**Molecular Simulation Study of Nanoscale Friction between Phosphocholine Self-Assembled Monolayer Surfaces Immersed in Aqueous Solution**

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**Statement of Purpose:** Tribology in biosystems is currently a rapidly growing area. While significant advances in the study of bio-lubrication systems have been made over the last few decades, the lubrication mechanism for the 'water-based' system is still poorly understood. It is crucial to have a fundamental understanding[3] of friction and adhesion for many biological applications such as joint replacement and contact lenses. Molecular simulation provides a unique tool to separate the intermingling interactions, look directly at the interaction surfaces, analyze friction properties, and obtain the molecular level understanding of the bio-lubrication mechanism. One of the most important properties of biological lubrication system is that the lubricant is often chemical attached to the surface, as occurs at the cartilage surface of joints. To mimic this, a phosphocholine self-assembly monolayer (PC-SAM) was studied as model system in this research. The purpose of this work is to study the bio-lubrication mechanism using molecular dynamics simulation in the hope of reaching a sufficient understanding for the intelligent design of bio-interfaces.

**Methods:** The simulation box used in this work was shown in Figure 1.The origin was located at the center of the box. This simulation box was constructed by placing a bulk solvent on each side along the y direction. Solvent molecules were confined between the two PC-SAM surfaces. Top and bottom surfaces had opposite sliding directions and the sliding directions were along the x direction. The Surfaces were infinite in the x direction, but finite in the y direction. Two dimensional periodic boundary conditions were applied to the entire simulation cell. The confined solvent was in contact with its bulk on both sides. Sodium Chloride was added to system at different ion concentrations.

For equilibrium Molecular Dynamics (MD), the starting configuration of PC-SAM, water, and counterions was taken from the final frame of the heating MD simulation. The velocity Verlet method was used for the integration of the Newton's equation in the NVT ensemble with a time step of 1.0 fs. The Berendsen method was used to maintain a constant temperature of 300K with a coupling constant of 0.1 ps. Initial velocities were assigned with a Maxwell-Bolzmann distribution at 300K. Each simulation system was placed in a rectangular box. The periodic boundary condition and minimum image convention were applied to the x and y directions only. There is a hard wall on both top and bottom of the simulation box and a reflective boundary condition is applied. All sulfur atoms of SAMs were fixed and all covalent bonds involving hydrogen atoms were constrained using the RATTLE algorithm. All simulations were performed on a 16-node Linux cluster using our BIOSURF program. We developed and extended this generalized molecular simulation program for the study of nanoscale friction between biological interfaces. All initial structures were built using the CHARMM package.

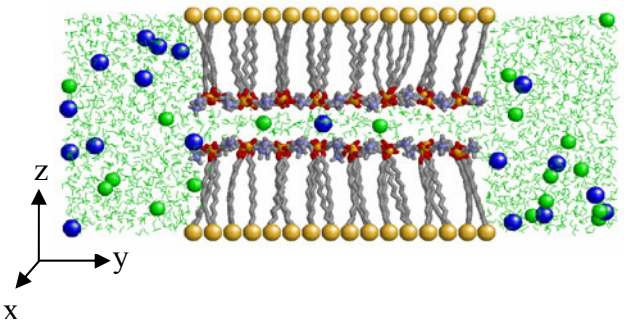


Figure 1 A schematic representation of the simulation box

**Results / Discussion:** The total length of each individual MD simulation run was about 1.5 ns. Configurations were saved every 1.0 ps after 1 ns for analysis. The short-range vdW interactions were calculated by the switch function at a twin range cutoff between 8 Å and 10 Å. The long-range electrostatic interactions were calculated by the force-shifting function at a cutoff distance of 12 Å. Early studies[1] showed that the atom-based force-shifting function can conserve energy, correctly predict the experimental data, and generate stable trajectories.

The effect of the concentration of sodium chloride on both friction coefficient and fluidity of PC-SAM was studied. Shearing velocity and pore size was also investigated to find their relations to friction properties. High concentration of sodium chloride had strong effect on the electrostatic interaction. The interaction between ion and PC-SAM surfaces was also investigated. Simulation results showed that friction between PC-SAM surfaces was lower than that between polyethylene (PE) surfaces, which indicated that PC-based materials may be an excellent candidate to reduce friction between PE surfaces in artificial joints. This conclusion was also supported by other experimental finding[2].

**Conclusions:** In this study, two PC-SAM surfaces were immersed in water and shearing against each other. Two water bulks were placed on both sides of surfaces. The high concentration of sodium chloride had strong effect on the electrostatic interaction, which will affect the fluidity of surfaces. It showed that the friction coefficient between PC-SAM is lower than that between PE surfaces. Thus, with its good biocompatibility, phosphoscholine has great potential applications in biomaterials.

**References:** 1. Zheng J, Li L, Tsao H, Chen S, Jiang S. *Biophysical Journal*, **2005**. 89 (1): 158-166.
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3. Urbakh M, Klafter J, Gourdon D, et al. *Nature*, **2004** 430 (6999): 525-528.