

Properties of Molecular Electrolytes

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The physical properties of complex molecular electrolytes are essential for biological function and of great interest to industry. They have been particularly difficult to describe theoretically and computationally given the presence of dielectric heterogeneities and the large number of disparate length scales involved in determining their physical properties. The Debye length, the Bjerrum length, the ion size, the molecular structure, and the special charge distribution along the molecules with charged and neutral groups such as amphiphiles and proteins determine their structure and their response to external stimuli. Computational, numerical and theoretical approaches to describe electrolytes in bulk, solutions and at interface will be described and a conceptual understanding of how charge dictates nano-scale structure and function will be provided.