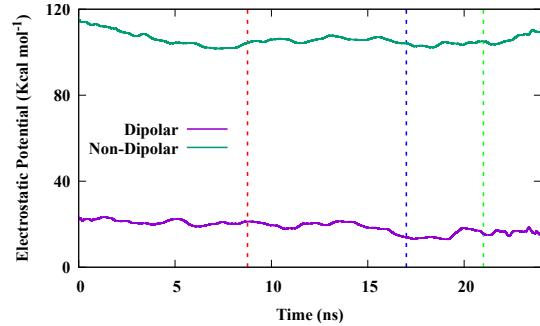


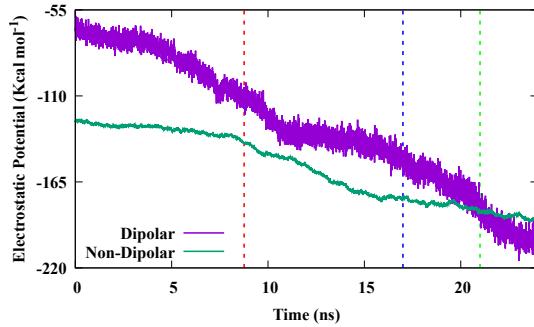
Figure S5: Lennard-Jones potential between nanoparticles and membrane comparision for (a) dipolar and non-dipolar nanoparticles and (b) two dipolar nanoparticles. Dashed vertical lines are the same as Figure 1.



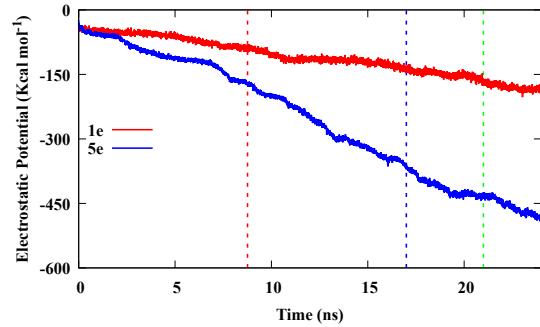
(a)



(b)

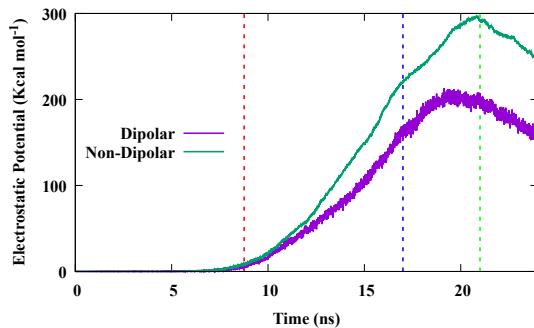


(c)

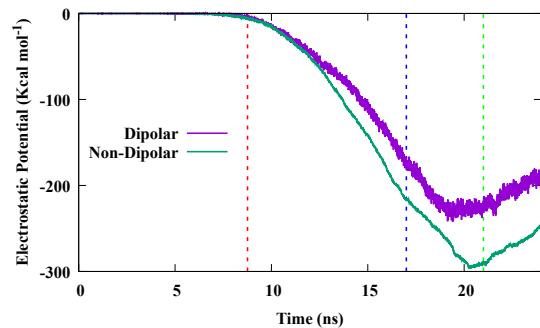


(d)

Figure S6: Electrostatic potential between nanoparticles and (a) negative and positive, (b) negative, (c) positive ions for nanoparticle with and without electric dipole, and (d) dipolar nanoparticles with two different dipole strengths with negative and positive. Dashed vertical lines are the same as Figure 1.



(a)



(b)

Figure S7: Electrostatic potential between nanoparticles, (a) negative, (b) positive head-groups of membrane. Dashed vertical lines are the same as Figure 1.