Abstract Submitted
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Fluids Density Functional Theory of Diblock Copolymers for Electrolyte Applications[1] JONATHAN R. BROWN, LISA M. HALL, Ohio State University — We use classical, fluids density functional theory (fDFT) to study microphase separation in block copolymer systems. We are motivated by systems used as battery electrolytes or in other transport applications, in which the two blocks of the system have different mechanical, dielectric, and transport properties that allow one phase to act as a charge/penetrant carrier and the other to make the film mechanically strong. We find density profiles of penetrants, showing to what degree they segregate into the A phase and their concentration near the interface, depending on the penetrant-A and penetrant-B interaction strengths as well as the A-B segregation strength. We also study the effect of tapering, or adding a gradient region (taper) between the pure A and B blocks of an AB diblock copolymer; the taper changes in composition along its length from pure A to pure B (or from B to A for an inverse taper). The effect of both penetrants and tapering on microphase domain spacing as a function of segregation strength will be discussed. Adjusting taper length allows one to tune the phase behavior of the system for easier processing or access to specific desired microphase structures.

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