

Abstract

Understanding the origin of life is one of the fundamental knowledge required to find life on extraterrestrial celestial. Among numerous phenomena that are driven by bio-molecules, self-assembly of the cellular membrane is considered as the most basic process in the origin of life. In water dominant environment of standard pressure and temperature, molecular interaction (Van der Waals force) among water molecules and phospholipids forces phospholipids to form lipid bilayer structure which is the proto structure of the cellular membrane. However, self-assembly of phospholipids in extremely pressurized wet environments has never been explored. Since liquid water in the solar system has been reported to reside inside the deep icy shell that is estimated to pressurize water up to 2GPa (Europa, Kah et al 2014) or deep ground (Mars, Orosei et al 2018), verifying the feasibility of self-assembly of phospholipids in a corresponding simulated environment must be explored. Here, we present the molecular dynamics simulation of phospholipid (DPPC) in 1 and 1,000 with GROMACS molecular dynamics simulation. We have verified the self-assembly of phospholipids in both conditions.

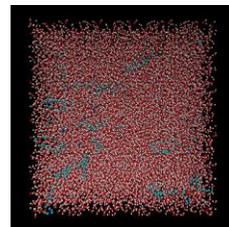
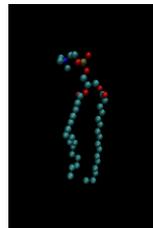
Thesis Statement: The self-assembly of phospholipids which is the fundamental process in the origin of life is not hindered by extreme pressure suggesting possible life existence on Europa and Mars

Introduction

The Hubble space telescope observation reported the existence of liquid water in the interior of Europa (Roth et al. 2014). Also, recent radar observation revealed possible liquid water in the underground of Mars (Orosei et al. 2018). This suggests a possible life existence in other worlds. However, in order to life to form, borderline which separates life from their surrounding environment, cellular membrane, must be present. Since liquid water in extraterrestrial celestial is inside the thick solid surfaces, they are considered to possess high pressure (Sheng et al 2011). In this study, we are to explore the possibility of self-assembly of cellular membrane analog structure in the extraterrestrial celestial environment.

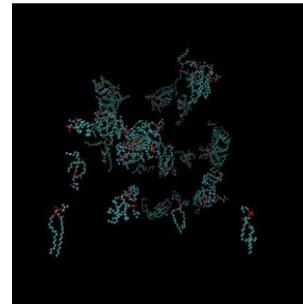
Simulation Conditions

GROMACS, which produces accurate calculation in molecular dynamics, is selected as the main software in this study (Spoel et al. 2015). The target molecule is selected as DPPC because of its common existence in cellular membranes among terrestrial life.

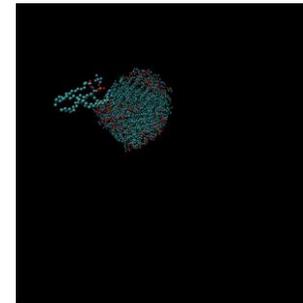


Simulation box : 10nm cubic
Simulated molecule : DPPC
Simulated Pressure : 1bar, 1,000 bar
Simulated temperature : 300K

Simulation Result (1bar)

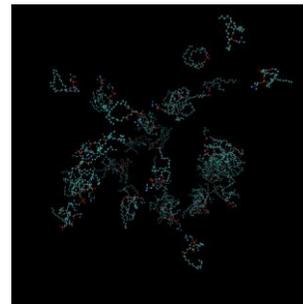


1ns

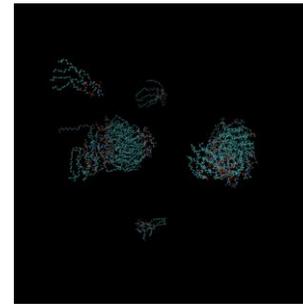


30ns

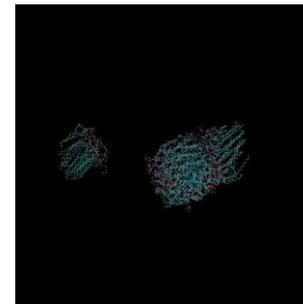
Simulation Result (1,000bar)



1ns



30ns



60ns

Conclusion

Self-assembly that is driven by the intramolecular interaction of DPPC is presented in both simulation conditions. This is well expected since the driving force corresponding interaction is well established (Marsh 2012). However, completion of self-assembly time is largely different between 1bar and 1,000bar indicating that in the higher pressurized water environment, self-assembly of phospholipid is delayed. Since the pressure of liquid water inside the Europa is expected to be higher than 10,000bar (Sheng et al. 2011), further simulations on higher pressure must be explored to determine whether the Europa could give birth to life. Furthermore, tested molecule (DPPC) is an evolved molecule that is produced by terrestrial life. Self-assembly of primitive molecules that were the main ingredients of primitive life should be tested in the presence of high pressure (Deamer 2017).

References

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