CU Physics Department Colloquium

Monday, November 30, 2009 4:10 PM 428 Pupin Hall

Molecular interaction in physics and biology:

from Poisson's equation to derivation of the universal density functional

Molecular interactions determine, for example, how transcription factors recognize their DNA binding sites, how proteins interact with each other, and consequently how a biological system functions. Since both proteins and DNAs are significantly charged, electric interactions are among the most important when studying biomolecular interactions. Despite a long history of research of complex systems such as biomolecules in solvent, these problems remain difficult even at the level of classical electrostatics and call for new schemes with controllable accuracy. When one wishes to study short range effects that require quantum mechanics, quantitative understanding is hindered by the presence of many electrons. It is known that interactions among electrons dominate, at low energy, properties of matter of various forms, including atomic clusters, biomolecules, nano- and bulk-materials. Pragmatic calculations, based on constructing many-electron wave functions, often suffer from accuracy loss and are stopped by an ``exponential wall'' when the number of electrons involved increases. The Density functional theory (DFT) and its applications, awarded the 1998 Nobel chemistry prize, use the 3D electronic density as the basic variable and thus are free from this wall. However, the proper execution of the DFT requires knowledge of a parameter-free universal density functional (UDF), which has remained elusive for decades. In this talk, I will describe the efforts we have invested in molecular interactions, ranging from correct classical and semi-classical to fully quantum-mechanical treatments. In particular, I will describe our recent derivation of the UDF, removing possibly ad hoc parameters from studies of many branches of science that include, in addition to physics, quantum chemistry, material science, nano-clusters, and biology.

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Meet the Speaker will be held in 705 Pupin Hall at 1:30 PM