by Debra E Blakely

The Path to a Nobel Prize

Many science editors may wonder whether papers crossing their desks can help win a Nobel Prize. Generally, however, a Nobel Prize is earned not for one paper but rather for a collective body of work. Because the Nobel Prize archives are not released until 50 years after a prize is given, most editors will never know which articles influenced the Nobel decision most.

The 1998 Nobel Prize in Chemistry went to Walter Kohn and John A Pople. Kohn, of the University of California, Santa Barbara, won for developing density functional theory (DFT), which simplifies the mathematical description of bonding between atoms in molecules. Pople, of Northwestern University, created a computational method that aids in applying DFT. The development of DFT in the 1960s, followed by its combination with a computational method in the 1990s, opened a highly productive field of research. Work drawing on DFT has now been reported in a wide array of general and specialized journals. Like much Nobel Prize winning research, work on DFT began as a highly specialized field but proved to have wide implications and applications. Here are five articles identified as significant to the body of research by Dennis R Salahub, University of Calgary, who has advanced DFT internationally.

Hohenberg P, Kohn W. Inhomogeneous electron gas. Phys Rev B 1964;136:B864-71.
This paper presents the theoretical basis for DFT, which "deals with the ground state of an interacting electron gas in an external potential. . . . It is proved that there exists a universal functional of the density." Publication of this paper marked the birth of DFT. *Physical Review* deals with similar topics, so it was a logical journal in which to publish this paper. At the time of its publication, work on DFT was too specialized for a more general journal. Only later would the implications of DFT be more broadly recognized.

Kohn W, Sham LJ. Self-consistent equations including exchange and correlation effects. Phys Rev A 1965;140:A1133-8.
A year after the previous paper, this paper converted the formal proofs of DFT into a form that could be used in practice. The Kohn-Sham version of DFT is now used in the vast majority of experiments and other applications drawing on the theory.

Gill PMW, Johnson BG, Pople JA, Frisch MJ. An investigation of the performance of a hybrid of Hartree-Fock and density functional theory. Int J Quantum Chem 1992;26:319-31.
An important transformation in DFT work occurred after 26 years. Pople had previously developed the computer software Gaussian, which is widely used in physics and chemistry experiments. This paper showed that combining DFT with Gaussian offered a solution to a previous problem in organic thermochemistry: inability to achieve high-accuracy calculations beyond small systems. Integrating DFT into Gaussian brought DFT to thousands of chemists who were already using Gaussian.

Gill PMW, Johnson BG, Pople JA. A standard grid for density functional calculations. Chem Phys Lett 1993;209:506-12.
This paper presents some of Pople's first work dealing specifically with DFT and the Gaussian computational method.

Becke AD. Density functional thermochemistry III: the role of exact exchange. J Chem Phys 1993;98: 5648-52.
This paper by Becke, a leading researcher in DFT, presents a prominent example of a publication drawing on the work of Kohn and Pople. Their work has since been used by many chemists.

For more information about DFT and those awarded the 1998 Nobel Prize, see *www.nobel.se/chemistry/laureates/1998/*.