

Abstract Submitted
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**Computational Study of the Bulk Properties of a Novel Molecule:
alpha-Tocopherol-Ascorbic Acid Surfactant**¹ SHANNON STIRLING, HYE-
YOUNG KIM, Southeastern Louisiana University, Hammond, LA 70471 — Alpha-
tocopherol-ascorbic acid surfactant (EC) is a novel amphiphilic molecule of antioxi-
dant properties, which has a hydrophobic vitamin E and a hydrophilic vitamin C
chemically linked [1]. We have developed atomistic force fields (g54a7) for a proto-
nated (neutral) EC molecule. Our goal is to carry out molecular dynamics (MD)
simulations of protonated EC molecules using the newly developed force fields and
study the molecular properties. First we ran energy minimization (EM) with one
molecule in a vacuum to obtain the low energy molecular configuration with emtol
=10. We then used Packmol to insert 125 EC molecules in a 3nm cube. We then
performed MD simulations of the bulk system composed of 125 EC molecules, from
which we measured the bulk density and the evaporation energy of the molecular
system. Gromacs2016 is used for the EM and MD simulation studies. We will
present the results of the ongoing research. [1] C.E. Astete, D. Dolliver, M. Whaley,
L. Khachatryan, and C.M. Sabliov, ACS Nano 5(12), 9313-9325 (2011).

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