Weekly Report: June 10 -June 14

-Vatsa Shah

Calculated Rate at which Radius of Ice-seed grows in water and rate of change of radius wrt time for all the systems of ice and water made in previous week ->

1) Used Fortran language to solve the problem. Made a code to take input from q6nave.xvg (nos. of molecules And Time) and stored it in inp.dat.
2) Using relation between radius and number of molecules, Calulated the radius at each time,

radius = (3.0 X (nos. Of molecules) / (4.0 X pi X rho)) ^ (1.0 / 3.0)

where rho = 30.38 molecules per (nm)^3 for Hexagonal Tip4p structure of ice and
rho = 31.05 molecules per (nm)^3 for Cubic Tip4p structure of ice.

3) By subtracting the consecutive radius's, we get the change of radius for each interval of time.
4) Stored the output of this code in radius.xvg and radiusgrad.xvg.

Read Following Research Papers->

1) Antifreeze Protein from Freeze-Tolerant Grass Has a Beta-Roll Fold with an Irregularly Structured Ice-Binding Site by Adam J.Middleton Christopher B.Marshall FrédérickFaucher MayaBar-Dolev IdoBraslavsky Robert L.Campbell Virginia K.Walker Peter L.Davies. (For 3ULT protein)

2) Mimicry of ice structure by surface hydroxyls and water of a b-helix antifreeze protein by Yih-Cherng Liou, Ante Tocilj, Peter L. Davies & Zongchao Jia. (For 1EZG protein)

Performed simulation to get stable Double Stranded TmAFP (Pdb Id code - 1EZG) Protein by energy minimization->

1) *gmx pdb2gmx -f 1ezg.pdb -o 1ezg_processed.gro*
2) *gmx editconf -f 1ezg_processed.gro -o 1ezg_14.8x14.8x14.8.gro -c -d 5 -bt cubic*
3) *gmx solvate -cp 1ezg_14.8x14.8x14.8.gro -cs tip4p.gro -o 1ezg_solv.gro -p topol.top*
4) *gmx grompp -f ions.mdp -c 1ezg_solv.gro -p topol.top -o ions.tpr*
5) *gmx genion -s ions.tpr -o 1ezg_solv_ions.gro -p topol.top -pname NA -nname CL -np 4*
6) *gmx grompp -f em.mdp -c 1ezg_solv_ions.gro -p topol.top -o em.tpr*
7) *gmx mdrun -v -deffnm em -ntmpi 4*
8) *Visualized the em.gro file in vmd.*

Performed simulation to get stable Double Stranded LpIBP (Pdb Id code - 3ULT) Protein by energy minimization ->

1) *removed residue EOH and EDO from the 3ult.pdb file.*
2) *gmx pdb2gmx -f 3ult.pdb -o 3ult_processed.gro -ignh*
3) *gmx editconf -f 3ult_processed.gro -o 3ult_15.6x15.6x15.6 .gro -c -d 5 -bt cubic*
4) *gmx solvate -cp 3ult_15.6x15.6x15.6.gro -cs tip4p.gro -o 3ult_solv.gro -p topol.top*
5) *gmx grompp -f ions.mdp -c 3ult_solv.gro -p topol.top -o ions.tpr -maxwarn 1*
6) *gmx genion -s ions.tpr -o 3ult_solv_ions.gro -p topol.top -pname NA -nname CL -np 6*

7) *gmx grompp -f em.mdp -c 3ult_solv_ions.gro -p topol.top -o em.tpr*
8) *gmx mdrun -v -deffnm em -ntmpi 4*
9) *Visualized the em.gro file in vmd.*