Special Program in Applied Mathematics and Applied Mechanics

Unified mean-field theory from ionic liquids to dilute electrolytes

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The Poisson-Nernst-Planck (PNP) theory is one of the most widely used analytical methods to describe electrokinetic phenomena for electrolytes. The model, however, considers isolated charges and thus is valid only for dilute ion concentrations. The key importance of concentrated electrolytes in applications has led to the development of a large family of generalized PNP models. In particular, the Bikerman model that takes into account the finite size of the ions has been one of the most commonly used extension to PNP

In this talk, we derive a thermodynamically consistent mean-field model for concentrated solutions. Our model recovers the Bikerman term, but shows that it is inconsistent in the sense that additional terms of equal magnitude should be taken into account. Furthermore, our study shows that the Bikerman approach inherently fails to describe finite-size effects at the highly concentrated regime, and presents a supplementary approach in this regime. The result is a modeling framework that is valid over the whole range of concentrations - from dilute electrolyte solutions to highly concentrated solution, such as ionic liquids. Importantly, the new model predicts distinct transport properties which are not governed by Einstein-Stokes relations, but are rather effected by inter-diffusion and even the emergence of nano-structure.This is a joint work with Doron Elad and Arik Yochelis.