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It is important to explain the broad context of your work. Leaving the details and specificities for the manuscript itself. Prof. Gregory D. Scholes

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The Journal of Physical Chemistry Letters

enclosed the manuscript "All-Atom Molecular Dynamics of a Spontaneously sicle" by Santos and co-workers which we would like to have considered for purnal of Physical Chemistry Letters.

ne of the most potent stimulators of the host innate immune system whose recognition m is essential to clear infections of invading bacterial pathogens. However, the role of ric forms of Lipid-A in the blood during the immune activation process remains part because the aggregation state of this complex glycolipid is unknown. We have d coarse-grained models of chemical variants of Lipid A based on the hybrid particleamics approach (hPF-MD) and applied it to investigate the aggregation behavior of n this letter we examine the validity of the vesiculation process predicted by the hPF-rming atomistic simulations of the spontaneously formed Lipid-A vesicle. Given the nature of Lipid-A, we believe this is the first atomistic simulation of a glycolipid vesicle

and an important benchmark for the hybrid particle-field/molecular dynamics approach.

We hope the work will be of as much interest to the JPCL readership as our previous Perspective (*J. Phys. Chem. Lett.* 2017, 8, 15, 3586–3594) on the subject, and thank you for your time.

With best regards,

Thereza A. Soares