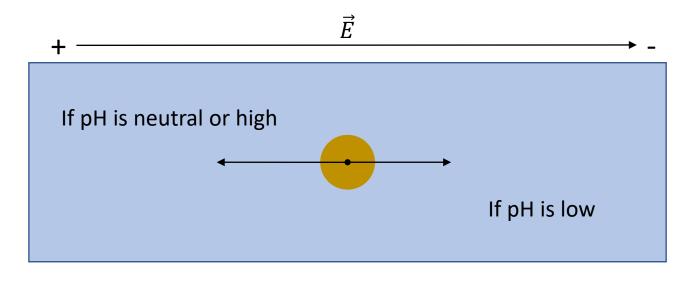
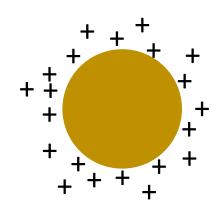
Movement of uncharged particles in the electrostatic field

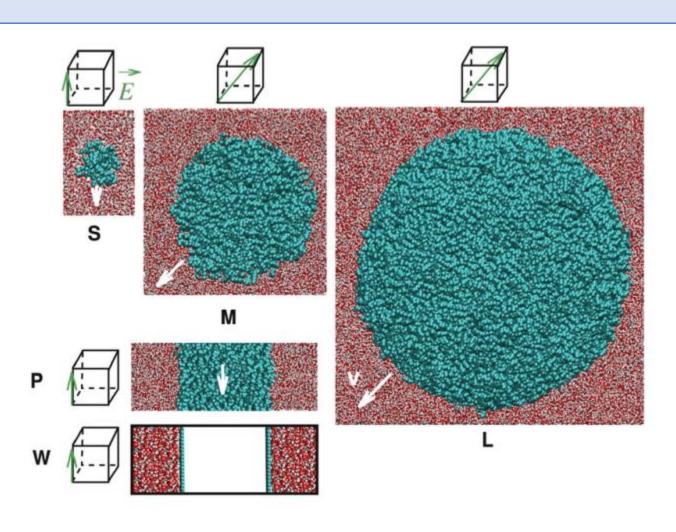
- Oil droplets in pure water show different mobilities depending on the pH
- Point of zero charge is at pH=6, but at that point there is negative mobility



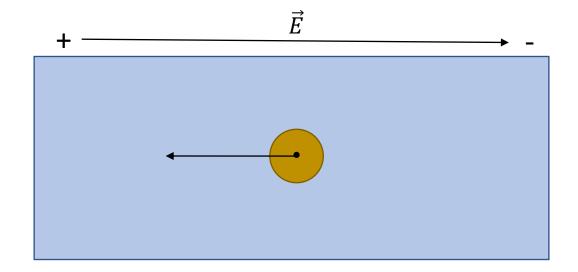


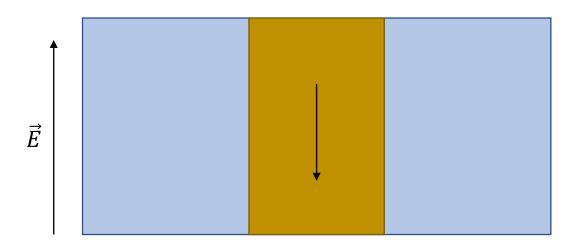
- Heptane droplet/slab in water
- Hydropobic wall in water

- Complete absence of ions
- Electric field

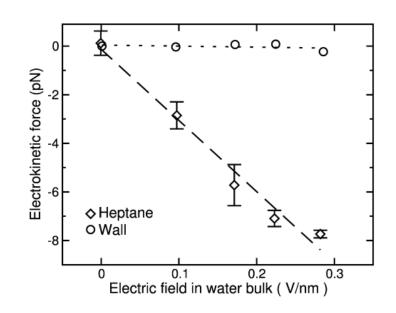


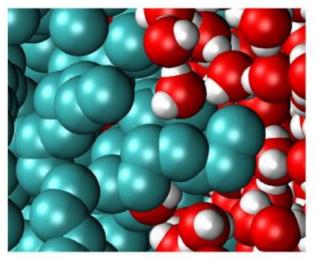
- Oil droplets migrate in the negative field direction
- Slab moves tangential to the interface
- Electrostatic potential of oil phase? positive

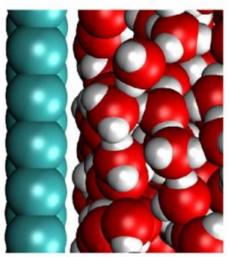




- Mobility contributions:
 electrophoretical force + frictional force
- Interface roughness is required for electrophoretic force







Electrophoretic mobility of oil - Conclusions

 Mobility in the absence of ions should be zero, but simulations show negative mobility

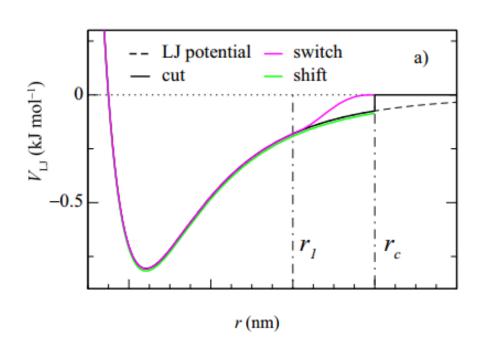
 Electrophoresis does not only reflect charge or electrophoretic potential of the droplet

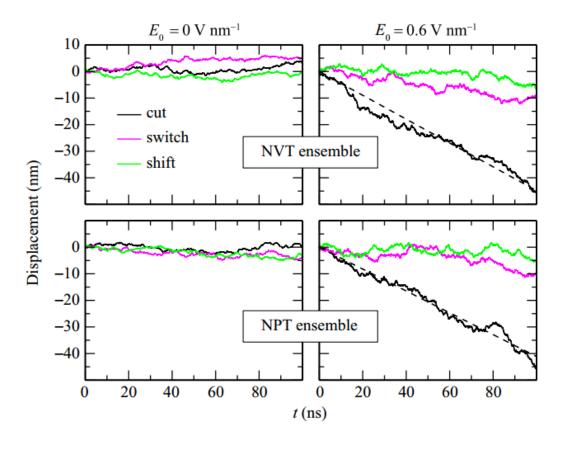
Mobility is attributed to partial charges of the atoms

• If true, electrophoretic experiments could me misleading

Electrophoretic mobility of oil - Explanation

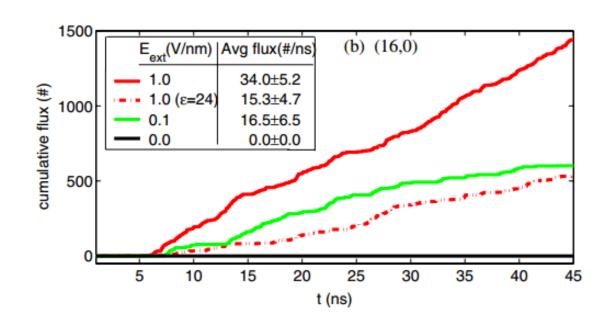
 Mobility only appears when using simple truncation method for LJ forces.

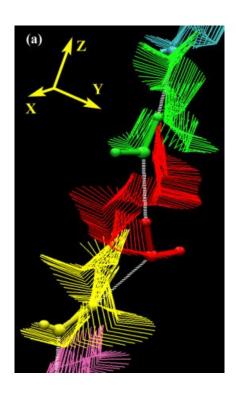




Water flow on carbon nanotubes

- Water oriented along one direction by aplying an external field
- Flux in the direction of the aligned water dipoles





Water flow on carbon nanotubes

 When using shift approach instead of truncated forces for LJ, mobilities dissapear.

• In LAMMPS, flux dissapears for smaller rc

