Fluids Density Functional Theory of Salt-Doped Block Copolymers[1] JONATHAN R. BROWN, LISA M. HALL, The Ohio State University — Block copolymers have attracted a great deal of recent interest as potential non-flammable, solid-state, electrolyte materials for batteries or other charge carrying applications. The microphase separation in block copolymers combines the properties of a conductive (though mechanically soft) polymer with a mechanically robust (though non-conductive) polymer. We use fluids density functional theory (fDFT) to study the phase behavior of salt-doped block copolymers. Because the salt prefers to preferentially solvate into the conductive phase, salt doping effectively enhances the segregation strength between the two polymer types. We consider the effects of this preferential solvation and of charge correlations by separately modeling the ion-rich phase, without bonding, using the Ornstein-Zernike equation and the hypernetted-chain closure. We use the correlations from this subsystem in the inhomogeneous fDFT calculations. Initial addition of salt increases the domain spacing and sharpens the interfacial region, but for high salt loadings the interface can broaden. Addition of salt can also drive a system with a low copolymer segregation strength to order by first passing through a two phase regime with a salt-rich ordered phase and a salt-poor disordered phase.

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