Weekly Report: July 8 - July 12

-Vatsa Shah

Performed simulation on 4 systems ->

1) chain A of tmafp protein on ice.
2) chain B of tmafp protein on ice.
3) chain A of lpibp protein on ice.
4) chain B of lpibp protein on ice.

Dimension of water system containing tmafp protein = 7.3 x 7.3 x 7.3 (nm)^3
Dimension of hexagonal ice used below the tmafp protein in water system = 7 x 7x 3 (nm)^3
Dimension of water system containing lpibp protein = 9.3 x 9.3 x 9.3 (nm)^3
Dimension of hexagonal ice used below the lpibp protein in water system = 9.3 x 9.4 x 3 (nm)^3

Changed the topol.top file by adding the SOL molecules of additional ice layer added at bottom.

1) Performing Energy minimization->

gmx grompp -f em.mdp -c protein_on_ice.gro -p topol.top -o em.tpr
gmx mdrun -s em.tpr -v -deffnm em -ntmpi 4

2) Performing NVT Equlillibrium step->

gmx grompp -f nvteq-t270.mdp -c em.gro -p topol.top -o eq_270_protein_on_ice.tpr
gmx mdrun -s eq_270_protein_on_ice.tpr -v -deffnm eq_270_protein_on_ice -ntmpi 4

3) Performing NVT Production run step->

gmx grompp -f nvtprod-t270.mdp -c eq_270_protein_on_ice.gro -p topol.top -o prod_270_protein_on_ice.tpr
gmx mdrun -s prod_270_protein_on_ice.tpr -v -deffnm prod_270_protein_on_ice -ntmpi 4

Result of above system can be found **/zfs/molecule/vatsashah** here.

In the output file, the ice dissociated to become water at 270K.

Hence, Ran another simulation in which both sides of hexagonal ice slabs were in contact with water box having protein in it.

1) Arrange the pbc box dimension such that two water-protein system and one ice slab can fit in it with some additional vaccum gap on top most and bottom most surface.

2) Change the topology file by adding additional molecules added to the system in same order as they stack up on one another.

3) Run the simulation commands same as in above points.

(I was not able to check result of above system due to shortage of time)