

Title: Energetic Variational Approaches in the Modeling of Ionic Solutions and Ion Channels

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Abstract: Ion channels are key components in a wide variety of biological processes. The selectivity of ion channels is the key to many biological process. We try to study these selectivity mechanisms in ion channels by developing reduced models, taking into consideration of dielectric coefficient and ion particle sizes, as well as their very different, however primary, structures and properties. These self-organized systems will be modeled and analyzed with energetic variational approaches (EnVarA) that were motivated by classical works of Rayleigh and Onsager. The resulting/derived multiphysics-multiscale systems automatically satisfy the Second Laws of Thermodynamics and the basic physics that are involved in the system. In this talk, I will discuss some of the related issues we had encountered in these projects.