Strong Electron Correlation

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Since the electronic Schrödinger equation is too complicated to be soluble for most interesting chemical systems, the task of the quantum chemist is to develop practical approximations that provide accurate models for the behavior of electrons in molecules. The difficulty of the underlying problem implies that these models are necessarily limited to certain special cases. For example, it is relatively easy to describe cases where the electrons in a molecule move nearly independently, so that the motion of one electron does not affect others very much. When this is not true, many of our conceptual precepts lose their utility because the notion of an electron configuration, and even the concept of orbitals, ceases to be relevant. In addition, when the independent-electron approximation breaks down, most conventional computational methods of quantum chemistry become unreliable. In this seminar, I will discuss quantum chemical models for strongly correlated molecules, focusing on alternatives to orbital-based models. Specifically, I will discuss models based on tensor-product decompositions, complexity-based truncations, and composite particles.