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Simulations of Volume Phase Transitions in Polyelectrolyte Networks Upon Counterion Exchange DE-WEI YIN, Dept of Chemical and Biological Engineering, Univ of Wisconsin-Madison, JUAN J. DE PABLO, Dept of Chemical and Biological Engineering, Univ of Wisconsin-Madison — Polyelectrolyte networks are known to undergo discontinuous volume phase transitions, the onset of which may be caused by a number of factors. We have shown through molecular dynamics simulations that the interplay between the counterion excluded-volume entropy and the electrostatic energy—factors not explicitly considered in the classical Flory–Tanaka model—appears to have an important role in driving the phase transitions [Yin, Yan, and de Pablo, J. Chem. Phys. 123(17):174909, (2005)]. In our current work, we examine how the exchange of monovalent and divalent counterions induces discontinuous phase transitions in polyelectrolyte networks. It is revealed that divalent counterions condense preferentially over monovalent counterions onto the polyelectrolyte network backbone, thereby screening the charges on the backbone, and thus the different counterion species contribute differently to the osmotic pressure and hence to the free energy of the system. We present our findings as they relate to experiments performed near physiological conditions.

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