Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

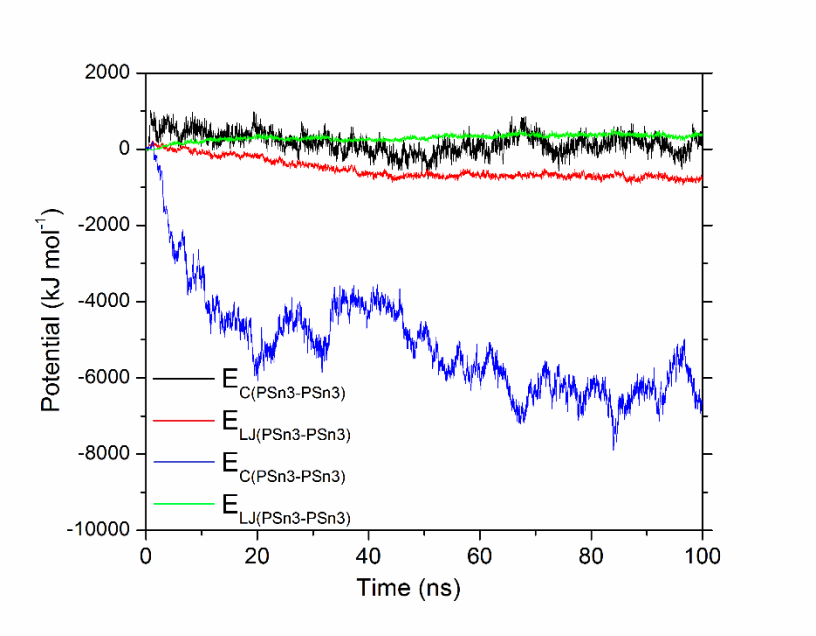
Supplementary Information

Molecular Dynamics Simulations Reveal the Assembly Mechanism of Polysaccharides in Marine Aerosols

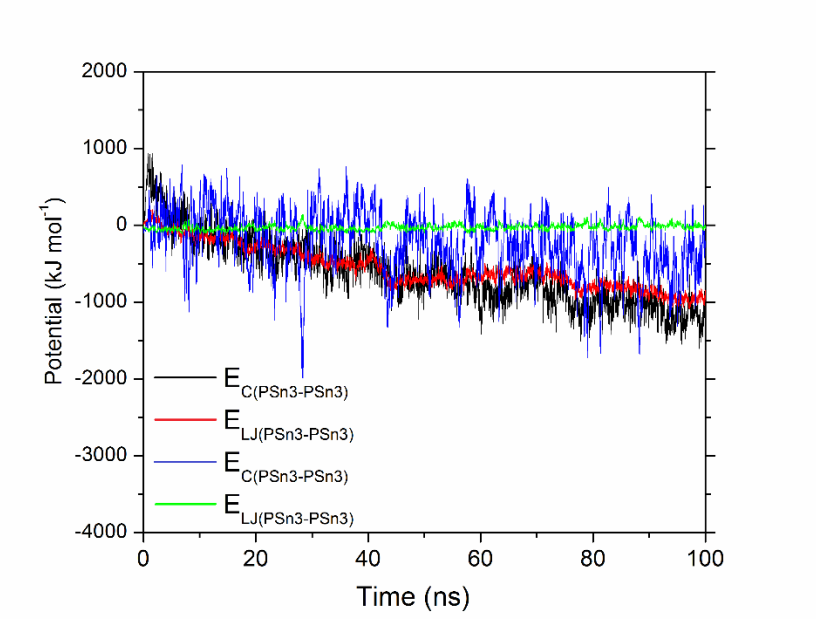
Lu Sun†, Xin Li[a], Thomas Hede[b], Yaoquan Tu[a], Caroline Leck[b], and Hans Ågren,[a]*

[a] Department of Theoretical Chemistry and Biology, School of Biotechnology, Royal Institute of Technology, S-10691 Stockholm, Sweden

[b] Department of Meteorology, Stockholm University, S-10691Stockholm, Sweden



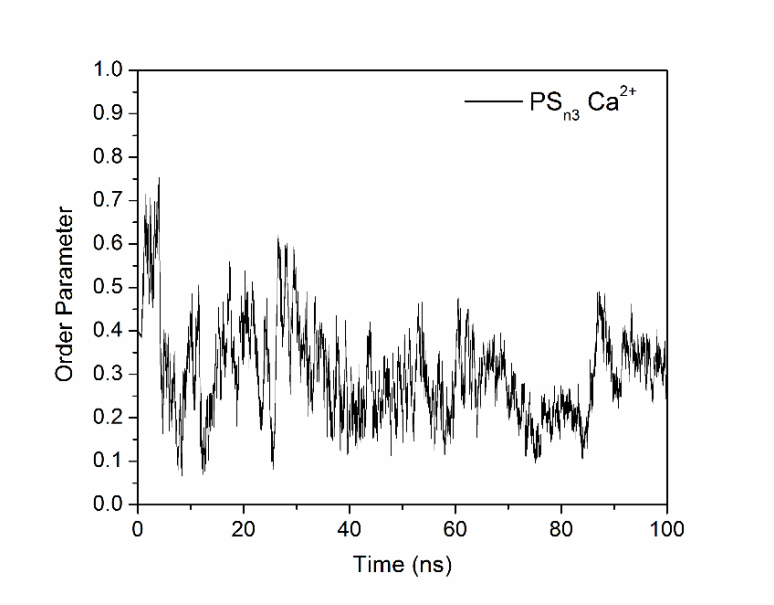
(a)



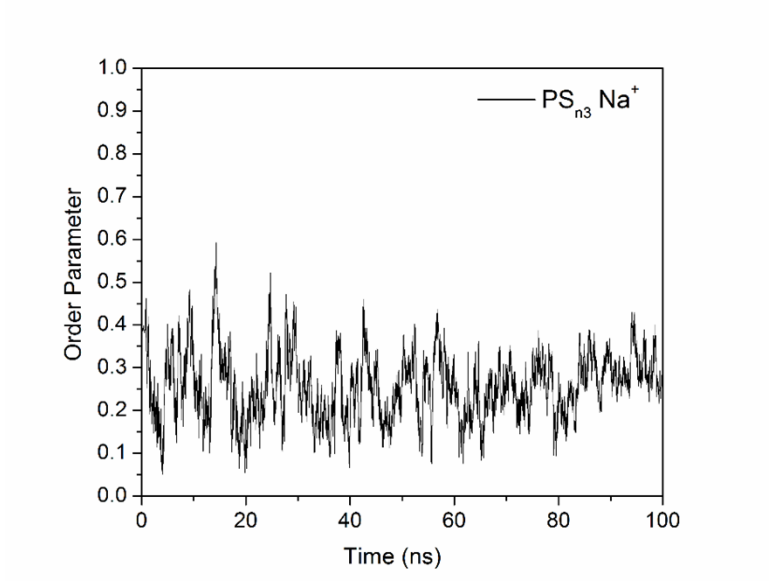
(b)

Figure S1. The electrostatic interaction and the Lennard-Jones interaction between polysaccharides and between cations. (a) For the system of three-unit polysaccharides with Ca^{2+} and (b) For the system of three-unit polysaccharides with Na^{2+}. In the presence of Ca^{2+}, the contribution of ionic bridges is significant and the electrostatic interaction between the polysaccharides hardly changes due to the formation of hydrogen bonds and the repulsion

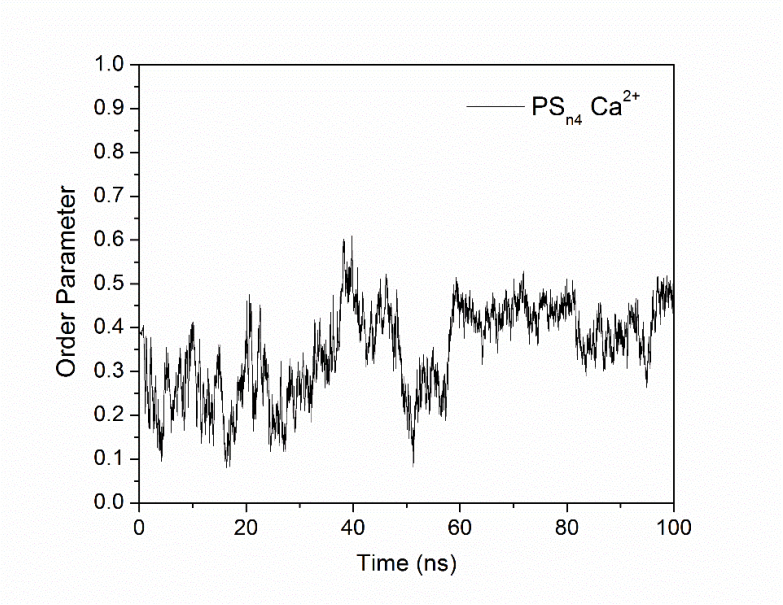
between the carboxyl groups. In contrast, in the absence of the ionic bridges, the formation of hydrogen bonds is the key to the assembly.



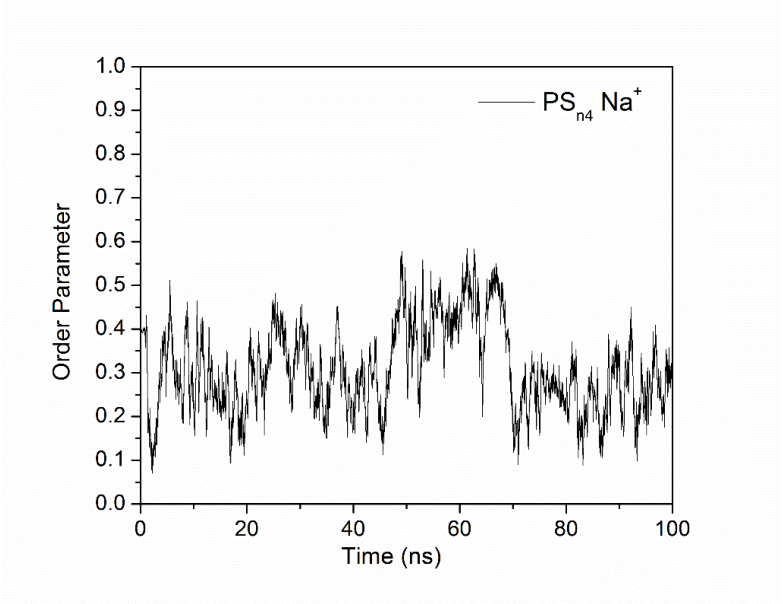
(a)



(b)

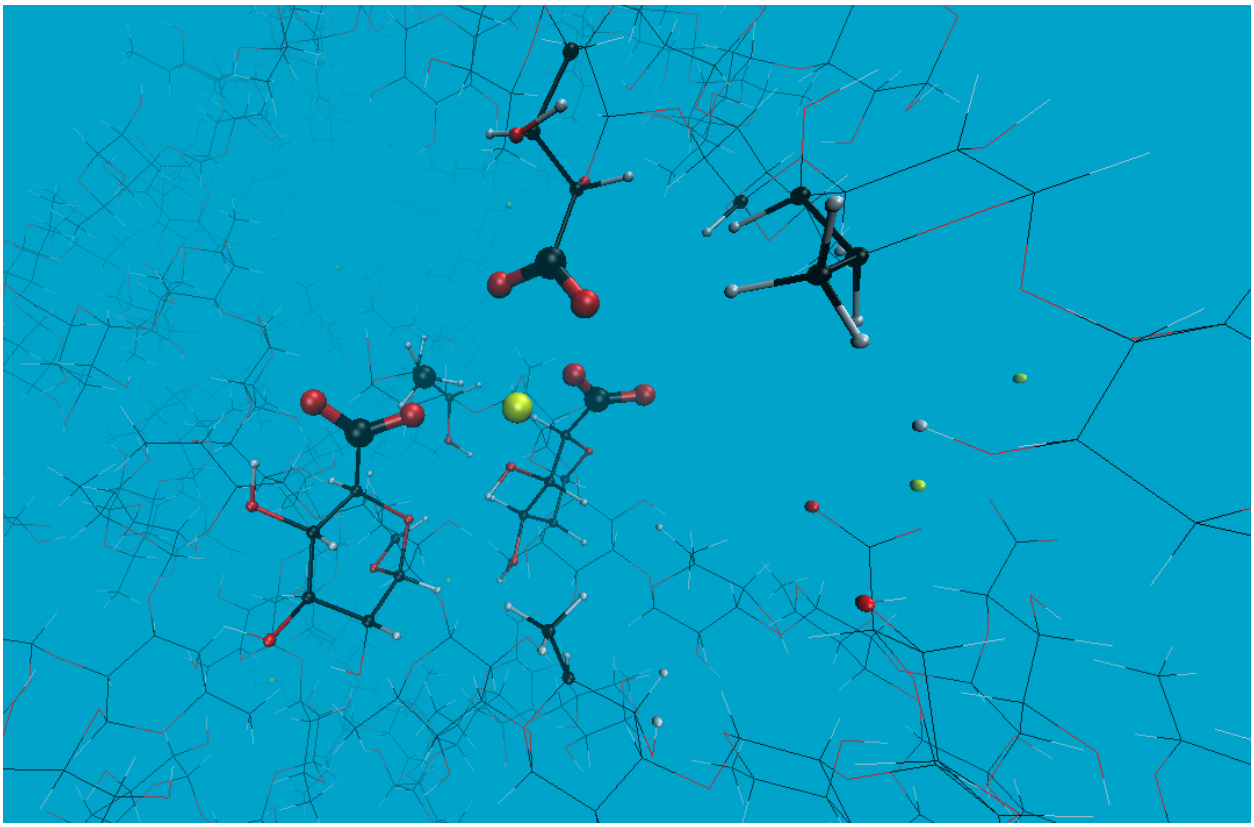


(c)

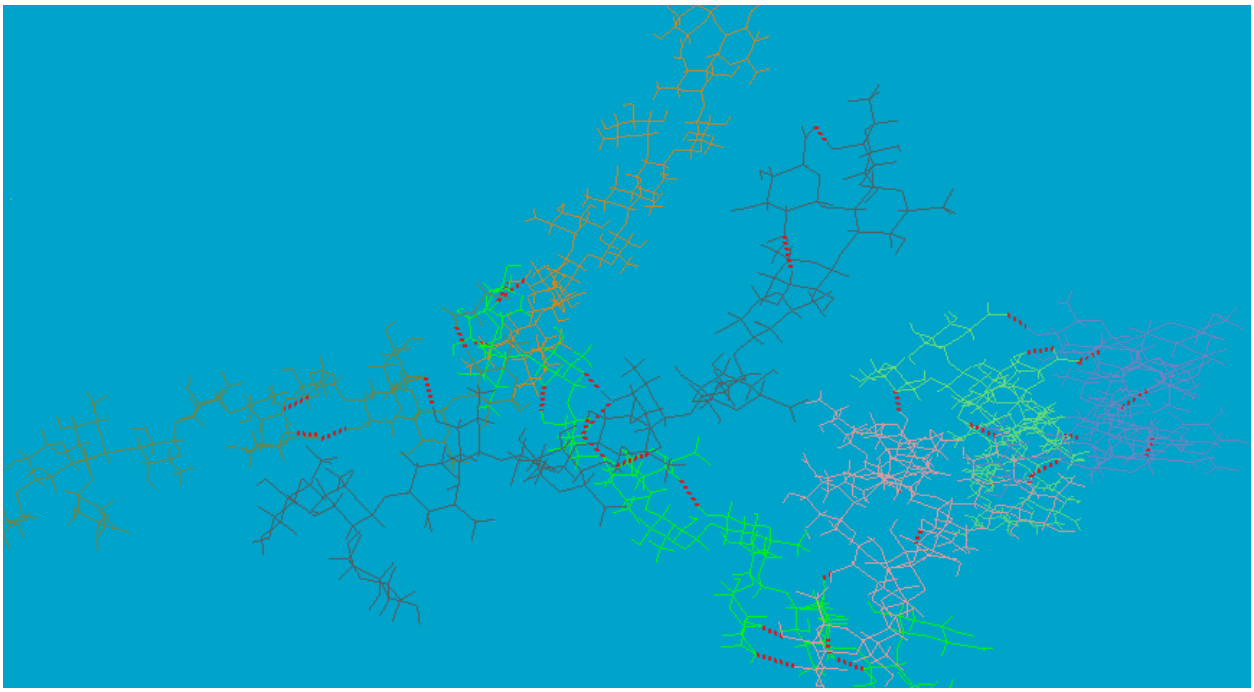


(d)

Figure S2. Evolution of the order parameter[1] (a) for the three-unit polysaccharides in the system with Ca^{2+}, (b) for the three-unit polysaccharides in the system with Na^{+}, (c) for the four-unit polysaccharides in the system with Ca^{2+}, and (d) for the four-unit polysaccharides in the system with Na^{+}(d).



(a)



(b)

Figure S3. (a) The $Ca^{2+}(COO^{-})_3^{-}$ ionic bridge, (b) The hydrogen bonds within the polymer assembly, with the hydrogen bonds denoted as red dashed lines. Both the visual configuration and gyration radius suggest that the structure is more compact than that without ionic bridge.

Reference

1. M. R. Wilson, *J. MOL. LIQ., 1996,* **68**, 23-31.