Molecular Simulation Study on the Antifouling Properties of Zwitterionic Materials

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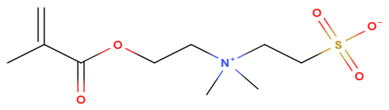
Introduction

Zwitterionic materials: A family of materials that possess both cationic and anionic groups.

- Biocompatible
- Resist nonspecific protein adsorption
- Many possible choices of cationic and anionic groups.



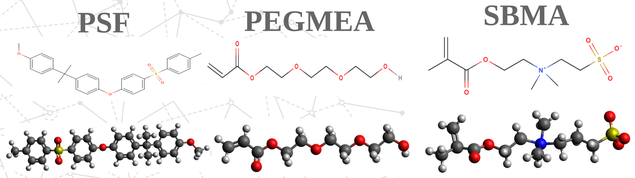
SBMA

Objectives

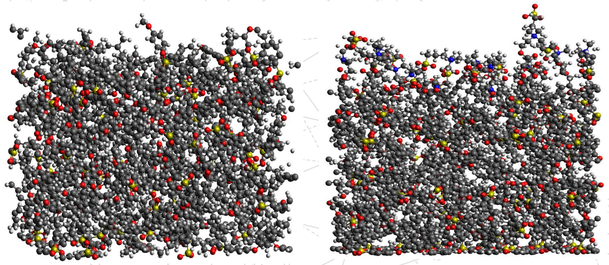
- Use molecular simulations to study the wetting behavior of water on SBMA functionalized polysulfone (PSF) membrane.
- Analyze dynamics of water near the membrane.
- Analyze the hydrogen bonds formed in the system.
- Provide an understanding on the antifouling properties of zwitterionic materials at molecular level.

Simulation Model

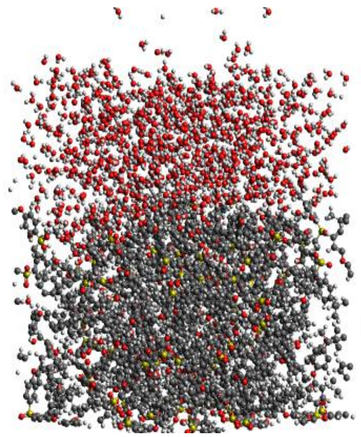
PSF PEGMEA SBMA



PSF Membrane SBMA-PSF Membrane



Simulation Snapshot

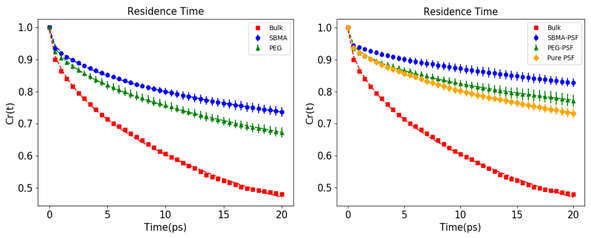


Water film

PSF membrane

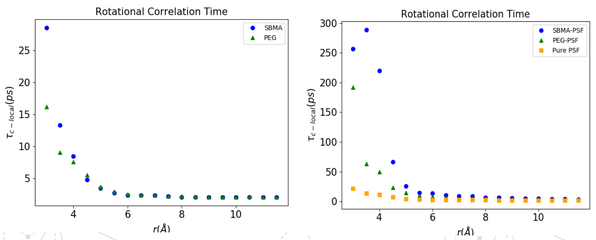
Water Dynamics Analysis

Residence Time



Water near SBMA has the longest residence time.

Rotational Dynamics



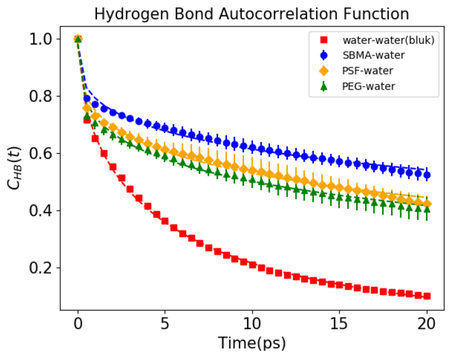
Water near SBMA has the slowest rotational motion.

Hydrogen Bond Analysis

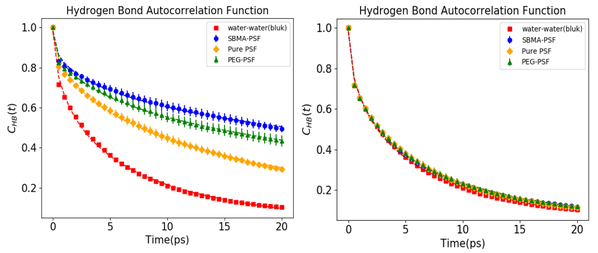
Geometry Criteria for Hydrogen Bonds:

- O-O distance less than 4.0 Å
- O-H-O angle larger than 120°

Hydrogen Bonds between Water and Polymer



Hydrogen Bonds between Water Molecules



water within 5.0Å from surface

water away from surface

Deeper Analysis on Hydrogen Bonds

Membrane Type	Number of Hbonds per Oxygen	Diffusion Coefficient for Bonded Water ($10^{-4}\ cm^2/s$)
Pure PSF	0.71610 ± 0.01261	0.10759 ± 0.00246
PEG-PSF	0.94270 ± 0.00924	0.097985 ± 0.00511
SBMA-PSF	1.6522 ± 0.01491	0.085663 ± 0.00194

Conclusion

- Both the transitional and rotational motions of water are retarded significantly by the polymer membranes.
- SBMA has the largest restriction effect on water dynamics and mobility.
- SBMA can form the most and strongest hydrogen bonds with water and it enhances the stability of the nearby water-water hydrogen bonds.
- Water molecules bonded to SBMA have the smallest average diffusion coefficient.
- The main reason for the antifouling properties of SBMA is its ability to contain a large amount of water by forming stable hydrogen bonds.

Future Research Plan

- Perform the analysis in an elementwise fashion to investigate which atom group contributes the most to antifouling.
- Study the influence of grafting density on the antifouling properties.
- Extend the analysis to other materials in the zwitterionic family.

References

1. Sau Lawrence Lee, Pablo G. Debenedetti, and Jeffrey R. Errington. (2014). A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. *The Journal of Chemical Physics 122, 204511 (2005); doi: 10.1063/1.1917745*.
2. Yi He, Jason Hower, Shengfu Chen, Matthew T. Bernards, Yung Chang, and Shaoyi Jiang. Molecular Simulation Studies of Protein Interactions with Zwitterionic Phosphorylcholine Self-Assembled Monolayers in the Presence of Water. *Langmuir 2008, 24, 10358-10364*