

Abstract Submitted
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Classical density functional theory of fluids as a multi-scale modeling tool for charged fluids: Electrical double layers, biological ion channels, dielectric interfaces¹ DIRK GILLESPIE, Rush University Medical Center — Classical density functional theory (DFT) of fluids (not quantum mechanical DFT of electron orbitals) has the potential to be a powerful modeling technique in many areas of science including ionic liquids, colloids, polymers, and proteins. DFT of fluids is a thermodynamic (statistical) theory in the grand canonical ensemble; given the particle interactions, equations are solved directly for the ensemble-averaged quantities. Because DFT is a thermodynamic theory where the ensemble-averaged quantities are computed directly, it computes results quickly (minutes for 1D problems, ~1 hour for 3D) and in arbitrarily low concentrations and it produces steady-state results. The DFT method is generally applicable to fluids in confining geometries or at interfaces. In this presentation the focus is on new results of DFT applications to electrolytes at charged interfaces and ion current through biological ion channels. A new technical advance of a DFT for dielectric interfaces will also be presented.

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