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Morphology of Tapered and Ion-containing Diblock Copolymers from Fluids Functional Density Theory JONATHAN R. BROWN, LISA M. HALL, The Ohio State University — We use classical, fluids density functional theory (fDFT) to study microphase separation in block copolymer systems. We focus on systems where local monomer scale ordering may be more important than for typical diblock copolymers, so fDFT allows us to generate more accurate density profiles and free energies at constant pressure. Specifically, we study the effect of tapering, or adding a gradient region (taper) between the pure A and B blocks of an AB diblock; the taper changes in composition smoothly from A to B. This additional control parameter allows one to increase the miscibility of the two blocks and change the effective segregation strength χN of the system. In contrast to our prior SCFT study, we capture the effect of the depletion of monomer density near the A-B interface, which changes as a function of taper length and interfacial width. Further, these methods can also be applied to ion containing systems, in which case monomer scale packing around ions is also important; we will show the fDFT predicted microphase morphology of block ionomers.

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