Investigating the Self-Assembly of Surfactant Molecules

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Abstract

Computational Chemistry provides a powerful means to study the dynamics of surfactant self assembly in various solvent conditions. This study aims to provide an understanding of the role of water models and salts on surfactant behavior. Towards this, we performed molecular dynamics (MD) simulations of the well-characterized dodecylphosphocholine (DPC) surfactant molecule using the SPC/E, TIP3P, TIP4P-Ew and TIP5P water models. In order to understand the influence of charges on surfactant conformational sampling and self-assembly, we performed additional simulations that included explicit Na^+Cl^- and K^+Cl^- ions. Our simulations identify the influence of water models and solvent conditions on conformational sampling in surfactants and help expand our understanding of the determinants of self-assembly processes

Dodecylphosphocholine

- DPC is a lipid-like polar surfactant
- It forms stable micelles in solutions and is good for simulating the eukaryotic environment of membranes
- Available thermodynamic and kinetic data from experiments will allow us to validate the results from our calculations

Hypothesis

- Changes in the conformational sampling of individual DPC molecules introduced by the choice of water models or the inclusion heavy metal ions influence the self-assembly process

Methods

- Amber molecular dynamics software – ff99sbildn and GAFF force fields.
- Each model was solvated in a truncated octahedral box of water molecules.
- Use of explicit Na^+, K^+ and Cl^+ ions – 12-6 potential
- Ambertools14 and VMD software suites were used to analyze data
- Energy minimization and equilbration performed prior to production MD at 300 K and 1 atm. pressure (NPT)
- Simulations were performed on LONI and LSU-HPC supercomputing resources

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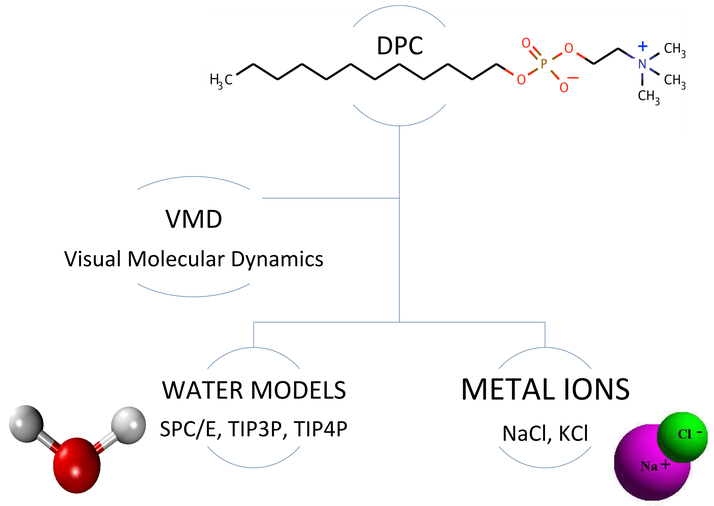
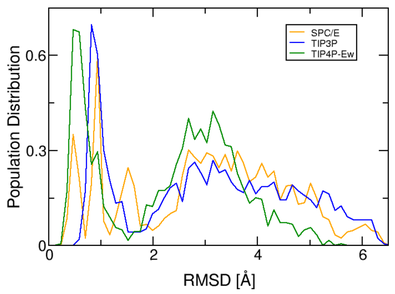


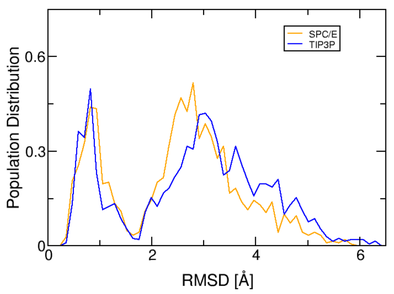
Results

0.4 M KCl Solution

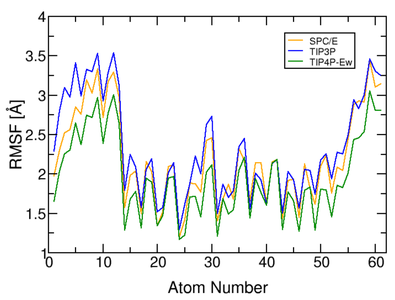
0.4 M NaCl Solution

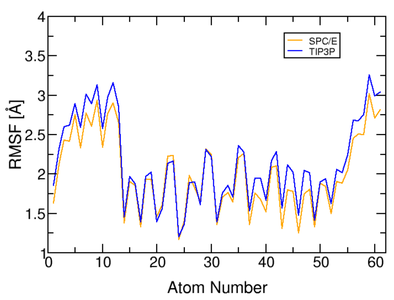
▪Structural changes



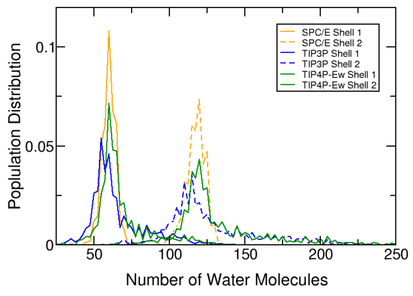


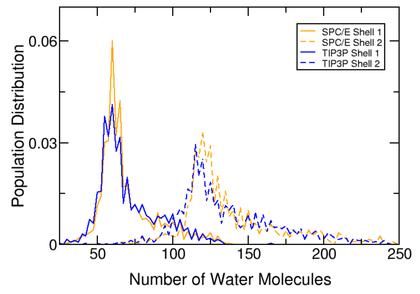
▪Fluctuations in atomic positions



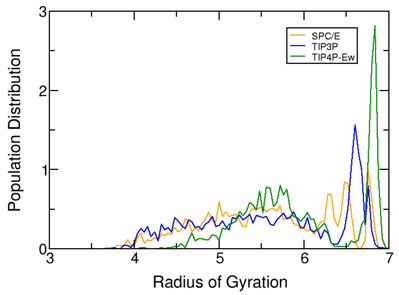


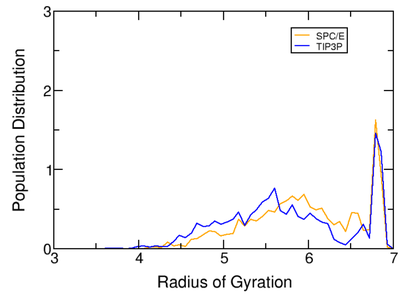
▪Solvent environment around surfactant





▪Changes in size





Conclusions and Future Directions

- Small changes in atomic motions were observed as a results of changing water models and introducing metal ions.
- *To investigate the influence of TIP5P water model and divalent ions on conformational dynamics of DPC.*
- *To simulate the self-assembly of DPC to form micelles*

Some References

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