

# BECKE'S *PERSPECTIVE* ON DFT

The *Journal of Chemical Physics* has produced a Special Topics issue on *Advances in Density Functional Theory*. I want to call to your attention the Perspective article by Becke titled “Perspective: Fifty years of density-functional theory in chemical physics”.<sup>1</sup> Becke writes a personal account of the history of DFT and makes a number of interesting points and observations. He rightly notes that DFT is exact and we should more properly refer to our actual implementations as Density Functional Approximations (DFA). He also notes that use of the term *ab initio* as a synonym for wavefunction theory is inappropriate as DFT is just as *ab initio* as HF and post-HF theories.

A common perception about DFT (well, DFA) is that there is no way to systematically improve functionals. Becke exposes a true underlying logic that *has* driven much of DFA development.

Lastly, Becke is discouraged by the more recent developments that have included virtual orbitals, such as double hybrid methods. His approach is that true DFT is *occupied orbitals only* (for which he pointedly does not want to adopt the acronym *OOO*), and that developments that include the virtual orbitals might toll the “death knell” for DFT.

For those interested in a pretty accessible account of the history of DFT, Becke’s *Perspective* is an excellent place to get started.

Source: <http://comporgchem.com/blog/?p=3303>