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Polymer Physics Prize Talk

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Polymer electrolytes have been particularly difficult to describe theoretically given the large number of disparate length scales involved in determining their physical properties. The Debye length, the Bjerrum length, the ion size, the chain length, and the distance between the charges along their backbones determine their structure and their response to external fields. We have developed an approach that uses multi-scale calculations with the capability of demonstrating the phase behavior of polymer electrolytes and of providing a conceptual understanding of how charge dictates nano-scale structure formation. Moreover, our molecular dynamics simulations have provided an understanding of the coupling of their conformation to their dynamics, which is crucial to design self-assembling materials, as well as to explore the dynamics of complex electrolytes for energy storage and conversion applications.