Density-functional calculations with exact exchange

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In this talk, I will discuss theory and recent applications (1-4) of exact-exchange (EXX) Kohn-Sham and related density-functional methods, with an emphasis on results for semiconductors and insulators.

EXX Kohn-Sham approaches treat the exchange part of the electron-electron interaction exactly, without resorting to the commonly used local-density (LDA) or generalized gradient (GGA) approximations. The key quantities in the EXX formalism are the exact exchange energy E_x and the exact local exchange potential $V_x(\mathbf{r}) = \frac{\delta E_x}{\delta n(\mathbf{r})}$, defined as the functional derivative of E_x with respect to the density $n(\mathbf{r})$. A prominent feature of the EXX scheme! is that $V_x(\mathbf{r})$ is self-interaction free and exhibits the correct $-\frac{1}{r}$ asymptotic behavior for (neutral) localized systems. This causes EXX eigenvalue spectra to be markedly closer to both the exact Kohn-Sham and to the experimental excitation spectra than their LDA or GGA counterparts.

I will illustrate these and other conceptual advantages of the EXX method, discuss EXX results for total energies and Kohn-Sham eigenvalues of a variety of systems, compare with standard LDA and GGA results, and comment on the prospects of exact-exchange schemes. In addition, the utilization of exact local and nonlocal exchange potentials (screened and unscreened) in density-functional schemes will be addressed.

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