

## SUPPORTING INFORMATION

### Effect of oxidation on POPC lipid bilayers:

### Anionic carboxyl group plays a major role

Behnaz Bagheri,<sup>\*,†,‡</sup> Phansiri Boonnoy,<sup>¶,§</sup> Jirasak Wong-ekkabut,<sup>¶,§</sup> and Mikko  
Karttunen<sup>||,⊥</sup>

<sup>†</sup>*Department of Applied Physics and Science Education, Technical University of Eindhoven,  
PO Box 513, 5600 MB, Eindhoven, The Netherlands*

<sup>‡</sup>*Institute for Complex Molecular Systems, PO Box 513, 5600 MB, Eindhoven, The  
Netherlands.*

<sup>¶</sup>*Department of Physics, Faculty of Science, Kasetsart University, 50 Ngamwongwan Rd,  
Chatuchak, Bangkok, Thailand 10900*

<sup>§</sup>*Computational Biomodelling Laboratory for Agricultural Science and Technology  
(CBLAST), Faculty of Science, Kasetsart University, 50 Ngamwongwan Rd, Chatuchak,  
Bangkok, Thailand, 10900*

<sup>||</sup>*Department of Physics and Astronomy, The University of Western Ontario, 1151  
Richmond Street, London, Ontario N6A 3K7, Canada*

<sup>⊥</sup>*Department of Chemistry, The University of Western Ontario, 1151 Richmond Street,  
London, Ontario N6A 5B7, Canada*

E-mail: b.bagheri@tue.nl,jirasak.w@ku.ac.th,mkarttu@uwo.ca

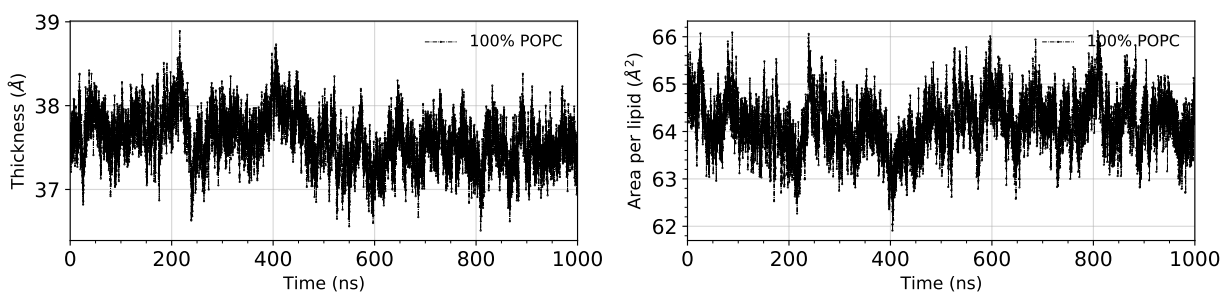


Figure S1: Bilayer thickness (left) and area per lipid (right) as a function of time for the pure POPC bilayer.

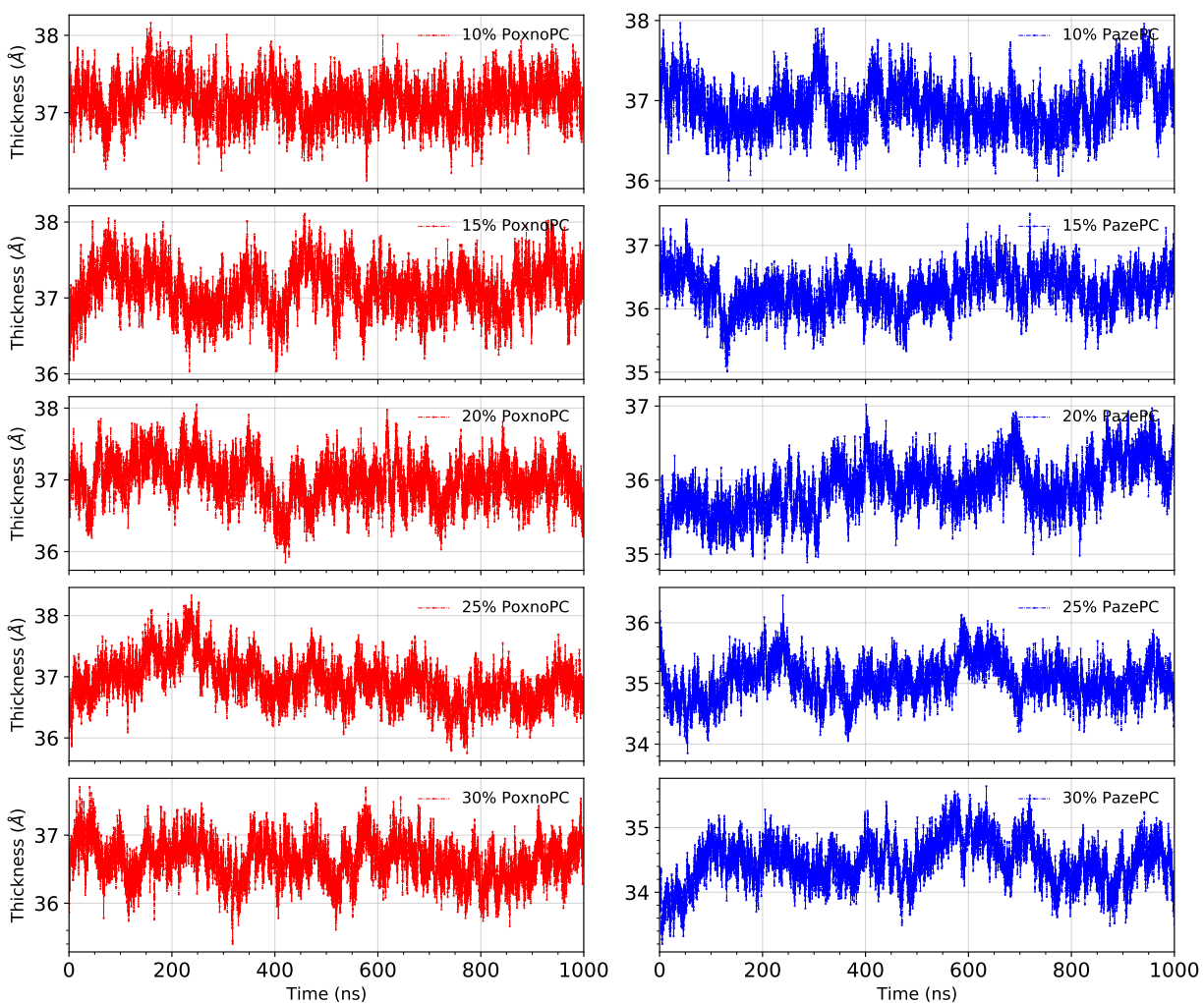


Figure S2: Bilayer thickness as a function of time for the POPC bilayers containing 10%, 15%, 20%, 25%, and 30% PoxnoPC (left) and PazePC (right).

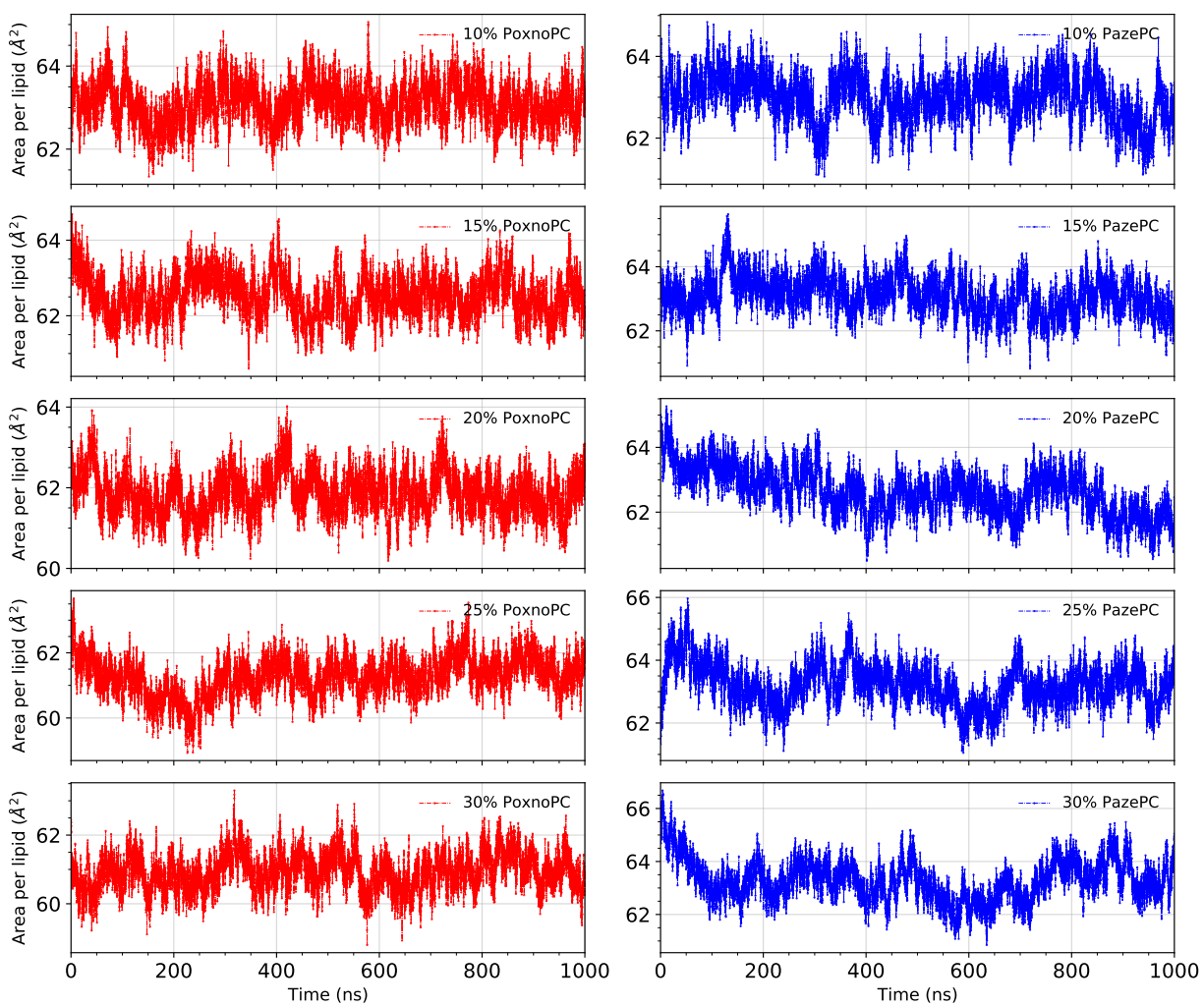


Figure S3: Area per lipid as a function of time for the POPC bilayers containing 10%, 15%, 20%, 25%, and 30% PoxnoPC (left) and PazePC (right).

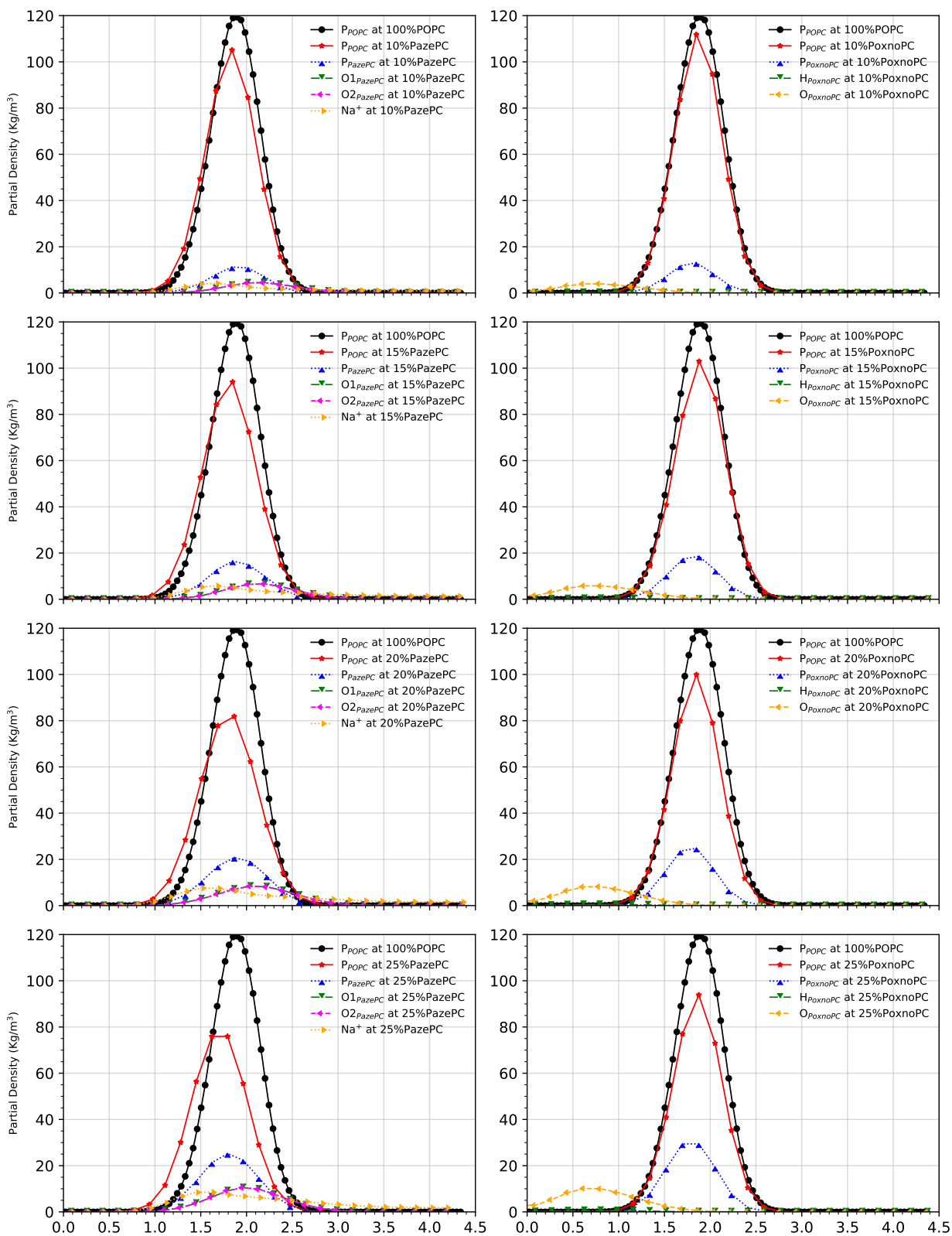


Figure S4: Density distributions of the lipid head groups and oxidized functional groups along the  $z$ -axis with respect to the distance from the bilayer center for the POPC bilayer containing 10%, 15%, 20%, and 25% PazePC (left) and PoxnoPC (right).