

Weekly Report: May 20 -May 24

-Vatsa Shah

Read following research paper's to get acquainted with project.

- 1) Davies_2016_IcebindingProteinAndFunctions_AnnualRevBiochem
- 2) Sanz_2016_SeedingPaper_MD
- 3) Supporting information for: Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates -Nils E. R. Zimmermann, Bart Vorselaars, David Quigley, and Baron Peters.

Created box of water (tip4p) of known dimension (eg. $4 \times 4 \times 4 \text{ nm}^3$, $6 \times 6 \times 6 \text{ nm}^3$, $8 \times 8 \times 8 \text{ nm}^3$, $10 \times 10 \times 10 \text{ nm}^3$) through simulations and performed energy minimization. Further did simulations to bring this box of water to fix temperature of 300K ,to fixed volume and fixed number of molecules.

To create box of water ->

```
gmx solvate -box 4 4 4 -cs tip4p -o box.gro -p tip4p-ice.top
```

Energy Minimization ->

```
gmx grompp -c box.gro -f em.mdp -o em.tpr -p tip4p-ice.top
gmx mdrun -s em.tpr -v -deffnm em
```

Bringing system to fixed factors like Temperature, volume and number of molecules ->

```
gmx grompp -f nvteq-t300.mdp -c em.gro -p tip4p-ice.top -o nvt_300k_4x4x4_eq.tpr
gmx mdrun -s nvt_300k_4x4x4_eq.tpr -v -deffnm nvt_300k_4x4x4_eq
```

Visualized the .gro file in vmd ->

```
vmd em.gro em.xtc
vmd nvt_300k_4x4x4_eq.gro nvt_300k_4x4x4_eq.xtc
```

Added ice seed in the equilibrium box of water using Python files ->

```
cut_cap_slab.py      -to cut a sphere out of a box
combine_grofile.py   -combining two gro files
```

- 1) carved out sphere of different radius (1.7 nm, 2.5 nm, 3.1 nm, 4.2 nm) from *Ih_15x15x15.gro* file and *Ic_15x15x15.gro* file.
- 2) carved out sphere from *nvt_300k_4x4x4_eq.gro* file.
- 3) combined the shere of ice from 1st step and box with hole from 2nd step.

Performed above steps with different Dimensions of boxes of water and visualized the ice-water.gro file in each case.