

Supplementary Information

Cholesterol suppresses membrane leakage by decreasing water penetrability

Bing Bu^{a,‡}, Michael Crowe^{b,‡}, Jiajie Diao^{b,*}, Baohua Ji^{a,c,*} and Dechang Li^{a,*}

a. Biomechanics and Biomaterials Laboratory, Department of Applied Mechanics, Beijing Institute of Technology, Beijing 100081, China.

b. Department of Cancer Biology, University of Cincinnati College of Medicine, Cincinnati, Ohio 45267, United States.

c. Institute of Applied Mechanics, Department of Engineering Mechanics, Zhejiang University, Hangzhou 310027, China.

* Corresponding authors: jiajie.diao@uc.edu; bhji@zju.edu.cn; dcli@bit.edu.cn.

‡ These authors contributed equally to this work.

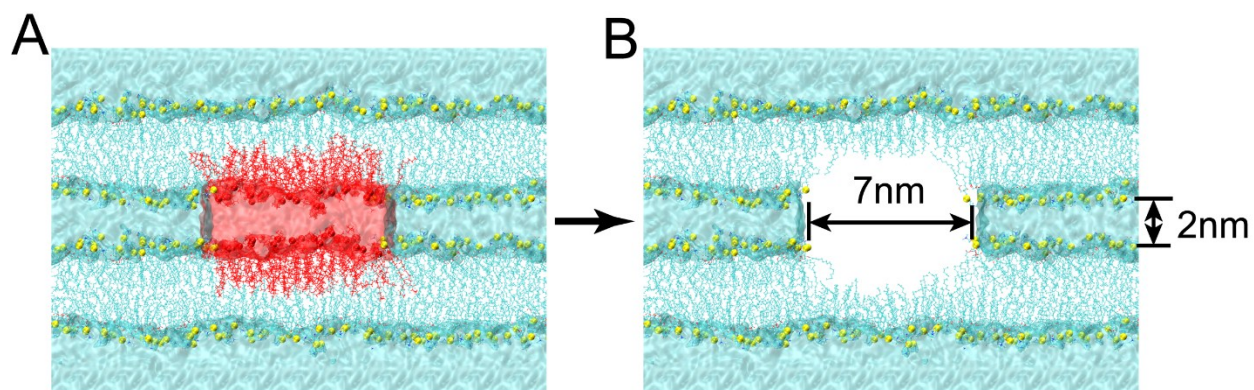


Figure S1. The initial setup of the membrane structure. (A) Two membrane was put close contact with a distance of $\sim 2\text{nm}$. The lipids and water molecules in red color in the contact region in (A) were removed to generate the HD structure. (B) The structure of two membranes after removing of partial lipids and water molecules of the two contacted leaflets.

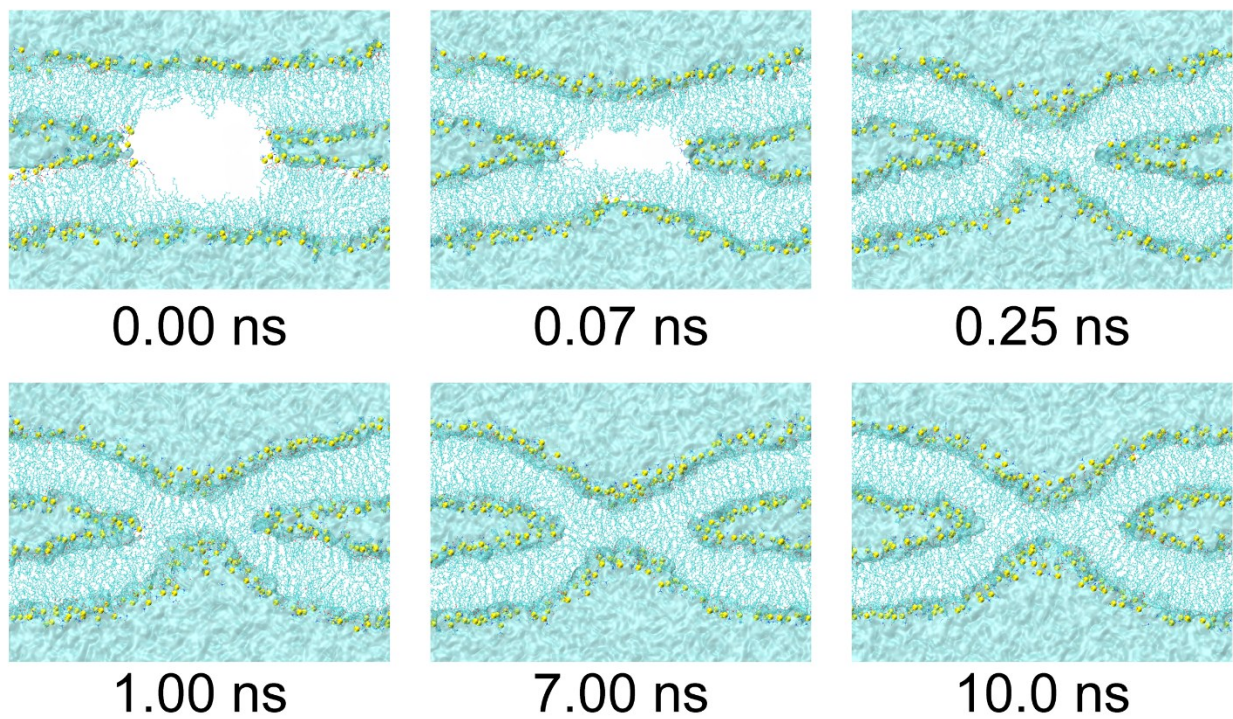


Figure S2. Structure evolution during equilibration simulation. A HD structure was formed after 10 ns equilibration simulation. The equilibrated structure at 10 ns was used for the product simulations.

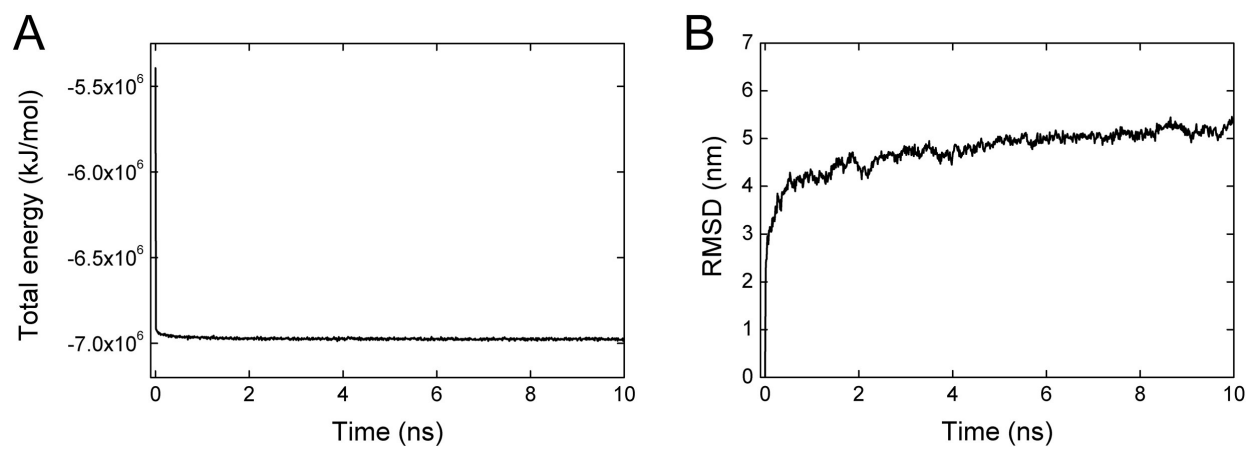


Figure S3. The total energy of the system and the RMSD of lipids during the equilibration simulation. It showed that the structure was well equilibrated after 10 ns simulation.