University of Texas at San Antonio

Department of Physics & Astronomy

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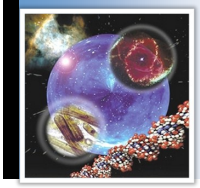
Friday, February 22, 2013
3:00 p.m.-4:00 p.m.
BB 3.04.18

An Olympic View of the Density Functional Theory

In this talk, I will present a family of density functional theories (DFT) that are unified within the same mathe-matical framework, i.e., Mermin's generalization of the Hohenberg-Kohn theorems. I will discuss a systematic approach for formu-lation and implementation of the DFT methods to predict the structural and physiochemi-cal properties of complex mo-lecular systems including electrolyte solu-tions, ionic liquids, polymers, and bi-ologi-cal systems. The DFT-based methods will be compared with conventional statis-tical-mechanical theo-ries of liquids and poly-mers, and their unique capabil-ity will be illustrated with practical exam-ples.



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