TCI SEMINAR

Putting the statistics back in statistical mechanics

Monday, October 28, 2013
3:00 p.m. Room 9341

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Statistical mechanics provides the basic connection between molecular scale details and macroscopic thermodynamic properties. Traditionally, analytical approaches such as mean field approximation and integral equations have been used to simplify the complicated multidimensional integrals statistical mechanics gives us. However, as computers have become increasingly powerful, they have allowed us to explore the statistical mechanics of increasingly complicated systems by instead estimating these integrals using sampling from the physical probability distributions. In this talk, I will examine ways that powerful new (and not-so-new) techniques borrowed from statisticians can be reapplied in physical contexts to accelerate molecular simulations and more efficiently analyze the simulation data collected. I'll discuss the application of these methods in the context of both for model systems and computing protein-ligand binding free energies.

Theoretical Chemistry Institute Seminar Series