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

Electronic Supplementary Information:

Molecular clustering characteristics in ternary trehalose and choline dihydrogen phosphate solutions

Nikita Nikulsin,[a] *E. R. Azhagiya Singam,*[a‡] *Gloria Elliot,*[b] *and Donald Jacobs**[a]

[a]Department of Physics and Optical Science, University of North Carolina at Charlotte, 9201 University City Blvd, Charlotte, NC 28223, USA.

[b]Department of Mechanical Engineering and Engineering Science, University of North Carolina at Charlotte, 9201 University City Blvd, Charlotte, NC 28223, USA.

[‡]Present address: College of Veterinary Medicine, Kansas State University, 1620 Denison Avenue, 228 Coles Hall, Manhattan, KS 66506, USA.

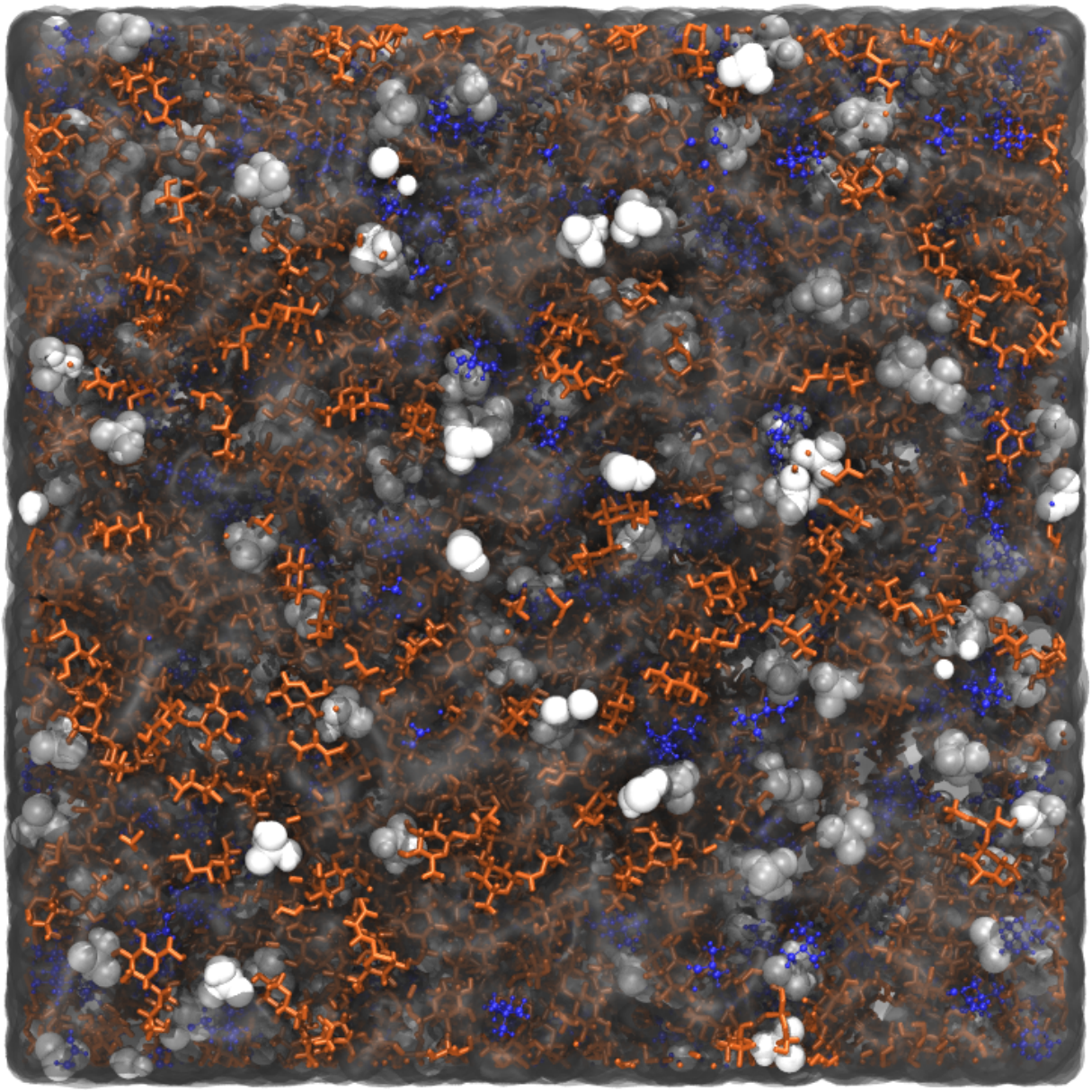

Figure S1. A large-scale view of the 50% solute by weight system. The orange molecules are trehalose, blue ions are cholines and white ions are dihydrogen phosphates. Water is represented by the translucent fluid in the figure.

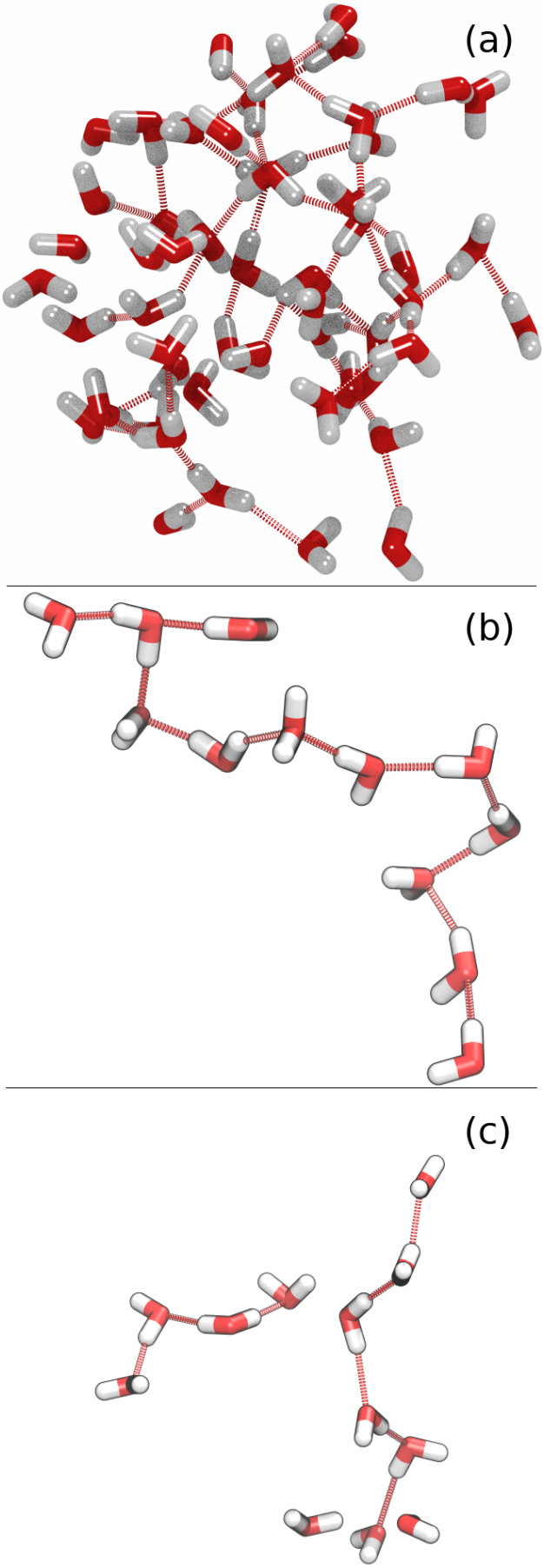

Figure S2. A section of a large cluster in the 50% system (a), and two clusters of comparable size in the (b) 83% system, and (c) 95% system. The dotted lines represent hydrogen bonds.

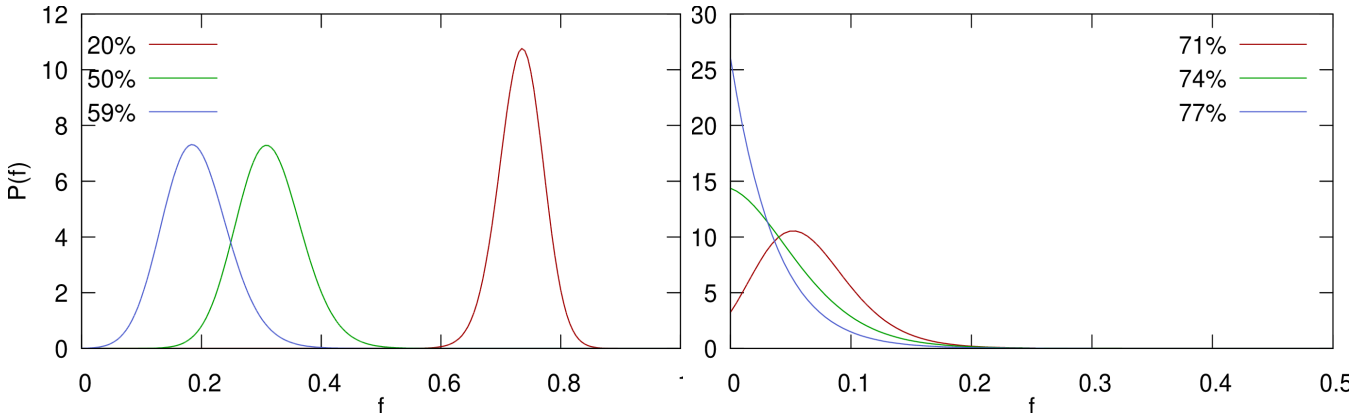

Figure S3. Probability distribution functions *P(f)* of fractions of time *f* that a particular choline ion spends being fully solvated.

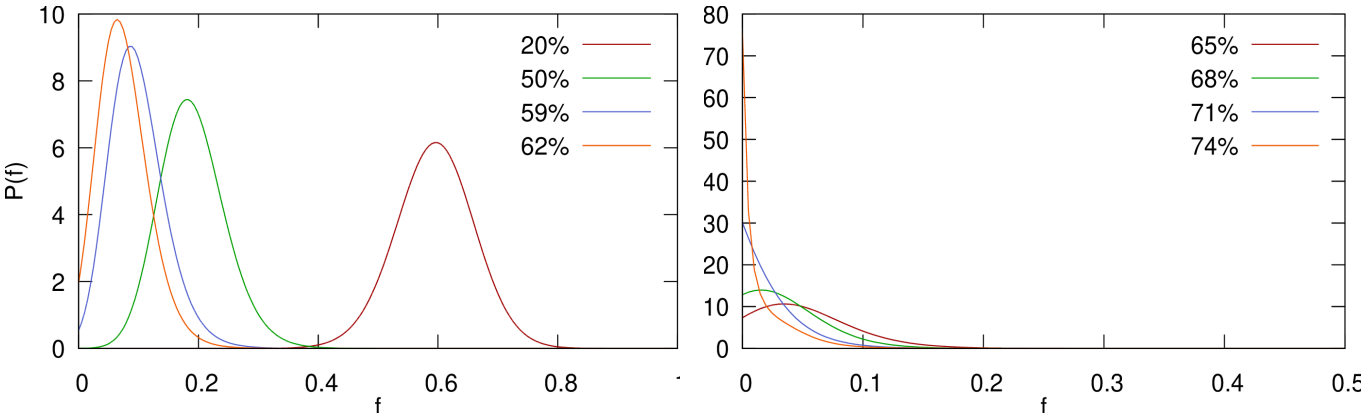

Figure S4. Probability distribution functions *P(f)* of fractions of time *f* that a particular phosphate ion spends being fully solvated.

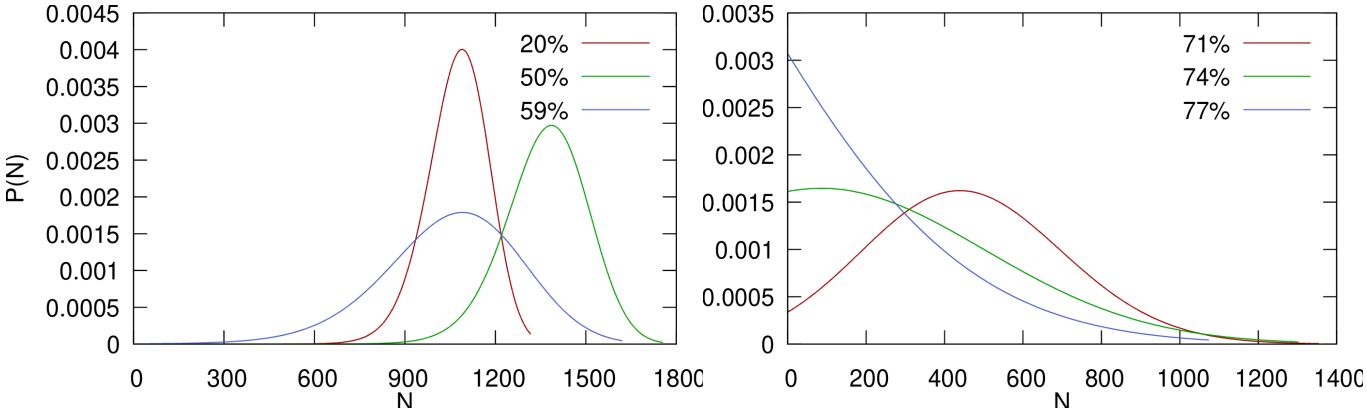

Figure S5. Probability distribution functions *P(N)* of the numbers of times *N* that a particular choline ion switches its category from fully solvated to interfacial and vice versa.

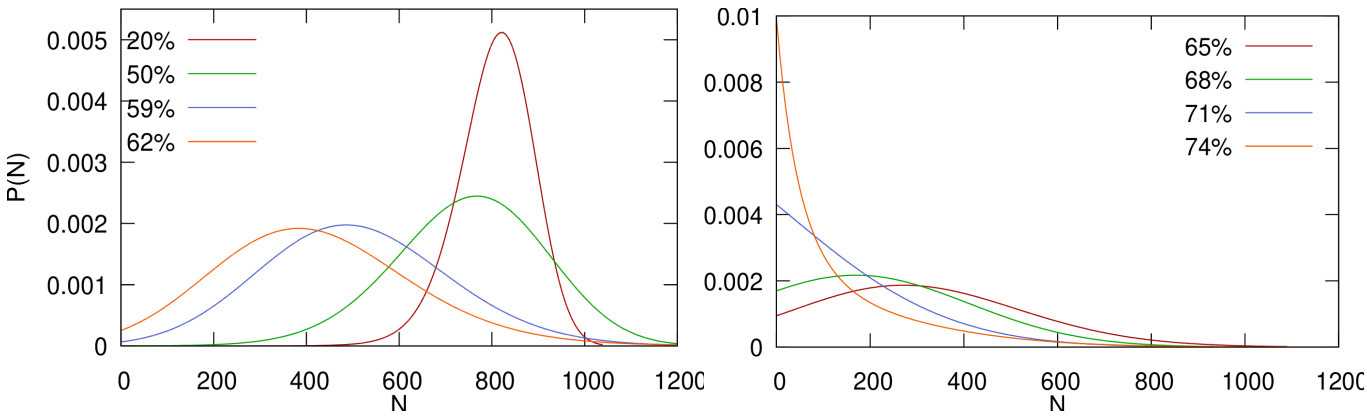

Figure S6. Probability distribution functions *P(N)* of the numbers of times *N* that a particular phosphate ion switches its category from fully solvated to interfacial and vice versa.

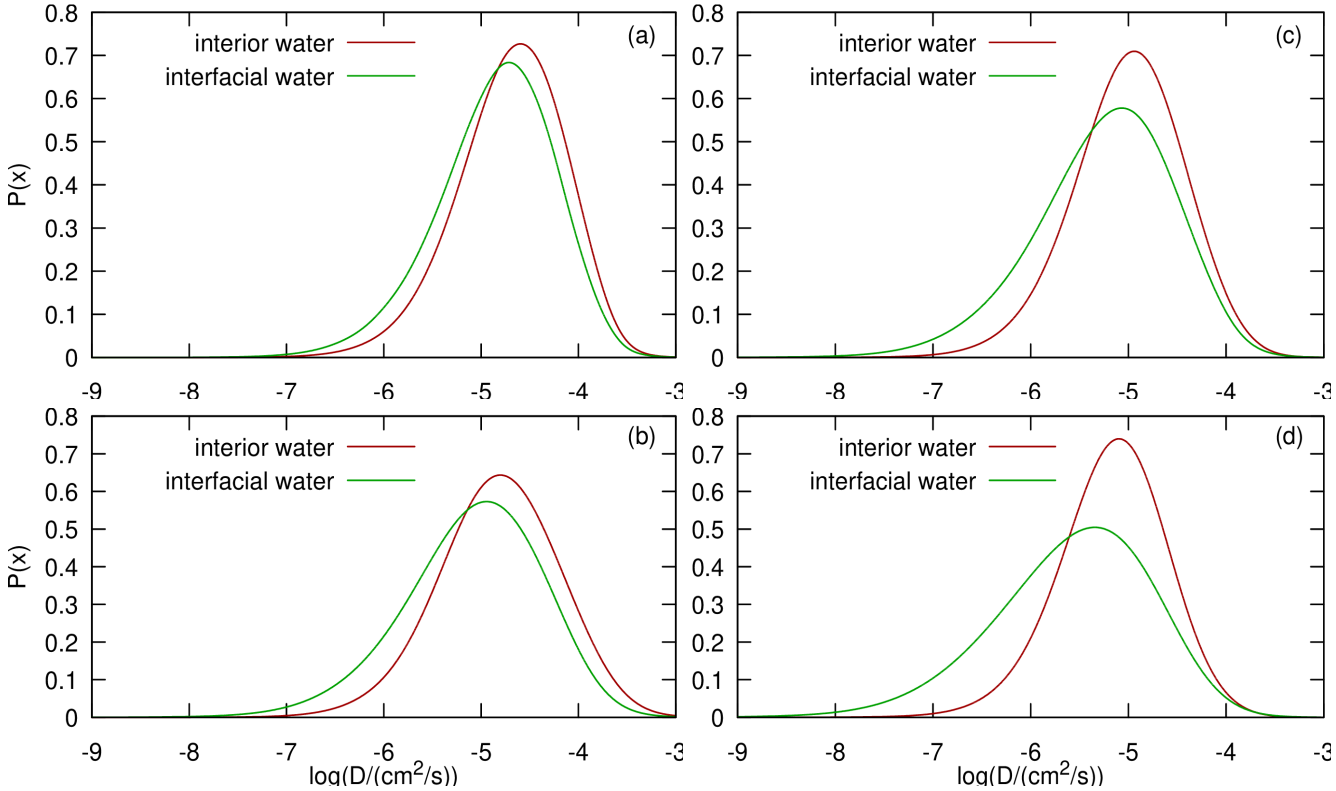

Figure S7. Probability distribution functions *P(x)* of the logarithms $x = log(D/(\mathrm{cm}^2/\mathrm{s}))$ of all recorded diffusivities of interior or interfacial water molecule instances in (a) 71% system, (b) 81.5% system, (c) 83% system and (d) 89% system.

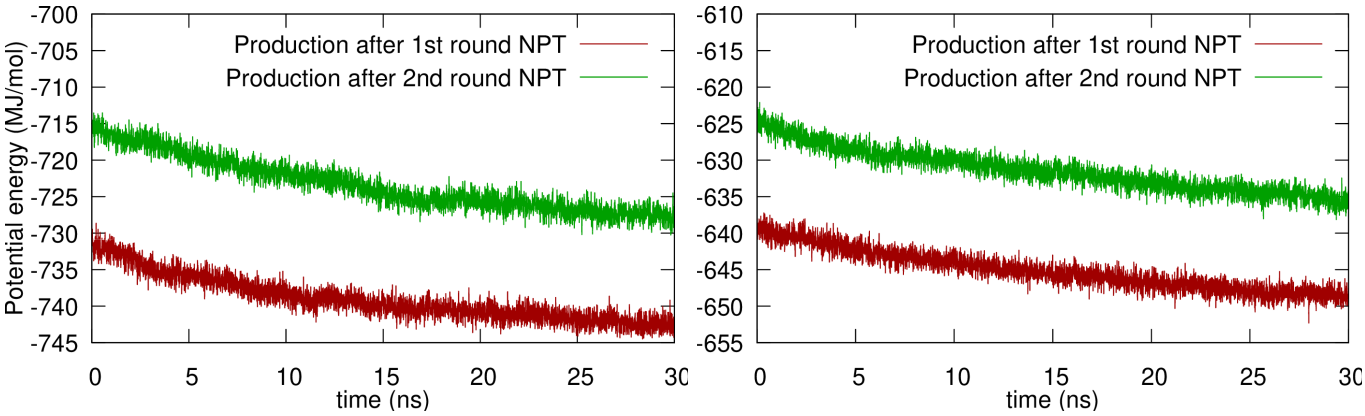

Figure S8. Potential energies as functions of time for production runs of the (a) 95% systems and (b) 100% systems.